Efficient PAC Learnability of Dynamical Systems Over Multilayer Networks

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Abstract. Networked dynamical systems are widely used as models of real-world cascade phenomena such as the spread of disease and information. Prior research has addressed the problem of learning the behavior of an unknown dynamical system when the underlying network has a single layer. In this paper, we study the learnability of dynamical systems over *multilayer* networks, which are much more realistic and challenging. First, we propose an efficient PAC learning algorithm with provable guarantees, and establish bounds on the sample complexity. Our results show that even though the hypothesis space grows exponentially in the number of layers, the proposed learner only requires a small number of training examples. Further, we provide a tight analysis of the Natarajan dimension, which measures the expressive power of the hypothesis class. Our results show that, asymptotically, our bound on the Nararajan dimension is tight for *almost all* multilayer graphs. The techniques and insights in our paper provide the theoretical foundations for future investigation of learning problems for multilayer systems.

1 Introduction

Networked dynamical systems are mathematical models for numerous cascade processes such as the spread of social behaviors, information, diseases, and biological phenomena [6, 31, 33, 35, 39, 50, 52]. In general, a networked dynamical system consists of an *underlying graph* where vertices are entities (e.g., individuals, genes), and edges are relationships between the entities. Further, each vertex has a *state* and *interaction functions* (i.e., behavior), which specify how the state evolves over time. The system dynamics proceeds in discrete time, with vertices updating states using interaction functions.

Inferring the unknown components of a networked system is an active area of research [2, 10, 12, 15, 38, 42]. One ongoing line of work is to learn the unknown *interaction functions* of entities (i.e., vertices) in a networked dynamical system. Interaction functions play a critical role in the system dynamics. In particular, these functions specify the decision rules that entities use to update their contagion states (e.g., whether or not to believe a rumor). One example is the class of threshold interaction functions [24], which are widely used to model the spread of social contagions [37, 58]. Specifically, each entity in the network has a decision threshold that represents the tipping point for a behavioral (i.e., state) change. In the case of a rumor, a person's belief changes when the number of neighbors believing in the rumor reaches a certain threshold. Overall, the interaction functions define the underlying mechanism of the cascade process, which also describes the system's global behavior (often complex and nonlinear) over time [24]. Therefore, when the interaction functions in a system are unknown, learning these missing components is of great interest.

Existing methods for learning interaction functions in networked systems only apply to the case when the underlying graph has a *single-layer*. To our knowledge, the problem for the more complex and realistic *multilayer* setting (that gives rise to multi-relational networks) has not received attention in the literature. In this work, we fill this gap through a formal study of **the learnability of the interaction functions in dynamical systems over multilayer networks**. Specifically, the graph in our target system consists of multiple layers with generally *different* set of edges in each layer. This is a classic setting for multilayer networks, and the ability of such networks to model complex real-world phenomena has been widely recognized (e.g., [25, 34, 44]). In particular, multilayer networks allow heterogeneous ties between vertices, with edges in each layer capturing a particular type of interaction (e.g., close friend, acquaintance) [17, 34, 44]. The framework also permits more complex cascades that involve *cross-layer interactions* [7, 16, 49].

Problem description. Consider a multilayer networked system where the interaction functions of vertices are *unknown*. By inferring these functions, our goal is to learn a system that captures the behavior of the true unknown system, with performance guarantees under the Probably Approximately Correct (PAC) model [55]. We learn from *snapshots of the true system's dynamics*, a common scheme considered in related papers (e.g., [9, 12, 59]). Since our problem setting involves multiclass learning, we also examine the *Natarajan dimension* [43], a well-known generalization of the VC dimension [57]. The Natarajan dimension measures the expressive power of the hypothesis class and characterizes the sample complexity of learning [51]. Overall, we aim to answer the following questions: (i) *How does one efficiently learn the true underlying multilayer system, and how many training examples are sufficient?* (ii) *What is the expressive power of the hypothesis class of multilayer networked systems?*

Challenges. The multilayer setting poses new challenges. First, the number of hypotheses grows exponentially in the number of layers; thus, a learner needs to find an appropriate hypothesis in a much larger space. Further, a learner must carefully analyze the complex *cross-layer interactions*. For example, while the training data (snapshots of dynamics) indicates a vertex's state change, it *does not* provide information about which layer(s) triggered the change. Additionally, when establishing a learner's performance, the analysis should account for the fact that a wrong prediction could be caused by any subset of layers. The intertwined connections between vertices in the multilayer setting also introduce complications in analyzing the Natarajan dimension. Overall, these challenges make our problem significantly different from the corresponding problem for single-layer networks.

Our contributions are as follows:

- **PAC learning.** We show that a small training set is sufficient to efficiently PAC learn the multilayer system. Specifically, we obtain the following results. (i) We develop an efficient PAC learner with provable guarantees: w.p. at least $1 - \delta$, the prediction error is at most ϵ, for any $\epsilon, \delta > 0$. (ii) For any fixed ϵ and δ, the number of training exampled used by our algorithm is only $O(\sigma k \log(\sigma k))$, where k is the number of layers and σ is the number of vertices with unknown interaction functions. Thus, when σ is fixed, the size of an adequate training set does *not* increase with the network size or density. This result also provides an upper bound on the sample complexity that is tighter than the general information-theoretic bound [26]. (iii) We further extend the learner to the Probably

Mostly Approximately Correct setting [3] and prove that the amount of training data can be further reduced under a relaxed notion of successful predictions by a learner. (*iv*) Using real-world and synthetic multilayer networks, we also experimentally explore the relationship between the algorithm's performance and system parameters under various scenarios.

- **Natarajan dimension.** We provide a tight analysis of the Natarajan dimension (Ndim), which measures the expressive power of the hypothesis class of multilayer systems. (*i*) We present a novel combinatorial structure and establish its equivalence to shatterable sets. (*ii*) Based on this connection, we present an (efficient) method for constructing shatterable sets and show that when restricting the system to an individual layer, Ndim is *exactly* σ, the number of vertices with unknown interaction functions. This precise characterization could be of independent interest. (*iii*) We then extend the argument to show that for a k-layer system, Ndim is between σ and $k\sigma$ and present classes of instances where the bounds are tight. Our result also provides a lower bound on the sample complexity. (*iv*) Lastly, using a probabilistic argument, we show that asymptotically for *almost all graphs* with n vertices and $k \geq 2$ layers, Ndim is *exactly* $k\sigma$.

Related work. Learning unknown components of networked systems is an active line of research. For *single-layer* networks, many researchers have developed methods to address problems related to *cascade inference* (e.g., learning the diffusion functions at vertices, edge parameters, source vertices, and contagion states of vertices) by observing propagation dynamics. For instance, Chen et al. [9] infer the edge probability and source vertices under the independent cascade model. Conitzer et al. [12] investigate the problem of inferring opinions (states) of vertices in stochastic cascades under the PAC scheme. Lokhov [38] studies the problem of reconstructing the parameters of a diffusion model given infection cascades. Other representative results include [10, 13, 14, 15, 18, 23, 28, 29, 32, 42, 59]. Questions on learning the network structure based on the outcomes of cascades have also been studied; see, for example [30, 46, 1, 19, 41, 22, 53]. To our knowledge, the problem of learning the interaction functions of networked multilayer systems has not been examined.

The paper that is most closely related work is by Adiga et al. [2], where the PAC learnability of threshold interaction functions in *single-layer* networked systems is studied. They present a consistent learner when there are only positive examples and show the hardness of learning when negative examples are also included. They also bound the sample complexity based on VC dimension. As mentioned earlier, the multilayer setting introduces new *challenges* that do not arise in the single-layer setting. For these reasons, the results in [2] cannot be directly applied to our multilayer setting, which requires new techniques developed in our work.

2 Preliminaries

Our setting follows the existing research on learning networked systems. For the readers' reference, we have included a table of the settings for several related papers in the Appendix (Section 6.1).

