Inferring Dynamic Bayesian Networks using Frequent Episode Mining

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Abstract
Motivation: Several different threads of research have been proposed for modeling and mining temporal data. On the one hand, approaches such as dynamic Bayesian networks (DBNs) provide a formal probabilistic basis to model relationships between time-indexed random variables but these models are intractable to learn in the general case. On the other, algorithms such as frequent episode mining are scalable to large datasets but do not exhibit the rigorous probabilistic interpretations that are the mainstay of the graphical models literature.

Results: We present a unification of these two seemingly diverse threads of research, by demonstrating how dynamic (discrete) Bayesian networks can be inferred from the results of frequent episode mining. This helps bridge the modeling emphasis of the former with the counting emphasis of the latter. First, we show how, under reasonable assumptions on data characteristics and on influences of random variables, the optimal DBN structure can be computed using a greedy, local, algorithm. Next, we connect the optimality of the DBN structure with the notion of fixed-delay episodes and their counts of distinct occurrences. Finally, to demonstrate the practical feasibility of our approach, we focus on a specific (but broadly applicable) class of networks, called excitatory networks, and show how the search for the optimal DBN structure can be conducted using just information from frequent episodes. Application on datasets gathered from mathematical models of spiking neurons as well as real neuroscience datasets are presented.

Availability: Algorithmic implementations, simulator codebases, and datasets are available from our website at http://neural-code.cs.vt.edu/dbn.

Keywords: Event sequences, dynamic Bayesian networks, temporal probabilistic networks, frequent episodes, temporal data mining.

1 Introduction

Probabilistic modeling of temporal data is a thriving area of research. The development of dynamic Bayesian networks as a subsuming formulation to HMMs, Kalman filters, and other such dynamical models has promoted a succession of research aimed at capturing probabilistic dynamical behavior in complex systems. DBNs bring to modeling temporal data the key advantage that traditional Bayesian networks brought to modeling static data, i.e., the ability to use graph theory to capture probabilistic notions of independence and conditional independence. They are now widely used in bioinformatics, neuroscience, and linguistics applications.

A contrasting line of research in modeling and mining temporal data is the counting based literature, exemplified in the KDD community by works such as [9, 7]. Similar to frequent itemsets, these papers define the notion of frequent episodes as objects of interest. Identifying frequency measures that support efficient counting procedures (just as support does for itemsets) has been shown to be crucial here.

It is natural to question whether these two threads, with divergent origins, can be related to one another. Many researchers have explored precisely this question. The classic paper by Pavlov, Mannila, and Smyth [13] used frequent itemsets to place constraints on the joint distribution of item random variables and thus aid in inference and query approximation. Chao and Parthasarathy [16] view probabilistic models as summarized representations of databases and demonstrate how to construct MRF (Markov random field) models from frequent itemsets. Closer to the topic of this paper, the work by Laxman et al. [7] linked frequent episodes to a generative HMM-like model of the underlying data.

Similar in scope to the above works, we present a unification of the goals of dynamic Bayesian network inference with that of frequent episode mining. Our motivations are not merely to establish theoretical results but also to inform the computational complexity of algorithms and spur faster algorithms targeted for specific domains. The key contributions are:

1. We show how, under reasonable assumptions on data characteristics and on influences of random variables, the optimal DBN structure can be established using a greedy, local, approach, and how this structure can be computed using the notion of fixed-delay episodes and their counts of distinct occurrences.
2. We present a specific (but broadly applicable) class of networks, called excitatory networks, and show how the search for the optimal DBN structure can be conducted using just information from frequent episodes.

3. We demonstrate a powerful application of our methods on datasets gathered from mathematical models of spiking neurons as well as real neuroscience datasets.

2 Bayesian Networks: Static and Dynamic

Formal mathematical notions are presented in the next section, but here we wish to provide some background context to past research in Bayesian networks (BNs). As is well known, BNs use directed acyclic graphs to encode probabilistic notions of conditional independence, such as that a node is conditionally independent of its non-descendants given its parents (for more details, see [5]). The earliest known work for learning BNs is the Chow-Liu algorithm [2]. It showed that, if we restricted the structure of the BN to be a tree, then the optimal BN can be computed using a minimum spanning tree algorithm. It also established the tractability of BN inference for this class of graphs.

More recent work, by Williamson [17], generalizes the Chow-Liu algorithm to show how (discrete) distributions can be generally approximated using the same ingredients that are used by the Chow-Liu approach, namely mutual information quantities between random variables. Meila [10] presents an accelerated algorithm that is targeted toward sparse datasets of high dimensionality. The approximation thread for general BN inference is perhaps best exemplified by Friedman’s sparse candidate algorithm [3] that presents various approaches to greedily learn (suboptimal) BNs.

Dynamic Bayesian networks are a relatively newer development and best examples of them can be found in the example sequence (1), where

\[
E_1, \ldots, E_n \subset \{A, B, C, \ldots, Z\},
\]

of \( M = 26 \) event-types:

\[
\langle (A, 2), (B, 3), (D, 3), (B, 5), (C, 9), (A, 10), (D, 12) \rangle
\]

The maximum time tick is given by \( T = 12 \). Each \( X(t), t = 1, \ldots, 12 \), is a vector of \( M = 26 \) indicator random variables. Since there are no events at time \( t = 0 \) in the example sequence (1), we have \( X(1) = 0 \). At time \( t = 2 \), we will have \( X(2) = [1000 \cdots 0]^T \). Similarly, \( X(3) = [0101 \cdots 0]^T \), and so on.