2.1 Multilayer Networked Dynamical Systems

Multilayer networks. All the graphs considered are undirected. For any integer $k \geq 1$, let $[k]$ denote the set $\{1, \ldots, k\}$. A *multilayer network* [34] is a sequence of graphs $\mathcal{M} = \{\mathcal{G}_i\}_{i=1}^{k}$, $\mathcal{G}_i = (\mathcal{V}, \mathcal{E}_i)$, where $\mathcal{V}$ is a set of n vertices *shared* by all graphs in $\mathcal{M}$, and $\mathcal{E}_i$ is the set of edges in $\mathcal{G}_i$, $i \in [k]$. Note that the edge sets of graphs in $\mathcal{M}$ are generally *different*. Overall, one can view $\mathcal{M}$ as a k-layer network where $\mathcal{G}_i \in \mathcal{M}$ is the graph on the ith layer.

Dynamical systems. Dynamical systems on multilayer networks is a generalization of dynamical systems over a single-layer network, as studied in previous works, e.g., [4]; we also follow their notation. A *Multilayer Synchronous Dynamical System* (**MSyDS**) over the Boolean domain $\mathbb{B} = \{0, 1\}$ is a triple $h^* = (\mathcal{M}, \mathcal{F}, \Psi)$:

- $\mathcal{M} = \{\mathcal{G}_i\}_{i=1}^{k}$ is an underlying multilayer network with k layers. Each vertex has a state from $\mathbb{B}$.
- $\mathcal{F} = \{f_{i,v} : i \in [k], v \in \mathcal{V}\}$ is a collection of functions, with $f_{i,v}$ denoting vertex v's **local interaction function** on the ith layer $\mathcal{G}_i$.
- $\Psi = \{\psi_v : v \in \mathcal{V}\}$ is a collection of functions, with ψ_v denoting the **master function** of vertex v.

The system dynamics proceeds in discrete time. Starting from the initial states of vertices, at each step, vertices update states *synchronously* using interaction functions and master functions. Specifically, for any $t \geq 0$, the state of each vertex v at time $t + 1$ is computed as follows:

- For each $\mathcal{G}_i \in \mathcal{M}$, the interaction function $f_{i,v} \in \mathcal{F}$ is evaluated, where the inputs are the states of vertices in v's closed neighborhood (i.e., v and its neighbors) in $\mathcal{G}_i$ at time t; $f_{i,v}$ then outputs a value in $\mathbb{B}$. This gives a k-vector $\mathbf{W}_v$ for each v, where $\mathbf{W}_v(i)$ is the output of $f_{i,v}$, $i \in [k]$.
- Next, the master function ψ_v is evaluated, with $\mathbf{W}_v$ as the input. The output of ψ_v, which is a value in $\mathbb{B}$, is the **next state** of v (i.e., its state at time $t + 1$).

Interaction functions. We focus on *threshold* interaction functions, a classic framework to model spreads of social contagions [24, 58]. In particular, each $v \in \mathcal{V}$ has an integer threshold $\tau_i(v) \in [0, \deg_i(v) + 2]$ for each layer $\mathcal{G}_i$, $i \in [k]$; here, $\deg_i(v)$ is the degree of v in $\mathcal{G}_i$. The interaction function $f_{i,v} \in \mathcal{F}$ outputs 1 if the number of active (i.e., state-1) vertices in v's closed neighborhood in $\mathcal{G}_i$ is **at least** $\tau_i(v)$; $f_{i,v}$ outputs 0 otherwise. If $f_{i,v}$ outputs 1, we say that the **threshold condition** of v is satisfied on $\mathcal{G}_i$.

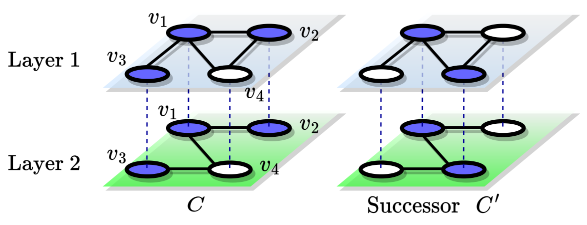

Figure 1: A 2-layer system with threshold interaction functions and `OR` master functions. Threshold values of vertices v_1 to v_4 in the first layer are $(2, 3, 3, 2)$, and in the second layer are $(3, 3, 2, 1)$. State-1 vertices are in blue. The configuration $\mathcal{C} = (1, 1, 1, 0)$, and it can be verified that its successor is $\mathcal{C}' = (1, 0, 0, 1)$.

Master functions. The two classes of master functions proposed in the literature are `OR` and `AND` [8, 36]. When function ψ_v is `OR`, the next state of v is 1 iff **there exists** a layer $i \in [k]$ where the interaction function $f_{i,v}$ evaluates to 1. In other words, v's next state is 1 iff its threshold condition is satisfied in at least one layer. Analogously, for `AND` functions, the next state of v is 1 iff $f_{i,v}$ evaluates to 1 in all the layers. An example of the dynamics for the `OR` master function is shown in Fig. 1.

A **configuration** $\mathcal{C}$ is an n-bit binary vector that specifies the state of each vertex at a particular time step. We use $\mathcal{C}(v)$ to denote the state of vertex v in $\mathcal{C}$. A configuration $\mathcal{C}'$ is the **successor** of $\mathcal{C}$ under a system h^* if $\mathcal{C}'$ evolves from $\mathcal{C}$ in one time step; this is $\underline{\text{denoted by } \mathcal{C}' = h^*(\mathcal{C})}$. Overall, the evolution of system h^* can be represented as a time-ordered sequence of configurations.

2.2 The Learning Problem

Hypothesis class. There is a ground truth MSyDS h^*. The learner is given partial information about h^*, where the thresholds (on all layers) of a subset $\mathcal{V}' \subseteq \mathcal{V}$ of vertices in h^* are *unknown*. Let $\sigma = |\mathcal{V}'|$. The *hypothesis class* $\mathcal{H}$ consists of $O(n^{\sigma k})$ MSyDSs over all possible threshold values of vertices in $\mathcal{V}'$. The goal is then to learn an MSyDS $h \in \mathcal{H}$ that is a good approximation of h^* by inferring the unknown thresholds. When $\mathcal{V}' = \mathcal{V}$, the thresholds of all vertices must be learned.

PAC learning. We learn the target system h^* from snapshots of its dynamics. Formally, let $\mathcal{X} = \{0,1\}^n$ be the set of all n-bit binary vectors. Let $\mathcal{T} = \{(\mathcal{C}_j, \mathcal{C}'_j)\}_{j=1}^q$ be a *training set* of q examples, which consists of the snapshots of system dynamics. In particular, examples in $\mathcal{T}$ are *configuration pairs*, where $\mathcal{C}_j$ is a drawn i.i.d. from an unknown distribution $\mathcal{D}$ over $\mathcal{X}$, and $\mathcal{C}'_j = h^*(\mathcal{C}_j)$ is the successor of $\mathcal{C}_j$ under h^*. We use $\mathcal{T} \sim \mathcal{D}^q$ to denote such a training set. For a new $\mathcal{C} \sim \mathcal{D}$ sampled, a hypothesis $h \in \mathcal{H}$ makes a successful prediction if $h(\mathcal{C}) = h^*(\mathcal{C})$. The **true error** of a hypothesis h is defined as $L_{(\mathcal{D},h^*)}(h) \coloneqq \Pr_{\mathcal{C}\sim\mathcal{D}}[h(\mathcal{C}) \neq h^*(\mathcal{C})]$. In the PAC model, when $\mathcal{T}$ is sufficiently large, the goal of a learner is to output an $h \in \mathcal{H}$ s.t. with probability at least $1-\delta$ over $\mathcal{T} \sim \mathcal{D}^q$, it holds that $L_{(\mathcal{D},h^*)}(h) \leq \epsilon$, for any given $\epsilon, \delta \in (0,1)$. The minimum number of training examples needed by any PAC learner to learn $\mathcal{H}$ is called the *sample complexity* of $\mathcal{H}$.