A Dynamic Bayesian Network [11] is essentially a DAG with nodes representing random variables and arcs representing conditional dependency relationships. In this paper, we model the random process \( X(t) \) (or equivalently, the event stream \( s \)), as the output of a Dynamic Bayesian Network. Each event-indicator, \( X_j(t), t = 1, \ldots, T \) and \( j = 1, \ldots, M \), corresponds to a node in the network, and is assigned a set of parents, which is denoted as \( \pi(X_j(t)) \) (or \( \pi_j(t) \)). A parent-child relationship is represented by an arc (from parent to child) in the DAG. In a Bayesian Network, nodes are conditionally independent of their non-descendants given their parents. The joint probability distribution of the random process, \( X(t) \), under the DBN model, can be factorized as a product of conditional probabilities, \( P[X_j(t) \mid \pi_j(t)] \), for various \( j, t \).

In general, given a node, \( X_j(t) \), any other \( X_k(\tau) \) can belong to its parent set, \( \pi_j(t) \). However, since each node has a time-stamp, it is reasonable to assume that a random variable, \( X_k(\tau) \), can only influence future random variables (i.e. those random variables associated with later time indices). Also, we can expect the influence of \( X_k(\tau) \) to diminish with time, and so we assume that \( X_k(\tau) \) can be a parent of \( X_j(t) \) only if time \( t \) is within \( W \) time-ticks of time \( \tau \) (Typically, \( W \) will be small, like say, 5 to 10 time units). All of this constitutes our first constraint, A1, on the DBN structure.

A1 : For user-defined parameter, \( W > 0 \), the set, \( \pi_j(t) \), of parents for the node, \( X_j(t) \), is a subset of event-indicators out of the \( W \)-length history at time-tick, \( t \), i.e. \( \pi_j(t) \subset \{ X_k(\tau) : 1 \leq k \leq M, (t - W) \leq \tau < t \} \).

The DBN essentially models the time-evolution of the event-indicator random variables associated with the \( M \) event-types in the alphabet, \( E \). By learning the DBN
structure, we expect to unearth relationships like “event $B$ is more likely to occur at time $t$, if $A$ occurred 3 time-ticks before $t$ and if $C$ occurred 5 time-ticks before $t$.” In view of this, it is reasonable to assume that the parent-child relationships depend on relative (rather than absolute) time-stamps of random variables in the network. We refer to this as translation invariance of the DBN structure, and is specified below as the second constraint, A2, on the DBN structure.

A2 : If $\pi_j(t) = \{X_{j1}(t_1), \ldots, X_{jt}(t_t)\}$ is an $\ell$-size parent set of $X_j(t)$ for some $t > W$, then for any other $X_j(t')$, $t' > W$, its parent set, $\pi_j(t')$, is simply a time-shifted version of $\pi_j(t)$, and is given by $\pi_j(t') = \{X_{j1}(t_1 + \delta), \ldots, X_{jt}(t_t + \delta)\}$, where $\delta = (t' - t)$.

The data stream, $s$, is a long stream of events which we will regard as a realization of the stochastic process, $X(t)$, $t = 1, \ldots, T$. While A2 is a sort of structural stationarity constraint on the DBN, in order to estimate marginals of the joint distribution from the data stream, we will also require that the distribution does not change when shifted in time. The stationarity assumption is stated in A3 below.

A3 : For all $j, \delta$, given any set of $\ell$ event-indicators, say, $\{X_{j1}(t_1), \ldots, X_{jt}(t_t)\}$, the stationarity assumption requires that, $P[X_{j1}(t_1), \ldots, X_{jt}(t_t)] = P[X_{j1}(t_1 + \delta), \ldots, X_{jt}(t_t + \delta)]$.

The joint probability distribution, $Q[\cdot]$, under the Dynamic Bayesian Network model can be written as:

$$Q[X(1), \ldots, X(T)] = P[X(1), \ldots, X(W)] \times \prod_{t=W+1}^{T} \prod_{j=1}^{M} P[X_j(t) | \pi_j(t)]$$  \hspace{1cm} (2)

Learning the structure of the network involves learning the map, $\pi_j(t)$, for each $X_j(t)$, $j = 1, \ldots, M$ and $t = (W + 1), \ldots, T$. In this paper, we derive an optimal structure for a Dynamic Bayesian Network, given an event stream, $s$, under assumptions A1, A2 and A3. Our approach follows the lines of [2, 17] where structure learning is posed as a problem of approximating the discrete probability distribution, $P[\cdot]$, by the best possible distribution from a chosen model class (which, in our case, is the class of Dynamic Bayesian Networks constrained by A1 and A2). The Kullback-Leibler divergence between the underlying joint distribution, $P[\cdot]$, of the stochastic process, and the joint distribution, $Q[\cdot]$, under the DBN model is given by

$$D_{KL}(P||Q) = \sum_{A} \left( P[X(1), \ldots, X(T)] \times \log \frac{P[X(1), \ldots, X(T)]}{Q[X(1), \ldots, X(T)]} \right)$$  \hspace{1cm} (3)

where $A$ represents the set of all possible assignments for the $T M$-length random vectors, $\{X(1), \ldots, X(T)\}$. Denoting the entropy of $P[X(1), \ldots, X(T)]$ by $H(P)$, the entropy of the marginal, $P[X(1), \ldots, X(W)]$, by $H(P_W)$, and substituting for $Q[\cdot]$ from Eq. (2), we get

$$D_{KL}(P||Q) = -H(P) - H(P_W) - \sum_{A} \left( P[X(1), \ldots, X(T)] \times \sum_{j=1}^{M} \sum_{t=W+1}^{T} \log P[X_j(t) | \pi_j(t)] \right)$$  \hspace{1cm} (4)

We now expand the conditional probabilities in Eq. (4) using Bayes rule, switch the order of summation and marginalize $P[\cdot]$ for each $j, t$. Denoting, for each $j, t$, the entropy of the marginal $P[X_j(t)]$ by $H(P_j(t))$, the expression for KL divergence now becomes:

$$D_{KL}(P||Q) = -H(P) - H(P_W) - \sum_{j=1}^{M} \sum_{t=W+1}^{T} H(P_j(t)) - \sum_{j=1}^{M} \sum_{t=W+1}^{T} I[X_j(t); \pi_j(t)]$$  \hspace{1cm} (5)

$I[X_j(t); \pi_j(t)]$ denotes the mutual information between $X_j(t)$ and its parents, $\pi_j(t)$, and is given by

$$I[X_j(t); \pi_j(t)] = \sum_{A_{j,t}} \left( P[X_j(t), \pi_j(t)] \times \log \frac{P[X_j(t), \pi_j(t)]}{P[X_j(t)] P[\pi_j(t)]} \right)$$  \hspace{1cm} (6)

where $A_{j,t}$ represents the set of all possible assignments for the random variables, $\{X_j(t), \pi_j(t)\}$. Under the translation invariance constraint, A2, and the stationarity assumption, A3, we have $I[X_j(t); \pi_j(t)] = I[X_j(t'); \pi_j(t')]$ for all $t > W$, $t' > W$. This gives us the following final expression for $D_{KL}(P||Q)$:

$$D_{KL}(P||Q) = -H(P) - H(P_W) - \sum_{j=1}^{M} \sum_{t=W+1}^{T} H(P_j(t)) - (T - W) \sum_{j=1}^{M} I[X_j(t); \pi_j(t)]$$  \hspace{1cm} (7)

where $t$ is any time-tick satisfying $(W < t \leq T)$. We note that in Eq. (7), the entropies, $H(P)$, $H(P_W)$ and $H(P_j(t))$ are independent of the DBN structure (i.e. they do not depend on the $\pi_j(t)$ maps). Since $(T - W) > 0$ and since $I[X_j(t); \pi_j(t)] \geq 0$ always, the KL divergence, $D_{KL}(P||Q)$, is minimized when the sum of $M$ mutual information terms in Eq. (7) is maximized. Further, from A1 we know that all parent nodes of $X_j(t)$ have time-stamps strictly less than $t$, and hence, no choice of $\pi_j(t)$, $j = 1, \ldots, M$ can result in a cycle in the network (in which case, the structure will not be a DAG, and in-turn, it will not represent a valid DBN). This ensures that, under the restriction of A1, the optimal
DBN structure (namely, one that corresponds to a $Q[.]$ that minimizes KL divergence with respect to the true joint probability distribution, $P[.]$, for the data) can be obtained by independently picking the highest mutual information parents, $\tau_j(t)$, for each $X_j(t)$ for $j = 1, \ldots, M$ (and, because of A2 and A3, we need to carry-out this parents’ selection step only for the $M$ nodes in any one time slice, $t$, that satisfies $(W < t \leq T)$).

4 Fixed-delay episodes

Frequent episode discovery is a popular framework in temporal data mining [8, 12, 1]. The data in this framework is a single long stream of events over a finite alphabet, as defined at the beginning of Sec. 3 (cf. Example 1). In the formalism of [9], an $\ell$-node (serial) episode, $\alpha$, is defined as a tuple, $(V_\alpha, \prec_\alpha, g_\alpha)$, where $V_\alpha = \{v_1, \ldots, v_\ell\}$ denotes a collection of nodes, $\prec_\alpha$ denotes a total order\(^1\) such that $v_i \prec_\alpha v_{i+1}$, $i = 1, \ldots, (\ell - 1)$. If $g_\alpha(v_j) = A_{j1}, j = 1, \ldots, \ell$, we use the graphical notation $(A_{j1} \rightarrow \cdots \rightarrow A_{ji})$ to represent $\alpha$. An occurrence of $\alpha$ in an event stream, $s = ((E_1, t_1), (E_2, t_2), \ldots, (E_n, t_n))$, is a map $h : V_\alpha \rightarrow \{1, \ldots, n\}$ such that (i) $E_{h(v_j)} = g(v_j) \forall v_j \in V_\alpha$ and (ii) for all $v_i \prec_\alpha v_j$ in $V_\alpha$, the times of occurrence of the $i^{th}$ and $j^{th}$ event in the occurrence are related according to $t_{h(v_i)} \leq t_{h(v_j)}$ in $s$.

Example 2 Consider a 3-node episode $\alpha = (V_\alpha, \prec_\alpha, g_\alpha)$, such that, $V_\alpha = \{v_1, v_2, v_3\}$, $v_1 \prec_\alpha v_2$, $v_2 \prec_\alpha v_3$ and $v_1 \prec_\alpha v_3$, and $g_\alpha(v_1) = A$, $g_\alpha(v_2) = B$ and $g_\alpha(v_3) = C$. The graphical representation for this episode is $\alpha = (A \rightarrow B \rightarrow C)$, indicating that in every occurrence of $\alpha$, an event of type $A$ must appear before an event of type $B$, and the $B$ must appear before an event of type $C$. For example, in sequence (1), the subsequence $[(A, 1), (B, 3), (C, 9)]$ constitutes an occurrence of $(A \rightarrow B \rightarrow C)$. For this occurrence, the corresponding $h$-map is given by, $h(v_1) = 1$, $h(v_2) = 2$ and $h(v_3) = 5$.