Natarajan dimension. Learning a hypothesis $h \in \mathcal{H}$ in our context can be cast as a *multiclass classification* problem, since h maps a configuration $\mathcal{C}$ to one of the possible 2^n configurations (classes). To characterize the expressive power of the hypothesis class $\mathcal{H}$, we consider the Natarajan dimension [43], which is a generalization of the VC dimension to the multiclass setting. The Natarajan dimension measures the *complexity* and *expressiveness* of the hypothesis class. Formally, a set $\mathcal{R} \subset \mathcal{X}$ is **shattered** by $\mathcal{H}$ if for every $\mathcal{C} \in \mathcal{R}$, one can find two associated configurations, denoted by $\mathcal{C}^A, \mathcal{C}^B \in \mathcal{X}$, such that (i) $\mathcal{C}^A \neq \mathcal{C}^B$, and (ii) for every subset $\mathcal{R}' \subseteq \mathcal{R}$, there exists $h \in \mathcal{H}$ such that $\forall \mathcal{C} \in \mathcal{R}'$, $h(\mathcal{C}) = \mathcal{C}^A$ and $\forall \mathcal{C} \in \mathcal{R} \setminus \mathcal{R}'$, $h(\mathcal{C}) = \mathcal{C}^B$. The **Natarajan dimension** of $\mathcal{H}$, denoted by $\text{Ndim}(\mathcal{H})$, is the *maximum* size of a shatterable set. Further, $\Omega((\text{Ndim}(\mathcal{H}) + \log(1/\delta))/\epsilon)$ is a lower bound on the sample complexity of learning $\mathcal{H}$ [51]. Overall, the larger the value of $\text{Ndim}(\mathcal{H})$, the higher the expressive power of $\mathcal{H}$.

3 PAC Learnability of Multilayer Networked Systems

In this section, we establish the efficient PAC learnability of the hypothesis class $\mathcal{H}$, defined in Section 2. We first develop an efficient learner by exploring the mechanism of cross-layer interactions. We then show that a training set of size $\lceil 1/\epsilon \cdot \sigma k \cdot \log(\sigma k/\delta) \rceil$ is sufficient for the learner to achieve the (ϵ,δ)-PAC guarantee. Lastly, we show that our learner can also handle the more general PMAC learning setting [3], which permits a more relaxed notion of predictions. Due to space limits, **full proofs appear in the Appendix, Section 6.2**.

3.1 An Efficient PAC Learner

For a configuration $\mathcal{C}$, a vertex $v \in \mathcal{V}$ and a layer $i \in [k]$, let $\Gamma_i[\mathcal{C}, v]$ be the number of 1's in the input to the interaction function $f_{i,v}$ under $\mathcal{C}$ (i.e., the number of state-1 vertices in v's closed neighborhood in $\mathcal{G}_i$). We call $\Gamma_i[\mathcal{C}, v]$ the **score** of v in $\mathcal{G}_i$ under $\mathcal{C}$. Let $\tau_i^h(v)$ be the *learned threshold* of v for the ith layer in h, and let $\tau_i^{h^*}(v)$ be v's *true threshold* in the target system h^*.

PAC Learner. Our algorithm learns a hypothesis $h \in \mathcal{H}$ by inferring the unknown thresholds in the target system h^*. Suppose the master function is `OR`. Given a training set $\mathcal{T} \sim \mathcal{D}^q$, for each vertex v in the set $\mathcal{V}'$ of vertices with unknown thresholds, for each layer $\mathcal{G}_i \in \mathcal{M}$, assign $\tau_i^h(v) = \max_{(\mathcal{C},\mathcal{C}')\in\mathcal{T}:\mathcal{C}'(v)=0}\{\Gamma_i[\mathcal{C},v]\}+1$. If $\mathcal{C}'(v) = 1$ for all $(\mathcal{C},\mathcal{C}') \in \mathcal{T}$, assign $\tau_i^h(v) = 0$.

On the other hand, if the master function is `AND`, assign $\underline{\tau_i^h(v) = \min_{(\mathcal{C},\mathcal{C}')\in\mathcal{T}:\mathcal{C}'(v)=1}\{\Gamma_i[\mathcal{C},v]\}}$. If $\mathcal{C}'(v) = 0$ for all $(\mathcal{C},\mathcal{C}') \in \mathcal{T}$, assign $\underline{\tau_i^h(v) = \deg_i(v) + 2}$, where $\deg_i(v)$ is the degree of v in $\mathcal{G}_i$. Lastly, the algorithm returns the corresponding system $h \in \mathcal{H}$. One can easily verify that h has zero empirical risk. Further, the running time is $O(nk \cdot |\mathcal{T}|)$. Since $\mathcal{H}$ is finite, it follows that the class $\mathcal{H}$ is efficiently PAC learnable [51].

Theorem 3.1. The class $\mathcal{H}$ is efficiently PAC learnable.

3.2 The Sample Complexity

We now show that our algorithm does not require too many training examples to PAC-learn $\mathcal{H}$. To begin with, a well-known general result in [26] implies that the sample complexity $m_{\mathcal{H}}(\delta,\epsilon)$ of $\mathcal{H}$ is upper bounded by $(1/\epsilon)\log(|\mathcal{H}|/\delta)$, where $\epsilon, \delta \in (0,1)$ are the two parameters in the PAC scheme. In our case, one can derive that

$$m_{\mathcal{H}}(\delta,\epsilon) \;\le\; \frac{1}{\epsilon}\cdot(\sigma k \cdot \log(d_{\text{avg}}(\mathcal{V}')) + \log(\frac{1}{\delta}), \tag{1}$$

where $\sigma = |\mathcal{V}'|$, k is the number of layers, and $d_{\text{avg}}(\mathcal{V}')$ is the average degree of the vertices of $\mathcal{V}'$ in the network where all the layers are merged into a single layer with parallel edges removed.

An alternative bound. The bound (1) depends explicitly on the average degree since a denser network always leads to a larger hypothesis class. Nevertheless, we now establish an alternative bound on the training set size $|\mathcal{T}|$ for our algorithm; this bound *does not depend explicitly on any graph parameters* (e.g., d_{avg}) except for the number of layers k.

A key lemma. For a configuration $\mathcal{C} \sim \mathcal{D}$, and a vertex v, let $B(\mathcal{C},v)$ denote the event that "$h^*(\mathcal{C})(v) = 0$", i.e., in the true system h^*, in every layer, $\mathcal{C}$ does not satisfy the threshold condition of v. For a layer $i \in [k]$ and a system $h \in \mathcal{H}$, let $A(\mathcal{C},i,v,h)$ be the "bad" event that "(1) the threshold condition of v on the ith layer is satisfied under h, and (2) $B(\mathcal{C},v)$ occurs". Formally, $A(\mathcal{C},i,v,h)$ is the event that "$\Gamma_i[\mathcal{C},v] \ge \tau_i^h(v)$ and $\forall j \in [k]$, $\Gamma_j[\mathcal{C},v] < \tau_j^{h^*}(v)$".

We now bound the probability (over $\mathcal{T} \sim \mathcal{D}^q$) of our algorithm learning a "bad" $h \in \mathcal{H}$ s.t. $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \ge \alpha$, for a given $\alpha \in (0,1)$.

Lemma 3.2. For a $v \in \mathcal{V}'$ and an $i \in [k]$, suppose $\tau_i^{h^*}(v) \ge 1$. Let $h \in \mathcal{H}$ be a hypothesis learned from a training set $\mathcal{T}$ of size $q \ge 1$. For a given $\alpha \in (0,1)$, and an integer $\rho_i(v) \in [0, \tau_i^{h^*}(v))$:

(1) If all $\rho_i(v)$ satisfy $\Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C},v)$ and $\Gamma_i[\mathcal{C},v] \ge \rho_i(v)] < \alpha$. Then $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] < \alpha$.

(2) Even if (1) does not hold, that is, there is a $\rho_i(v)$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C},v)$ and $\Gamma_i[\mathcal{C},v] \ge \rho_i(v)] \ge \alpha$, then $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \ge \alpha$ holds with probability **at most** $(1-\alpha)^q$ over $\mathcal{T} \sim \mathcal{D}^q$.

For an error rate $\alpha \in (0,1)$, Lemma 3.2 states that the probability (over $\mathcal{T} \sim \mathcal{D}^q$) of the algorithm learning a "bad" hypothesis h where $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \ge \alpha$ is at most $(1-\alpha)^q$. Using this lemma, we now present the result on the size of an adequate training set for our algorithm.