In the episode formalism reviewed so far, the exact time-stamps on the events in the data stream are only used to check the time-order of events constituting an episode occurrence. There are many ways to incorporate explicit time-duration constraints in episode occurrences (like the windows-width constraint of [9], or the dwelling time constraint of [8]). Episodues with inter-event gap constraints were introduced in [12]. For example, the framework of [12] can express the temporal pattern “$B$ must follow $A$ within 5 time-ticks and $C$ must follow $B$ within 10 time-ticks.” Such a pattern is represented using the graphical notation, $(A \overset{5-5}{\rightarrow} B \overset{[0-10]}{\rightarrow} C)$. In this paper, we use a simple sub case of the inter-event gap constraints, in the form of fixed inter-event time-delays.

Here, each inter-event time constraint is represented by a single delay rather than a range of delays. We will refer to such episodes as fixed-delay episodes. For example, $(A \overset{5}{\rightarrow} B \overset{10}{\rightarrow} C)$ represents a fixed-delay episode, every occurrence of which must comprise an $A$, followed by a $B$ exactly 5 time-ticks later, which in-turn is followed by a $C$ exactly 10 time-ticks later.

Definition 4.1 An $\ell$-node fixed-delay episode is defined as a pair, $(\alpha, D)$, where $\alpha = (V_\alpha, \prec_\alpha, g_\alpha)$ is the usual (serial) episode of [9], and $D = (\delta_1, \ldots, \delta_{\ell-1})$ is a sequence of $(\ell - 1)$ non-negative delays. Every occurrence, $h$, of the fixed-delay episode in an event sequence, $s = ((E_j, t_1), \ldots, (E_{j_n}, t_n))$, must satisfy the inter-event constraints, $\delta_i = (t_{h(v_{i+1})} - t_{h(v_i)})$, $i = 1, \ldots, (\ell - 1)$. ($A_{j_i}, \delta_1 \rightarrow \cdots \rightarrow A_{j_{i+1}}$) is the graphical notation for inter-event episode, $(\alpha, D)$, where $A_{j_i} = g_\alpha(v_i)$, $i = 1, \ldots, \ell$.

The framework of frequent episode discovery requires the notion of episode frequency. This can be defined in many ways [9, 6]. In this paper, we use the notion of distinct occurrences to define the frequency of fixed-delay episodes.

Definition 4.2 Two occurrences, $h_1$ and $h_2$, of a fixed-delay episode, $(\alpha, D)$, are said to be distinct, if they do not share any events in the data stream, $s$. Given a user-defined, $W > 0$, frequency of $(\alpha, D)$ in $s$, denoted $f_\alpha(\alpha, D, W)$, is defined as the total number of distinct occurrences of $(\alpha, D)$ in $s$ that terminate strictly after $W$.

In general, counting distinct occurrences of episodes suffers from computational inefficiencies [6]. (Each occurrence of an episode $(A \rightarrow B \rightarrow C)$ is a substring that looks like $A \ast B \ast C$, where $\ast$ denotes a variable-length don’t-care, and hence, counting all distinct occurrences in the data stream can require an unbounded number of automata for each episode). However, in case of fixed-delay episodes, it is easy to track distinct occurrences efficiently. For example, when counting frequency of $(A \overset{3}{\rightarrow} B \overset{5}{\rightarrow} C)$, if we encounter an $A$ at time $t$, to recognize an occurrence involving this $A$ we only need to check for a $B$ at time $(t + 3)$ and for a $C$ at time $(t + 8)$. In addition to being attractive from an efficiency point-of-view, we will show next in Sec. 4.1 that the distinct occurrences-based frequency count for fixed-delay episodes will allow us to interpret relative frequencies as probabilities of DBN marginals. (Note that the $W$ in Definition 4.2 is same as length of the history window used in the constraint A1. Skipping any occurrences terminating in the first $W$ time-ticks makes it easy to normalize the frequency count into a probability measure).
4.1 Marginals from episode frequencies

In Sec. 3 we derived the optimal DBN structure for an event sequence under constraints A1 and A2, and assumption A3. The main result was that for \( t > W \), the (optimal) parents of a node, \( X_j(t) \), corresponds to the subset, \( \pi_j(t) \subseteq \{X_1(t) : 1 \leq k \leq M; (t - W) \leq \tau < t \} \), which maximizes the mutual information, \( I[X_j(t); \pi_j(t)] \).

In this section, we describe how to compute this mutual information from the frequency counts of fixed-delay episodes.

Every subset of event-indicators in the network is associated with a fixed-delay episode.

**Definition 4.3** Let \( \{X_j(t) : j = 1, \ldots, M; t = 1, \ldots, T\} \) denote the collection of event-indicators used to model event stream, \( s = ((E_1, t_1), \ldots (E_n, t_n)) \), over alphabet, \( \mathcal{E} = \{A_1, \ldots, A_M\} \). Consider an \( \ell \)-size subset, \( \mathcal{X} = \{X_{j_1}(t_1), \ldots, X_{j_\ell}(t_\ell)\} \), of these indicators, and without loss of generality, assume \( t_1 \leq \cdots \leq t_\ell \). Define the \((\ell - 1)\) inter-event delays in \( \mathcal{X} \) as follows: \( \delta_j = (t_{j+1} - t_j), j = 1, \ldots, (\ell - 1) \). The fixed-delay episode, \((\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X}))\), that is associated with the subset, \( \mathcal{X} \), of event-indicators is defined by \( \alpha(\mathcal{X}) = (A_{j_1} \rightarrow \cdots \rightarrow A_{j_\ell}) \), and \( \mathcal{D}(\mathcal{X}) = \{\delta_1, \ldots, \delta_{\ell-1}\} \). In graphical notation, the fixed-delay episode associated with \( \mathcal{X} \) can be represented as follows:

\[
(\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X})) = (A_{j_1}^{\delta_1} \cdots \delta_{\ell-1} A_{j_\ell}).
\]

For computing mutual information using Eq. (6), we need the marginals of various subsets of event-indicators in the network. Given a subset like \( \mathcal{X} = \{X_{j_1}(t_1), \ldots, X_{j_\ell}(t_\ell)\} \), we need estimates for probabilities of the form, \( P[X_i(t_1) = a_1, \ldots, X_i(t_\ell) = a_\ell] \), where \( a_j \in \{0, 1\}, j = 1, \ldots, \ell \). The fixed-delay episode, \((\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X}))\), that is associated with \( \mathcal{X} \) is given by Definition 4.3 and its frequency in the data stream, \( s \), is denoted by \( f_s(\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X}), W) \) (as per Definition 4.2) where \( W \) denotes length of history window as per A1. Since an occurrence of the fixed-delay episode, \((\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X}))\), can terminate in each of the \((T - W)\) time-ticks in \( s \), the probability of an all-ones assignment for the random variables in \( \mathcal{X} \) is given by:

\[
P[X_{i_1}(t_1) = 1, \ldots, X_{i_\ell}(t_\ell) = 1] = \frac{f_s(\alpha(\mathcal{X}), \mathcal{D}(\mathcal{X}), W)}{T - W}
\]

For all other assignments (i.e. for assignments that are not all ones) we need to use the inclusion-exclusion formula to obtain corresponding probabilities. The inclusion-exclusion principle has been used before in data mining, e.g. for approximating queries using frequent itemsets [14]. The idea is to obtain exact or approximate frequency counts for arbitrary boolean queries using only counts of frequent itemsets in the data. In our case, counting distinct occurrences of fixed-delay episodes facilitates use of the inclusion-exclusion formula for obtaining the probabilities needed in the mutual information expression of Eq. (6).

Consider the set, \( \mathcal{X} = \{X_{j_1}(t_1), \ldots, X_{j_\ell}(t_\ell)\} \), of \( \ell \) event-indicators, and let \((a_1, \ldots, a_\ell)\), \( a_j \in \{0, 1\}, j = 1, \ldots, \ell \), be any general assignment for the event-indicators in \( \mathcal{X} \). Let \( \mathcal{U} \subseteq \mathcal{X} \) denote the set of indicators out of \( \mathcal{X} \) for which corresponding assignments in \( \mathcal{A} \) are all 1’s, i.e. \( \mathcal{U} = \{X_{j_k} \in \mathcal{X} : k \text{ s.t. } a_k = 1 \text{ in } \mathcal{A}, 1 \leq k \leq \ell \} \). The inclusion-exclusion formula can now be used to compute the probabilities as follows:

\[
P[X_{j_1} = a_1, \ldots, X_{j_\ell} = a_\ell] = \sum_{\mathcal{U} \subseteq \mathcal{Y} \subseteq \mathcal{X}} (-1)^{|\mathcal{Y}\setminus\mathcal{U}|} \left( \frac{f_s(\mathcal{Y})}{T - W} \right)
\]

where we use \( f_s(\mathcal{Y}) \) as short-hand for \( f_s(\alpha(\mathcal{Y}), \mathcal{D}(\mathcal{Y}), W) \), the distinct occurrences-based frequency (cf. Definition 4.2) of the fixed-delay episode, \((\alpha(\mathcal{Y}), \mathcal{D}(\mathcal{Y}))\). It is possible to verify that summing the expression in Eq. (10) over all possible binary \( \ell \)-tuples, \((a_1, \ldots, a_\ell)\), always yields 1. Thus, in case of fixed-delay episodes, suitably-normalized frequency counts can be regarded as corresponding marginal probabilities.

5 Excitatory networks

In this section, we describe a restricted class of networks, called **excitatory networks** where only certain kinds of conditional dependencies among nodes are permitted. In general, each event-type from the alphabet can have some propensity of random occurrence (and this of course, can be different for different event-types). In so-called excitatory networks the only way to increase the propensity of occurrence of an event-type is by the occurrence of specific event-types at specific delays in the immediate past. For example, we can have a conditional dependency such as, “whenever \( A \), \( B \), and \( C \) occur (say) 2 time-ticks apart, the probability of occurrence of \( D \) increases.” No other kinds of conditional dependencies are permitted in excitatory networks. In other words, one or more event-types cannot increase the propensity of another by not occurring in the data stream. This kind of constraint appears naturally in neuroscience, where one is interested in unearthing conditional dependency relationships among neuron spiking patterns. There are several regions in the brain that are known to exhibit predominantly excitatory characteristics and in these cases a neuron cannot increase the firing rate of another by not firing.

In the context of DBN structure learning, this restriction translates to event-types frequently appearing alongside their respective parents (with specific delays).
This motivates the use of frequent episodes to restrict the search space for parent sets. We note that, in general, it is difficult to infer an optimal network by inspection of the set of frequent episodes and/or the association rules that can be derived from it. This is because, there can be several frequent episodes/rules ending in the same event-type and these may even be of different sizes. There is no obvious way to systematically analyze frequencies and confidence values among these candidates to pick the optimal parent(s) in the network. In Sec. 7, we will present some examples to illustrate the shortcomings of our frequency based approach in detecting higher order causative relationships.