Theorem 3.3. For any $\epsilon, \delta \in (0,1)$, with a training set of size $q = \lceil 1/\epsilon \cdot \sigma k \cdot \log(\sigma k/\delta) \rceil$, the proposed algorithm learns a hypothesis $h \in \mathcal{H}$ such that with probability at least $1-\delta$ (over $\mathcal{T} \sim \mathcal{D}^q$), $\Pr_{\mathcal{C}\sim\mathcal{D}}[h(\mathcal{C}) \neq h^*(\mathcal{C})] < \epsilon$.

Implication on the sample complexity. Theorem 3.3 provides an upper bound on the sample complexity $m_{\mathcal{H}}(\delta, \epsilon)$ of learning $\mathcal{H}$. Specifically, $m_{\mathcal{H}}(\delta, \epsilon) \leq \lceil \frac{1}{\epsilon} \cdot \sigma k \cdot \log(\frac{\sigma k}{\delta}) \rceil$.

Remark. With the proposed learner, Theorem 3.3 shows that an adequate number of examples to PAC-learn $\mathcal{H}$ does *not* explicitly depend on the average degree or the size of the multilayer graph. Thus, when other parameters are fixed, the sample complexity of learning $\mathcal{H}$ does not grow as the graph gets larger or denser. Further, Our bound in Theorem 3.3 is tighter than Ineq (1) in several regimes. For instance, for a fixed σ, the bound in Ineq (1) grows as $d_{avg}(\mathcal{V}')$ gets larger; on the other hand, our bound remains unchanged.

Extension to the PMAC Model. Our PAC learner can handle a more general Probably Mostly Approximately Correct (PMAC) framework [3], where the goal is to make predictions that are good *approximations* for the true values. Specifically, the learned hypothesis h makes a successful prediction if $h(\mathcal{C})$ agrees with $h^*(\mathcal{C})$ on the states of more than $(1-\beta)$ fraction of the vertices in $\mathcal{V}'$, for a given factor $\beta \in (0,1)$. Foramally, let $W(h(\mathcal{C}), h^*(\mathcal{C}))$ be the number of vertices in $\mathcal{V}'$ whose states in $h(\mathcal{C})$ are *different* from those in $h^*(\mathcal{C})$. For given $\epsilon, \delta, \beta \in (0,1)$, the goal is to learn a hypothesis $h \in \mathcal{H}$ such that with probability at least $1-\delta$ over $\mathcal{T} \sim \mathcal{D}^q$, $\Pr_{\mathcal{C}\sim\mathcal{D}}[W(h(\mathcal{C}), h^*(\mathcal{C})) \geq \beta\sigma] \ \leq \ \epsilon$.

The PMAC model has been used in many contexts, such as learning submodular functions [47, 3] and cascade inference [12]. Our next theorem shows that the training set can be significantly reduced under this setting.

Theorem 3.4. For any given $\epsilon, \delta, \beta \in (0,1)$, with a training set $\mathcal{T}$ of size $q = \lceil 1/\epsilon \cdot 1/\beta \cdot k \cdot \log(\sigma k/\delta) \rceil$, the proposed algorithm (Section 3.1) learns an $h \in \mathcal{H}$ such that with probability at least $1-\delta$ over $\mathcal{T} \sim \mathcal{D}^q$, h satisfies the condition $\Pr_{\mathcal{C}\sim\mathcal{D}}[W(h(\mathcal{C}), h^*(\mathcal{C})) \geq \beta\sigma] \ \leq \ \epsilon$.

Remark. Compared to the bound on the PAC sample complexity in Theorem 3.3, the size of an adequate training set under the PMAC model is reduced by a multiplicative factor of $\sigma\beta$. For instance, when β is a constant (i.e., to obtain a constant-factor approximation), the training set size is decreased by a linear (w.r.t. σ) factor. This demonstrates a trade-off between the quality of the prediction and the size of the training data: when our learner is allowed to make approximate predictions, it requires a much lower number of examples to learn an appropriate hypothesis.

4 Tight Analytical Results for Natarajan Dimension

Recall that the Natarajan dimension (Ndim) of a hypothesis class measures the expressiveness of the class and characterizes the sample complexity of PAC learning [43]. In particular, the higher the value of Ndim, the greater is the expressive power of the class. In this section, we examine the Natarajan dimension of the hypothesis class $\mathcal{H}$, denoted by Ndim($\mathcal{H}$), and develop the following results. **Proofs of all the results appear in the Appendix, Section 6.3.**

First, we present an efficient method for constructing shatterable sets based on an iterative search technique. Using this method, we establish that Ndim($\mathcal{H}$) is *exactly* σ when the underlying network has only one layer. Previously, Adiga et al. [2] showed that for the single-layer case where $\sigma = n$, the dimension of $\mathcal{H}$ is at least $n/4$. Our precise characterization of $\mathrm{Ndim}(\mathcal{H})$ provides both an improvement over their bound [2] and an extension to arbitrary σ.

Next, we show that for multilayer networks, $\mathrm{Ndim}(\mathcal{H})$ is bounded between σ and $k\sigma$. This proof uses an extended version of our argument for the single-layer case. Further, we present classes of instances where the bounds are tight. Our results also show that the best lower bound for sample complexity that one can obtain using this approach is $\Omega((\sigma + \log(1/\delta))/\epsilon)$.

Lastly, we further tighten our analysis by showing that asymptotically, for *almost all* graphs (i.e., the probability tends to 1) with n vertices and $k \geq 2$ layers, $\mathrm{Ndim}(\mathcal{H})$ of the corresponding hypothesis class $\mathcal{H}$ is *exactly* σk.

4.1 An Exact Characterization for a Single Layer

Consider the case where the underlying network of the true system h^* has a single layer. We present a combinatorial characterization of a shatterable set, which allows us to obtain an exact value for $\mathrm{Ndim}(\mathcal{H})$. We begin with some definitions.

Definition 4.1 (**Landmark Vertices**)**.** Suppose the underlying network has a single layer. Given a set $\mathcal{R} \subseteq \mathcal{X}$, a vertex $v \in \mathcal{V}'$ is a ***landmark*** vertex for a configuration $\mathcal{C} \in \mathcal{R}$ if the score $\Gamma[\mathcal{C}, v] \neq \Gamma[\hat{\mathcal{C}}, v]$ for all $\hat{\mathcal{C}} \in \mathcal{R} \setminus \{\mathcal{C}\}$.

The landmark vertices play a key role in $\mathcal{R}$ being shatterable. Given $\mathcal{R} \subseteq \mathcal{X}$, let $\mathcal{W}(\mathcal{R}) \subseteq \mathcal{V}'$ be the (possibly empty) set of vertices that are landmark vertices for at least one configuration in $\mathcal{R}$.

Definition 4.2 (**Canonical Set**)**.** Suppose the underlying network has a single layer. A set $\mathcal{R} \subseteq \mathcal{X}$ is ***canonical*** w.r.t. $\mathcal{H}$ if there exists an $\underline{\text{injective}}$ mapping from $\mathcal{R}$ to $\mathcal{W}(\mathcal{R})$ s.t. each $\mathcal{C} \in \mathcal{R}$ is mapped to a landmark vertex of $\mathcal{C}$.

Shattering. By the definition of shattering (see Section 2), each $\mathcal{C}$ in a shatterable set $\mathcal{R}$ is associated with two configurations, denoted by $\mathcal{C}^A$ and $\mathcal{C}^B$, where $\mathcal{C}^A \neq \mathcal{C}^B$.

Definition 4.3 (**Contested Vertices**)**.** We call a vertex v **contested** for a $\mathcal{C} \in \mathcal{R}$ if $\mathcal{C}^A(v) \neq \mathcal{C}^B(v)$.

By linking landmark vertices to contested vertices, our next Lemma shows that for a single-layer system, the property of being canonical is *equivalent* to being shatterable.

Lemma 4.4. When the underlying network has a single layer, a set $\mathcal{R} \subseteq \mathcal{X}$ can be shattered by $\mathcal{H}$ **if and only if** $\mathcal{R}$ is canonical w.r.t. $\mathcal{H}$.