6 Algorithms

In Secs. 3-4, we developed the formalism for learning an optimal DBN structure from event streams by using distinct occurrences-based counts of fixed-delay episodes to compute the DBN marginal probabilities. The top-level algorithm for discovering the network is to fix any time \( t > W \) and consider each \( X_i(t) \), \( i = 1, \ldots, M \), in turn. The best parent set, \( \pi_i(t) \), for \( X_i(t) \) is selected by searching over subsets of event-indicators (in the \( W \)-length history of \( X_i(t) \)) for the one that maximizes the mutual information, \( I[X_i(t) ; \pi_i(t)] \). To compute this mutual information we use the formalism of fixed-delay episodes. The marginal probabilities required in the computation of \( I[X_i(t) ; \pi_i(t)] \) are obtained using Eq. (10) which basically uses the frequencies of appropriate fixed-delay episodes in an inclusion-exclusion formula. Finally, since we are looking for only excitatory connections, we restrict our search space to frequent fixed-delay episodes. Thus the first step in our DBN learning algorithm is to detect all frequent fixed-delay episodes with a span less than \( W \). This is described in Sec. 6.1. These frequent episodes (along with their respective frequencies) are input to the actual parents-search algorithm (which constructs different parents and picks the one with highest mutual information). This is explained next in Sec. 6.2.

6.1 Discovering fixed-delay episodes

However for long patterns and low support thresholds, an Apriori like algorithm incurs substantial costs and further must repeatedly scan the entire database for each level. In Algorithm 1 we present a pattern-growth based algorithm for mining frequent episodes (with fixed delays).

The pattern-growth procedure given in Algorithm 1 takes as input an episode \( \alpha \), a set of integers \( D_\alpha \), and the actual event sequence \( S \). \( D_\alpha \) is a set time stamps \( t_i \) such that there is an occurrence of \( \alpha \) starting at \( t_i \) in \( S \). For example, say at level 1 we have \( \alpha = (C) \), then \( D_\alpha(C) = \{1, 4, 5, 8, 9\} \) for the event sequence \( S \) shown in Fig 1. The algorithm proceeds by obtaining counts for all episodes \( \beta \) generated by extending \( \alpha \) e.g. \( B \xrightarrow{0} C \), \( \ldots, A \xrightarrow{5} C \) etc. For an episode say \( \beta = B \xrightarrow{2} C \), the count is obtained looking for an occurrence of event \( B \) at time \( t_j = t_i - 2 \) where \( t_i \in D_B \). In the example \( t_j = \{2, 3, 6\} \). The number of such occurrences gives the count of \( B \xrightarrow{2} C \). At every step the algorithm tries to grow an episode with count \( > \theta \) otherwise stops.

6.2 Learning DBN structure

In Sec. 3 we derived the conditions of an optimal DBN structure. Based on our assumptions, it suffices to look at a one time instance \( t > W \) and ascertain the parents of each of the \( M \) nodes \( X(t) \). Translation invariance then automatically allows us to fix the parents of all other \( X(t)'s \) at time instance \( t > W \).

The algorithm considers one node corresponding to each event-type in the alphabet in-turn, and searches for its best parent set. Based on our discussion in Sec. 5, we restrict the search space to only frequent episodes (ending in the event-type). If there are no frequent episodes ending in an event-type, we declare it as a root node. In addition from mutual information theory we know that
in general
\[ I[X; Y] \geq I[X; Z], \forall Z \subset Y \quad (11) \]

where \( X \) is a single random variable and \( Y \) and \( Z \) are sets of random variables. But on removing the nodes that do not contribute in causing \( X_j \) from the parent set \( \pi_j \), the mutual information decreases only slightly. This is the basis of Algorithm 2 where at each step the parent set of size \( m \), \( \pi_j^m(t) \) is chosen from the frequent episode of size \( (m + 1) \) which gives the highest mutual information with \( X_j(t) \). In the case where a parent set of size \( n \), \( \pi_j^n(t) \) with \( n > m \) has already been selected for \( X_j(t) \) in an earlier iteration, the set \( \pi_j^m(t) \) replaces \( \pi_j^n(t) \) if \( I[X_j(t), \pi_j^m(t)] - I[X_j(t), \pi_j^n(t)] < \epsilon \) and \( \pi_j^n(t) \subset \pi_j^m(t) \).

In addition \( \pi_j^n \) replaces \( \pi_j^m \) if \( I[X_j, \pi_j^m] > I[X_j, \pi_j^n] \) for \( \pi_j^n \not\subset \pi_j^m \). Therefore using the \( \epsilon \) criteria we can iteratively remove nodes from the parent set that do not contribute in the information theoretic sense towards the cause of \( X_j \).

**Algorithm 2** DBN learning from frequent episodes

1. */ Initialize */
2. \( h = \{\} \) */ Empty hash-map */
3. for \( i = k \) down to 1 do
4. \( \text{for all } \alpha \in F_{i-1} \) do
5. */ \( F_{i+1} \): frequent episodes of size \( i + 1 \) */
6. \( A = \text{Last event of } \alpha \)
7. \( \text{par} = \text{prefix}(\alpha) \)
8. */ \( \text{par} \): first \( |\alpha| - 1 \) nodes chosen as candidate parents of \( A \) with delays corresponding to inter-event gaps in \( \alpha \) */
9. if \( A \notin h \) then
10. \( h(A) = (\text{par}, M I(A, \text{par}), i) \)
11. else
12. \( (\text{par}_{\text{prev}}, m_i, \text{level}) = h(A) \)
13. if \( \text{level} = i + 1 \) then
14. \( m_i = M I(A, \text{par}) \)
15. if \( |m_i - m_{\text{prev}}| < \epsilon \) or \( m_i > m_{\text{prev}} \) then
16. \( h(A) = (\text{par}, m_i, i) \)
17. else if \( \text{level} = i \) then
18. \( m_i = M I(A, \text{par}) \)
19. if \( m_i > m_{\text{prev}} \) then
20. \( h(A) = (\text{par}, m_i, i) \)
21. Output: \( \text{DBN} = \{(A, h[A], \text{par}) \}, \forall A \} \) gives the DBN

The time complexity of computing mutual information with a parent set of size \( k \) is \( O(2^k) \) as we have to compute \( 2^k \) value assignments to all the nodes in the parent set (which take values 0 or 1). But since \( k \) is a user-supplied parameter (and assumed constant for a given run of Algorithm 2), the time complexity is output-sensitive with linear dependence on the number of frequent episodes \( O(|F_{i+1}|) \) at each level \( i \).

### 7 Experimental Results

We present results on data gathered from both mathematical models of spiking neurons as well as real neuroscience datasets.

#### 7.1 Data generation model

Our approach here is to model each neuron as an inhomogeneous Poisson process\(^2\) whose firing rate is a complex function of the input received by the neuron:

\[ \lambda_i(t) = \frac{\lambda}{1 + \exp(-I_i(t) + \theta)} \quad (12) \]

Eq 12 gives the firing rate of the \( i^{th} \) neuron at time \( t \). The network inter-connect allowed by this model gives it the amount of sophistication required for simulating higher-order interactions. More importantly, the model allows for variable delays which mimic the delays in conduction pathways of real neurons.

\[ I_i(t) = \sum_j \beta_{ij} Y_{j(t-\tau_{ij})} + \ldots + \sum_j \beta_{ij...l} Y_{j(t-\tau_{i...l})} \ldots Y_{l(t-\tau_{i...l})} \quad (13) \]

In Eq 13, \( Y_{j(t-\tau_{ij})} \) is the indicator of the event of a spike on \( j^{th} \) neuron \( \tau_{ij} \) time earlier. The higher order terms in the input contribute to the firing rate only when the \( i^{th} \) neuron received inputs from all the neurons in the term with corresponding delays. With suitable choice of parameters \( \beta_{(\cdot)} \) one can simulate a wide range of networks.

#### 7.2 Types of Networks

In this section we demonstrate the effectiveness of our approach in unearthing different types of networks. Each of these networks was simulated by setting up the appropriate inter-connections, of suitable order, in our mathematical model.

**Causative Chains**: These are simple first order interactions forming linear chains. The parent set for each random variable is a single variable. Observe that this class includes loops in the underlying graph that would be ‘illegal’ in a static Bayesian network formulation. A causative chain is perhaps the easiest scenario for DBN inference. Here a network with 50 nodes is simulated for 60 sec on the multi-neuronal simulator, where the conditional probability is varied from 0.4 to 0.8. For a reasonably high conditional probability (0.8), we obtain 100% precision for a reasonably wide range of the frequency threshold (0.002, 0.038). The recall is also similarly high but drops a bit toward higher values of the frequency threshold. For the low conditional probability scenario, the number of frequent episodes mined drops to zero and hence no network is found (implying both a precision and recall of 0). A similar experiment was

\(^2\)simulator courtesy Mr. Raajay, M.S. Student, IISc, Bangalore.
conducted for different values of parameter $\epsilon$ and $k$. For this particular network, the results are robust as there are only first order interactions.

Higher-order causative chains: A higher-order chain is one where parent sets are not restricted to be of cardinality one. In the example network of Fig. 2(b) we have two disconnected components: one first order causative chain formed by nodes A, B, C and D and a higher-order causative chain formed by M, N, O and P. In the higher-order chain, O fires when both M and N fire with appropriate timing and P fires when all of M, N, and O fire. Looking only at frequent episodes, both $A \rightarrow B \rightarrow C \rightarrow D$ and $M \rightarrow N \rightarrow O \rightarrow P$ turn out to be frequent. But using the $\epsilon$ criteria for our algorithm we can distinguish the two components of the circuits to be of different orders. Table 1 demonstrates results on this network as $\epsilon$ is varied from 0.00001 to 0.01, and for the same range of conditional probabilities as before. A low $\epsilon$ results in a decrease of precision, e.g., our approach finds A and B to be parents of C. Conversely, for higher values of $\epsilon$ our algorithm might reject the set M, N, P as parents of P and retain some subset of them. A final observation is in reference to the times from Table 1; the values presented here includes the time to compute the mutual information terms plus the time to mine frequent patterns, and the significant component is the latter.