Remark. By definition, the size of a canonical set is at most $|\mathcal{V}'| = \sigma$. From Lemma 4.4, it follows that $\mathrm{Ndim}(\mathcal{H})$, which is the maximum size of a shatterable set, is **at most** σ when the underlying network has a single layer.

Next, we present an efficient method for constructing a canonical set of size σ based on depth-first search (see proof of Theorem 4.5 in the Appendix). Consequently, for *any* underlying single-layer network, **there exists a shatterable set of size exactly** σ. Overall, we obtain the tight result that for single-layer systems, $\mathrm{Ndim}(\mathcal{H}) = \sigma$. Formally:

Theorem 4.5. When the underlying network has a single layer, a shatterable set of size σ can be constructed. Thus, $\text{Ndim}(\mathcal{H}) = \sigma$.

Remark. Theorem 4.5 is interesting since for many problems [56, 5], including those on learning networked systems [2], known results on such dimensions are bounds rather than exact values. Further, our graph theoretic machinery (e.g., canonical set) may be of independent interest in studying other learning problems for dynamical systems.

4.2 Bounds on Ndim for Multilayer Systems

Based on the results developed in the previous section, we obtain bounds on $\text{Ndim}(\mathcal{H})$ when the underlying network $\mathcal{M}$ has $k \geq 2$ layers. We first prove that $\text{Ndim}(\mathcal{H}) \leq k\sigma$ by showing that each $v \in \mathcal{V}'$ is *contested* for at most k configurations in any shatterable set. We then show that $\text{Ndim}(\mathcal{H}) \geq \sigma$ by establishing that any shatterable set obtained by restricting the system to any single layer in $\mathcal{M}$ is also shatterable over the multilayer network $\mathcal{M}$. We start with the upper bound:

Lemma 4.6. If the network has $k \geq 2$ layers, then the size of any shatterable set $\mathcal{R}$ is at most $k\sigma$.

To establish a lower bound on the size of a shatterable set, we prove the following lemma.

Lemma 4.7. Suppose h^* is an MSyDS whose underlying network has $k \geq 2$ layers. Let $\hat{h}^*$ be a single-layer system obtained from h^* by using the network in any layer $i \in [k]$. If a set $\mathcal{R}$ is shatterable by the hypothesis class of $\hat{h}^*$, then it is also shatterable by the hypothesis class of h^*.

By Theorem 4.5, when the underlying network has a single layer, there exists a shatterable set of size σ. Thus, Lemma 4.7 implies that there also exists a shatterable set of size σ for the multilayer setting. Overall, we obtain the following bounds on $\text{Ndim}(\mathcal{H})$:

Theorem 4.8. Suppose the underlying network has $k \geq 2$ layers. Then $\sigma \leq \text{Ndim}(\mathcal{H}) \leq k\sigma$.

Remark. There are classes of multilayer systems where the bounds are tight. To match the lower bound, consider a class of 2-layer networks $\mathcal{M} = \{\mathcal{G}_1, \mathcal{G}_2\}$ where for *every* vertex v, the set of neighbors in $\mathcal{G}_2$ is a superset of its neighbor set in $\mathcal{G}_1$, with *exactly* one extra neighbor in $\mathcal{G}_2$. One can easily verify that $\text{Ndim}(\mathcal{H}) = \sigma$ in this case. On the other hand, in the next section, we show that the upper bound ($k\sigma$) is tight for *almost all* threshold MSyDSs.

Implications in the sample complexity. By a result in [51], our bounds on $\text{Ndim}(\mathcal{H})$ in Theorem 4.8 lead to the following bounds on the sample complexity for PAC learning $\mathcal{H}$.

$$c_1 \frac{\sigma + \log(1/\delta)}{\epsilon} \;\leq\; m_{\mathcal{H}}(\delta, \epsilon) \;\leq\; \frac{1}{\epsilon} \cdot \left(c_2 \cdot k\sigma \cdot \log\left(\frac{k\sigma}{\epsilon}\right) + k\sigma^2 + \log\left(\frac{1}{\delta}\right) \right) \tag{2}$$

for some constants $c_1, c_2 \geq 0$.

Remark. The upper bound in the above inequality has the dominant term $O(k\sigma^2)$, while our upper bound (established in Theorem 3.3) is $O(k\sigma \log(k\sigma))$. Thus, this general upper bound is weaker than our bound. As for the lower bound in Ineq (2), when the number of layers k is a constant (a realistic scenario in real-world networks by the Dunbar's number [20]), our upper bound on the sample complexity (Theorem 3.3) is within the factor $O(\log(\sigma))$ of the lower bound.

4.3 The Asymptotic Tightness of the Bounds

We have shown that for any k-layer system, $\mathrm{Ndim}(\mathcal{H})$ is at most $k\sigma$. In this section, we further explore the expressive power of the hypothesis class and prove that asymptotically (i.e., as $n \longrightarrow \infty$), for *almost all* graphs with n vertices and $k \geq 2$ layers, $\mathrm{Ndim}(\mathcal{H})$ of the corresponding hypothesis class is *exactly* $k\sigma$; i.e., the highest expressiveness possible which matches our upper bound.

Approach overview. Given a multilayer network $\mathcal{M}$, we first define a special set $\mathcal{Q}$ of vertex-layer pairs in $\mathcal{M}$. We then show that for each such set $\mathcal{Q}$, there is a shatterable set of size $|\mathcal{Q}|$ for the corresponding hypothesis class under $\mathcal{M}$. Next, consider a graph $\mathcal{M}$ chosen uniformly at random from the space of all k-layer graphs with n vertices. We prove that asymptotically with probability 1, $\mathcal{M}$ admits such a special set $\mathcal{Q}$ that contains *all the $k\sigma$ vertex-layer pairs*, thus implying the existence of a shatterable set of size $k\sigma$.

Vertex-layer set. For a k-layer network $\mathcal{M}$ and a subset $\mathcal{V}'$ of vertices, let $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ be a set of vertex-layer pairs $(v,i), v \in \mathcal{V}', i \in [k]$, such that every $(v,i) \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ satisfies the following condition: $N_{\mathcal{M}}[v,i] \setminus N_{\mathcal{M}}[v',i'] \neq \varnothing, \forall (v',i') \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}, (v',i') \neq (v,i)$, where $N_{\mathcal{M}}[v,i]$ is the closed neighborhood of v in the ith layer of $\mathcal{M}$. We first establish the correspondence between such a set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ and a shatterable set.

Lemma 4.9. Given a multilayer network $\mathcal{M}$ and a subset $\mathcal{V}'$ of vertices, for each set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$, there is a shatterable set of size $|\mathcal{Q}_{\mathcal{M},\mathcal{V}'}|$ for the corresponding hypothesis class over $\mathcal{M}$, where thresholds of vertices in $\mathcal{V}'$ are unknown.

Our next lemma shows that, asymptotically, almost all graphs $\mathcal{M}$ with n vertices and k layers have a set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ of size $k\sigma$, where $\mathcal{V}'$ is a subset of vertices and $\sigma = |\mathcal{V}'|$.

Lemma 4.10. Given $n \geq 1$, $k \geq 2$, and $\mathcal{V}' \subseteq [n]$, let $\mathcal{M}$ be a graph chosen uniformly at random from the space of all k-layer graphs with n vertices. With probability at least $1 - 4 \cdot (\sigma k)^2 \cdot (\frac{3}{4})^n$, $\mathcal{M}$ admits a set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ of size $k\sigma$, where $\sigma = |\mathcal{V}'|$.

Lastly, by Lemmas 4.9 and 4.10, we conclude that for any $k \geq 2$, asymptotically in n, almost all the hypothesis classes of threshold dynamical systems over k-layer graphs have Ndim exactly $k\sigma$.

Theorem 4.11. Given $k \geq 2$, as n approaches infinity, almost all the hypothesis classes of threshold dynamical systems over k-layer graphs have Ndim exactly σk.

Remark. "*Almost all*" is a standard term in the probabilistic method to indicate that the proportion of the graphs that satisfies a certain property *tends to one* as the number of nodes increases (e.g., see [21]). In our case, the proportion $1 - 4 \cdot (\sigma k)^2 \cdot (\frac{3}{4})^n$ approaches 1 quickly due to the exponent of n. In fact, we empirically found that for this proportion to be close to 1, n only needs to be around 1,000 (**See Appendix, Section 6.4**).