Table 1: DBN results for network shown in Fig. 2(b) for varying conditional probability (used in generation) and $\epsilon$ (used in mining); base firing rate = 20Hz.

| Cond. | Epsilon | Time (total) | Recall | Precision |
|-------|---------|--------------|--------|-----------|
| 0.8   | 0.00001 | 18.31        | 100    | 75        |
| 0.8   | 0.0001  | 18.31        | 100    | 100       |
| 0.8   | 0.001   | 18.3         | 88.89  | 100       |
| 0.8   | 0.01    | 18.31        | 77.78  | 100       |
| 0.4   | 0.00001 | 15.02        | 100    | 81.82     |
| 0.4   | 0.0001  | 14.98        | 100    | 100       |
| 0.4   | 0.001   | 14.98        | 100    | 100       |
| 0.4   | 0.01    | 14.98        | 88.89  | 100       |

Syn-fire Chains: Another important pattern often seen in neuronal spike train data is that of synfire chains. This consists of groups of synchronously firing neurons strung together repeating over time. In an earlier work [12], it was noted that discovering such patterns required a combination of serial and parallel episode mining. But the DBN approach applies more naturally to mining such network structures.

Polychronous Circuits: Groups of neurons that fire in a time-locked manner with respect to each other are referred to as polychronous groups. This notion was introduced in [4] and gives rise to an important class of patterns. Once again, our DBN formulation is a natural fit for discovering such groups from spike train data. An example of a polychronous circuit is shown in Fig 2(d) and its corresponding results in Table 2.

Table 2: DBN results for network shown in Fig. 2(d) for different Freq. thresh. and epsilon

| Cond. | Freq. Thresh. | Epsilon | Time (total) | Recall | Precision |
|-------|---------------|---------|--------------|--------|-----------|
| 0.8   | 0.002        | 0.0005  | 22.3         | 100    | 100       |
| 0.8   | 0.014        | 0.0005  | 18.8         | 40     | 100       |
| 0.8   | 0.002        | 0.0001  | 22.81        | 100    | 53.57     |
| 0.8   | 0.002        | 0.01    | 22.91        | 93.33  | 100       |
| 0.4   | 0.002        | 0.0005  | 15.48        | 53.33  | 100       |
| 0.4   | 0.014        | 0.0005  | 15.11        | 13.33  | 100       |
| 0.4   | 0.002        | 0.0001  | 15.28        | 53.33  | 61.54     |
| 0.4   | 0.002        | 0.01    | 15.3         | 46.67  | 100       |

7.3 Scalability

The scalability of our approach with respect to data length and number of variables is shown in Fig 3 and Fig 4. Here four different networks with 50, 75, 100 and 125 variables respectively were simulated for time durations ranging from 20 sec to 120 sec. The base firing rate of all the networks was fixed at 20 Hz. In each network 40% of the nodes were chosen to have up to 3 three parents. The parameters of the DBN mining algorithm were chosen such that recall and precision are both high.
Figure 3: Plot of time taken for mining frequent episodes vs. data length in sec

Figure 4: Plot of time taken for mutual information computation and searching for the parent set vs. data length in sec

Figure 5: Plot of total time taken for DBN discovery vs. network density

7.4 Sensitivity

Finally, we discuss the sensitivity of the DBN mining algorithm to the parameters ($\theta, \epsilon$). To obtain precision-recall curves for our algorithm applied to data sequences with different characteristics, we vary the two parameters $\theta$ and $\epsilon$ in the ranges {0.002, 0.008, 0.014, 0.026, 0.038} and {0.00001, 0.0001, 0.001, 0.01} respectively. The data sequence for this experiment is generated from the multi-neuronal simulator using different settings of base firing rate, conditional probability, number of nodes in the network, and the density of the network as defined earlier.

The set of precision-recall curves are shown in Fig 6. It can be seen that the proposed algorithm is effective for a wide range of parameter settings and also on data with sufficiently varying characteristics.

7.5 Mining DBNs from MEA recordings

Multi-electrode arrays (see Fig. 7) are high throughput ways to record the spiking activity in neuronal tissue and are hence rich sources of event data where events correspond to specific neurons (or clumps of neurons) being activated. We use data from dissociated cortical cultures gathered by Steve Potter’s laboratory at Georgia Tech [15] which gathered data over several days. The DBN shown in Fig. 8 depicts a circuit discovered from (> 80%). It can be seen in the figures that for a network with 125 variables, the total run-time is of the order of few minutes along with recall > 80% and precision at almost 100%.

Another way to study scalability is w.r.t. the density of the network, defined as the ratio of the number of nodes that are descendants for some other node to the total number of nodes in the network. Fig 5 shows the time taken for mining DBN when the density is varied from 0.1 to 0.6.
the first 15 min of recording on day 35 of culture 2-1. The overall mining process takes about 10 min with threshold $\theta = 0.0015$ with DBN search parameter $\epsilon = 0.0005$.

Figure 7: Micro electrode array (MEA) used to record spiking activity of neurons in tissue cultures.

In order to establish that this network is in fact significant we run our algorithm on several surrogate spike trains generated by replacing the neuron labels of each spikes in the real data with a randomly chosen neuron label. These surrogates are expected to break the temporal correlations in the data and yet preserve the overall summary statistics. No network structure was found in 25 such surrogate sequences. We are currently in the process of characterizing and interpreting the usefulness of such networks found in real data.

8 Discussion

We have presented the beginnings of research to relate inference of DBNs with frequent episode mining. The key contribution here is to show how, under certain assumptions on network structure, data and distributional characteristics, we are able to infer the structure of DBNs using the results from frequent episode mining. While our experimental results provide convincing evidence of the efficacy of our methods, in future work we aim to provide strong theoretical results supporting our experiences.

An open question of interest is to characterize (other) useful classes of DBNs that have both practical relevance (like excitatory circuits) and which also can be tractably inferred using sufficient statistics of the form studied here.

9 Repeatability

Supplementary material, algorithm implementations, and results for this paper are hosted at http://neural-code.cs.vt.edu/dbn.

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