5 Experimental Analysis

We present experimental studies on the relationships between model parameters and the empirical performance of our PAC algorithm. Our goal is to compare theoretical results with empirical findings and explore the performance of the algorithm on different networks [40, 45, 54, 11], shown in Table 1.

Dataset	Type	k	n	m	Avg. deg.
`Aarhus`	Social	5	61	620	20.33
`CKM-Phy`	Social	3	246	1,551	12.61
`Multi-Gnp`	Random	2	500	7,495	15
`PPI`	Biology	7	900	12,870	28.6
`Twitter`	Social	2	2000	10,233	10.23

Table 1: *List of multilayer networks.* Parameters k, n, and m are the number of layers, the number of vertices, and the total number of edges in a network, respectively.

Training and testing. For each network, we construct a target ground-truth system where the threshold of each vertex $v \in \mathcal{V}$ on each layer i is assigned uniformly at random from $[0, \deg_i(v) + 2]$. For each ground-truth MSyDS h^* defined above, a training set $\mathcal{T} = \{(\mathcal{C}_i, h^*(\mathcal{C}_i))\}_{i=1}^q$ is constructed, where each $\mathcal{C}_i$ is sampled from a distribution $\mathcal{D}$. We consider *distributions* where the state of each vertex in $\mathcal{C}_i \in \mathcal{T}$ is 0 w.p. p and 1 w.p. $1 - p$, for a fixed $p \in \{0.1, 0.5, 0.9\}$. In general, a higher p implies a distribution that is more biased towards vertices in state 0. Our PAC algorithm then uses $\mathcal{T}$ to learn a hypothesis $h \in \mathcal{H}$ where all the thresholds are inferred. To evaluate the quality of h, we sample 10,000 configurations from $\mathcal{D}$, and compute the *empirical loss* ℓ, which is the fraction of sampled configurations $\mathcal{C}$'s where $h(\mathcal{C}) \neq h^*(\mathcal{C})$. In presenting the results, each data point is the average over 50 learned hypotheses.

5.1 Experimental Results

Impacts of model parameters. We first examine the relationships between the loss ℓ and the training set size $|\mathcal{T}|$, over three distributions (of samples) specified by different values of p. Experimental results using the `Multi-Gnp` network (Table 1) are presented in Fig 2(a), where *the thresholds of all vertices must be learned* (i.e., $\sigma = n = 500$).

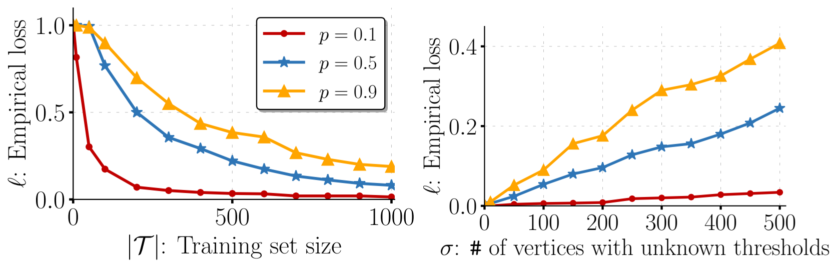

Figure 2: (a): ℓ vs $|\mathcal{T}|$ and (b): ℓ vs σ, over different distributions specified by p. The underlying network is `Multi-Gnp` (Table 1). The stdev for all data points is less than 0.09.

Observations. In Figure 2(a), as $|\mathcal{T}|$ increases, we observe a decrease in the loss ℓ. Such a relationship is expected since a larger sample usually provides more information about the underlying true system. Further, note that for each value of $|\mathcal{T}|$, the loss increases as the distribution of samples becomes more biased towards vertices having state 0. One reason for this behavior is that when states in $\mathcal{C} \sim \mathcal{D}$ consist mostly of 0's, the score of each vertex (on each layer) under $\mathcal{C}$ could be far from its true threshold. Since our algorithm learns thresholds based on these scores, it will require more examples to learn an appropriate hypothesis when there are more 0's in each training sample.

Next, we study the relationship between ℓ and σ, under a fixed training set size $|\mathcal{T}| = 500$ over different distributions. The results for the `Multi-Gnp` network (Table 1) are shown in Fig 2(b). From Fig 2(b), observe that ℓ increases with σ. This is because a larger σ leads to an (exponentially) larger hypothesis space. Since the amount of training data (i.e., $|\mathcal{T}|$) the algorithm receives is fixed, a learned hypothesis would incur a higher loss when σ is larger. Nevertheless, even though $|\mathcal{H}|$ is exponential in σ, the loss ℓ

under our algorithm grows much more slowly.

Impact of the number of layers. We study the effect of the graph structure on ℓ. We first examine the relationship between ℓ and $|\mathcal{T}|$ using the real-world multilayer networks in Table 1. In these experiments, we set $\sigma = n$ (i.e., *the thresholds of all vertices are to be learned*) and choose $\mathcal{D}$ as the uniform distribution. The results are shown in Fig 3(a).

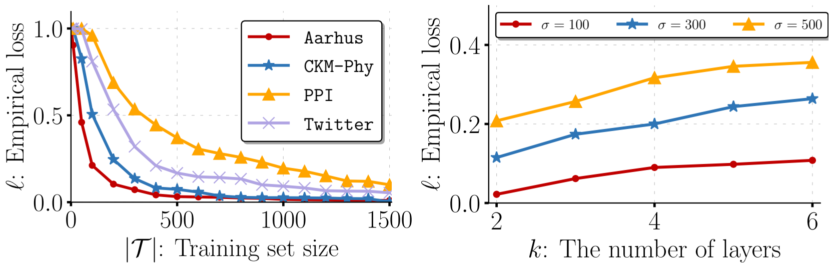

Figure 3: (a): ℓ vs $|\mathcal{T}|$, over different real-world networks (Table 1), and (b): ℓ vs k over different values of σ, where the underlying network is Gnp. The stdev for all data points is less than 0.08.

Observations. From Fig 3(a), we observe a joint effect of σ and k on the loss ℓ. In particular, if the network has more vertices (thus a larger $\sigma = n$), the learned hypothesis h usually has a higher loss ℓ, as one would expect. Further, even though the Twitter network has more vertices than the PPI network, the latter network has more layers. Since the size of the hypothesis class is exponential w.r.t k, for the same $|\mathcal{T}|$, observe that the h under the PPI network incurs a higher loss. Next, we study the effect of k on the loss ℓ using multilayer Gnp networks of size 500 and average degree (on each layer) of 10. We increase the number of layers from 2 to 6 while fixing $|\mathcal{T}|$ at 500. The result is shown in Fig 3(b) for three values of σ. Overall, we observe a positive correlation between k and ℓ; this is because a larger k leads to a larger hypothesis space.

6 Future Work

We studied the PAC learnability of *interaction functions* in dynamical systems over multilayer networks. One direction for future work is to improve our lower bound on the sample complexity for PAC learnability. The second direction is to tighten the gap between the lower and upper bounds on the Natarajan dimension for multilayer systems. A third direction is to consider a noisy setting where labels in the training set (i.e., the successor configurations) may be incorrect with a small probability.

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Appendix

6.1 The Settings of Existing Works

Our problem setting follows the line of existing research on learning networked systems. Here, we present the settings of a few illustrative papers on learning networked systems that span multiple authors and domains. These references are also cited in the main paper.

Vertex States	Update Scheme	Time Scale	Interaction Function	Venue
Binary	Synchronous	Discrete	Deterministic	AAAI-2022 [13]
Binary	Synchronous	Discrete	Threshold	ICML-2022 [48]
Binary	Synchronous	Discrete	Threshold	ICML-2021 [9]
Binary	Synchronous	Discrete	Susceptible-Infected	ICML-2021 [15]
Binary	Synchronous	Discrete	Independent Cascade	ICML-2021 [59]
Binary	Synchronous	Continuous	Probablistic	NeurIPS-2020 [27]
Binary	Synchronous	Discrete	Threshold	NeurIPS-2020 [37]
Binary	Synchronous	Discrete	Deterministic	ICML-2020 [12]
Binary	Synchronous	Discrete	Threshold	ICML-2019 [2]
Binary	Synchronous	Discrete	Threshold & Independent Cascade	NeurIPS-2016 [28]
Binary	Synchronous	Discrete	Threshold & Independent Cascade	NeurIPS-2015 [42]

Table 2: The problem settings of a few illustrative papers on learning networked systems.

6.2 Additional Material for Section 3

Duality between OR and AND master functions with respect to learning

The AND and OR master functions can be treated similarly in our context. For the OR master function, the state of a vertex v is 1 if the interaction function in at least one layer outputs a 1. Similarly, for the AND master function, the state of a vertex v is 0 if the interaction function on at least one layer outputs a 0. Due to this duality, all our results for OR master functions carry over to AND master functions.

Detailed Proofs in Section 3

Recall that $\tau_i^h(v)$ and $\tau_i^{h^*}(v)$ are the thresholds of v on the ith layer in a learned system (hypothesis) h and in the true system h^*, respectively. Fix a vertex v and layer $i \in [k]$. For a configuration $\mathcal{C} \sim \mathcal{D}$, let $B(\mathcal{C}, v)$ denote the event "the threshold condition for v is **not** satisfied in any of the layers under $\mathcal{C}$ in the true system h^*". For an $h \in \mathcal{H}$ and a configuration $\mathcal{C}$, let $A(\mathcal{C}, i, v, h)$ be the event such that (1) the threshold condition of v on the ith layer is satisfied under $\mathcal{C}$ in h, and (2) the event $B(\mathcal{C}, v)$ occurs. Formally, $A(\mathcal{C}, i, v, h)$ is the event "$\Gamma_i[\mathcal{C}, v] \geq \tau_i^h(v)$ for the given ith layer and $\Gamma_j[\mathcal{C}, v] < \tau_j^{h^*}(v),\ \forall j \in [k]$".

Lemma 3.2. *For a $v \in \mathcal{V}'$ and an $i \in [k]$, suppose $\tau_i^{h^*}(v) \geq 1$. Let $h \in \mathcal{H}$ be a hypothesis learned from a training set $\mathcal{T}$ of size $q \geq 1$. For a given $\alpha \in (0,1)$, and an integer $\rho_i(v) \in [0, \tau_i^{h^*}(v))$:*

(1) *If all $\rho_i(v)$ satisfy:*

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[\underbrace{\Gamma_j[\mathcal{C}, v] < \tau_j^{h^*}(v),\ \forall j \in [k]}_{Event\ B(\mathcal{C},v)} \text{ and } \Gamma_i[\mathcal{C}, v] \geq \rho_i(v)] < \alpha \tag{3}$$

then $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] < \alpha$.

(2), Even if (1) does not hold, that is, there is a $\rho_i(v)$ such that

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[\underbrace{\Gamma_j[\mathcal{C}, v] < \tau_j^{h^*}(v),\ \forall j \in [k]}_{Event\ B(\mathcal{C},v)} \text{ and } \Gamma_i[\mathcal{C}, v] \geq \rho_i(v)] \geq \alpha \tag{4}$$

*then the condition $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] \geq \alpha$ holds with probability **at most** $(1-\alpha)^q$ over $\mathcal{T} \sim \mathcal{D}^q$.*

Proof. We first consider the case where $\Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C}, v) \text{ and } \Gamma_i[\mathcal{C}, v] \geq \rho_i(v)] < \alpha$ for all integer $\rho_i(v) \in [0, \tau_i^{h^*}(v))$. This case implies that

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C}, v) \text{ and } \Gamma_i[\mathcal{C}, v] \geq 0] < \alpha \tag{5}$$

Let h be the learned hypothesis by our algorithm. We now argue that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] < \alpha$. In particular, note that the learned threshold $\tau_i^h(v)$ is always in the range $[0, \tau_i^{h^*}(v)]$. If $\tau_i^h(v) = \tau_i^{h^*}(v)$, the event $A(\mathcal{C}, i, v, h)$ does not occur. On the other hand, if $\tau_i^h(v) < \tau_i^{h^*}(v)$, then the event $\Gamma_i[\mathcal{C}, v] \geq \tau_i^h(v)$ is contained in the event $\Gamma_i[\mathcal{C}, v] \geq 0$; thus,

$$\begin{aligned}
\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] &= \Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C}, v) \text{ and } \Gamma_i[\mathcal{C}, v] \geq \tau_i^h(v)] & (6)\\
&\leq \Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C}, v) \text{ and } \Gamma_i[\mathcal{C}, v] \geq 0] & (7)\\
&< \alpha & (8)
\end{aligned}$$

Now consider the second case as stated in Ineq (4). Let $\rho_i(v)$ be the **maximal** integer in $[0, \tau_i^{h^*}(v))$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C}, v) \text{ and } \Gamma_i[\mathcal{C}, v] \geq \rho_i(v)] \geq \alpha$. We now establish the claim:

Claim 6.0.1. If $\exists\ (\mathcal{C}, \mathcal{C}') \in \mathcal{T}$ s.t. $B(\mathcal{C}, v)$ occurs and $\Gamma_i[\mathcal{C}, v] \geq \rho_i(v)$, then the algorithm learns an $h \in \mathcal{H}$ s.t. $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] < \alpha$.

Suppose such a pair $(\mathcal{C}, \mathcal{C}')$ exists in $\mathcal{T}$. Let h be the hypothesis returned by our algorithm using $\mathcal{T}$. Note that since $\Gamma_j[\mathcal{C}, v] < \tau_j^{h^*}(v),\ \forall j \in [k]$ (i.e., the event $B(\mathcal{C}, v)$), we must have $\mathcal{C}'(v) = 0$. By the definition of the PAC algorithm in the main manuscript, it follows that the learned threshold satisfies:

$$\tau_i^h(v) \geq \rho_i(v) + 1 \tag{9}$$

Recall that $A(\mathcal{C}, i, v, h)$ is the event "$\Gamma_i[\mathcal{C}, v] \geq \tau_i^h(v)$ and event $B(\mathcal{C}, v)$ occurs". If $\rho_i(v) = \tau_i^{h^*}(v) - 1$, then we learned the true threshold (i.e., $\tau_i^h(v) = \tau_i^{h^*}(v)$), and thus the event $A(\mathcal{C}, i, v, h)$ does not occur.

On the other hand, if $\rho_i(v) < \tau_i^{h^*}(v) - 1$, then

$$\begin{aligned} \Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] &= \Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C},v) \text{ and } \Gamma_i[\mathcal{C},v] \geq \tau_i^h(v)] & (10)\\ &\leq \Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C},v) \text{ and } \Gamma_i[\mathcal{C},v] \geq \rho_i(v)+1] & (11)\\ &< \alpha & (12)\end{aligned}$$

where the last inequality follows from the maximality of $\rho_i(v)$. This establishes the Claim. To complete the argument for the second case, let $\eta = \Pr_{\mathcal{C}\sim\mathcal{D}}[B(\mathcal{C},v) \text{ and } \Gamma_i[\mathcal{C},v] \geq \rho_i(v)]$. The probability (over $\mathcal{T}\sim\mathcal{D}^q$) that no such configuration $\mathcal{C}$ exists in $\mathcal{T}$ is $(1-\eta)^q \leq (1-\alpha)^q$, where the inequality follows from Eq (4). Therefore, with probability at most $(1-\alpha)^q$, it holds that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \geq \alpha$ for the learned hypothesis h. This concludes the proof. ∎

Theorem 3.3. *For any $\epsilon,\delta \in (0,1)$, with a training set of size $q = \lceil 1/\epsilon \cdot \sigma k \cdot \log(\sigma k/\delta)\rceil$, the proposed algorithm learns a hypothesis $h \in \mathcal{H}$ such that with probabilty at least $1-\delta$ (over $\mathcal{T}\sim\mathcal{D}^q$),*

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[h(\mathcal{C}) \neq h^*(\mathcal{C})] < \epsilon \tag{13}$$

Proof. For a vertex $v \in \mathcal{V}'$, an $h \in \mathcal{H}$ learned by the proposed algorithm, and a configuration $\mathcal{C}\sim\mathcal{D}$, recall that $h(\mathcal{C})$ denotes the successor of $\mathcal{C}$ under the system (hypothesis) h; $h(\mathcal{C})(v)$ is the state of v in $h(\mathcal{C})$. Let $A(\mathcal{C},v,h)$ be the bad event where $h(\mathcal{C})(v) \neq h^*(\mathcal{C})(v)$, that is, the next state of v predicted by h is wrong. For any layer $i \in [k]$, by the mechanisms of the PAC algorithm in the main manuscript:

$$\tau_i^h(v) = \max_{(\mathcal{C},\mathcal{C}')\in\mathcal{T}:\mathcal{C}'(v)=0}\{\Gamma_i[\mathcal{C},v]\} + 1. \tag{14}$$

We remark that the learned threshold $\tau_i^h(v)$ is *at most* the value of the true threshold $\tau_i^{h^*}(v)$.

We first establish the claim:

Claim 6.0.2. The event $A(\mathcal{C},v,h)$ occurs if and only if $h(\mathcal{C})(v) = 1$ and $h^*(\mathcal{C})(v) = 0$.

The necessity is trivially true. To prove sufficiency, we show that the case where $h(\mathcal{C})(v) = 0$ and $h^*(\mathcal{C})(v) = 1$ never occurs. Note that if $h(\mathcal{C})(v) = 0$, under `OR` master functions, the threshold condition of v is **not** satisfied in any layer under h. That is, $\Gamma_j[\mathcal{C},v] < \tau_j^h(v),\ \forall j \in [k]$. Since $\tau_j^h(v) \leq \tau_j^{h^*}(v), \forall j \in [k]$, it follows that the threshold condition of v is also **not** satisfied in any of the layers under h^*. Therefore, if $h(\mathcal{C})(v) = 0$, then we must have $h^*(\mathcal{C})(v) = 0$. This completes the proof of Claim 6.0.2.

Based on Claim 6.0.2, a useful interpretation of the event $A(C,v,h)$ is that the threshold condition of v is satisfied in **at least one** layer under $\mathcal{C}$ in h, but in the true system h^*, the threshold condition of v is **not** satisfied in any of the layers.

To arrive at the result in Ineq (13), we first bound the probability (over $\mathcal{T}\sim\mathcal{D}^q$) of learning a bad h where $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \geq \epsilon/(\sigma k)$. For a $\mathcal{C}\sim\mathcal{D}$, and a layer $i \in [k]$, recall that $A(\mathcal{C},i,v,h)$ is the event "$\Gamma_i[\mathcal{C},v] \geq \tau_i^h(v)$ and $\Gamma_j[\mathcal{C},v] < \tau_j^{h^*}(v),\ \forall j \in [k]$". Note that the event $A(\mathcal{C},v,h)$ occurs if and only if $A(\mathcal{C},i,v,h)$ occurs for at least one layer $i \in [k]$.

For any layer $i \in [k]$, if the true threshold $\tau_i^{h^*}(v) = 0$, the event $A(\mathcal{C},i,v,h)$ will never happen as the algorithm always learns the correct threshold, i.e., $\tau_i^h(v) = \tau_i^{h^*}(v)$. Now suppose $\tau_i^{h^*}(v) \geq 1$. We can apply Lemma 3.2 with $\alpha = \epsilon/(\sigma k)$ and conclude that with probability **at most** $(1-\epsilon/(\sigma k))^q$ over the choices of q examples $\mathcal{T}\sim\mathcal{D}^q$, the learned h is "bad"; that is, $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C},i,v,h)] \geq \epsilon/(\sigma k)$. Overall, when considering all the layers in the network, with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at most $k \cdot (1-\epsilon/(\sigma k))^q$, there exists a layer $i \in [k]$ such that

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] \geq \frac{\epsilon}{\sigma k} \tag{15}$$

Next, we bound the probability (over $\mathcal{T} \sim \mathcal{D}^q$) of learning a hypothesis $h \in \mathcal{H}$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq \epsilon/\sigma$, that is, the probability of h predicting wrong next state of v is at least ϵ/σ. In particular, note that if $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq \epsilon/\sigma$, then there must exist a layer $i \in [k]$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, i, v, h)] \geq \epsilon/(\sigma k)$. By our aforementioned argument for Ineq (15), it follows that with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at most $k \cdot (1-\epsilon/(\sigma k))^q$,

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq \frac{\epsilon}{\sigma} \tag{16}$$

Lastly, we consider the event where $h(\mathcal{C}) \neq h^*(\mathcal{C})$ for a configuration $\mathcal{C} \sim \mathcal{D}$, that is, the successor of $\mathcal{C}$ predicted by the learned hypothesis h is wrong. Note that if $\Pr_{\mathcal{C}\sim\mathcal{D}}[h(\mathcal{C}) \neq h^*(\mathcal{C})] \geq \epsilon$, then there exists a vertex $v \in \mathcal{V}'$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq \epsilon/\sigma$, which happens with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at most $\sigma k \cdot (1-\epsilon/(\sigma k))^q$. Setting $q = \lceil \frac{1}{\epsilon} \cdot \sigma k \cdot \log\left(\frac{\sigma k}{\delta}\right)\rceil$, one can verify that $\sigma k \cdot (1-\epsilon/(\sigma k))^q \leq \delta$. Overall, when $q = \lceil \frac{1}{\epsilon} \cdot \sigma k \cdot \log\left(\frac{\sigma k}{\delta}\right)\rceil$, with probability at least $1-\delta$ over the choices of q examples $\mathcal{T} \sim \mathcal{D}^q$, the learned $h \in \mathcal{H}$ satisfies the condition

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[h(\mathcal{C}) \neq h^*(\mathcal{C})] < \epsilon. \tag{17}$$

This completes the proof. ■

Theorem 3.2. *For any given $\epsilon, \delta, \beta \in (0,1)$, with a training set $\mathcal{T}$ of size $q = \lceil 1/\epsilon \cdot 1/\beta \cdot k \cdot \log(\sigma k/\delta)\rceil$, the proposed algorithm learns an $h \in \mathcal{H}$, such that with probability at least $1-\delta$ over $\mathcal{T} \sim \mathcal{D}^q$, h satisfies that $\Pr_{\mathcal{C}\sim\mathcal{D}}[W(h(\mathcal{C}), h^*(\mathcal{C})) \geq \beta\sigma] \leq \epsilon$.*

Proof. We follow the analysis in Theorem 3.3. Let $h \in \mathcal{H}$ be the hypothesis learned by the algorithm. Recall that $A(\mathcal{C}, v, h)$ is the "bad" event where $h(\mathcal{C})(v) \neq h^*(\mathcal{C})(v)$ for a vertex $v \in \mathcal{V}'$ and $\mathcal{C} \sim \mathcal{D}$. Using Lemma 3.2 where we set $\alpha = (\epsilon\beta)/k$, with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at most $k \cdot (1-(\epsilon\beta)/k)^q$, we have $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq (\epsilon\beta)$ for any vertex $v \in \mathcal{V}'$. Thus, with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at most $\sigma k \cdot (1-(\epsilon\beta)/k)^q$, there exists a vertex $v \in \mathcal{V}'$ such that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] \geq \epsilon\beta$.

Equivalently, with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at least $1-\sigma k \cdot (1-(\epsilon\beta)/k)^q$, it holds that $\Pr_{\mathcal{C}\sim\mathcal{D}}[A(\mathcal{C}, v, h)] < (\epsilon\beta)$ for all $v \in \mathcal{V}'$. Then by the linearity of expectation,

$$\mathbb{E}_{\mathcal{C}\sim\mathcal{D}}[W(h(\mathcal{C}), h^*(\mathcal{C}))] < \epsilon\beta \cdot \sigma \tag{18}$$

Using Markov Inequality, it follows that with probability (over $\mathcal{T} \sim \mathcal{D}^q$) at least $1-\sigma k \cdot (1-(\epsilon\beta)/k)^q$, the learned $h \in \mathcal{H}$ satisfies

$$\Pr_{\mathcal{C}\sim\mathcal{D}}[W(h(\mathcal{C}), h^*(\mathcal{C})) \geq \beta\sigma] \leq \epsilon \tag{19}$$

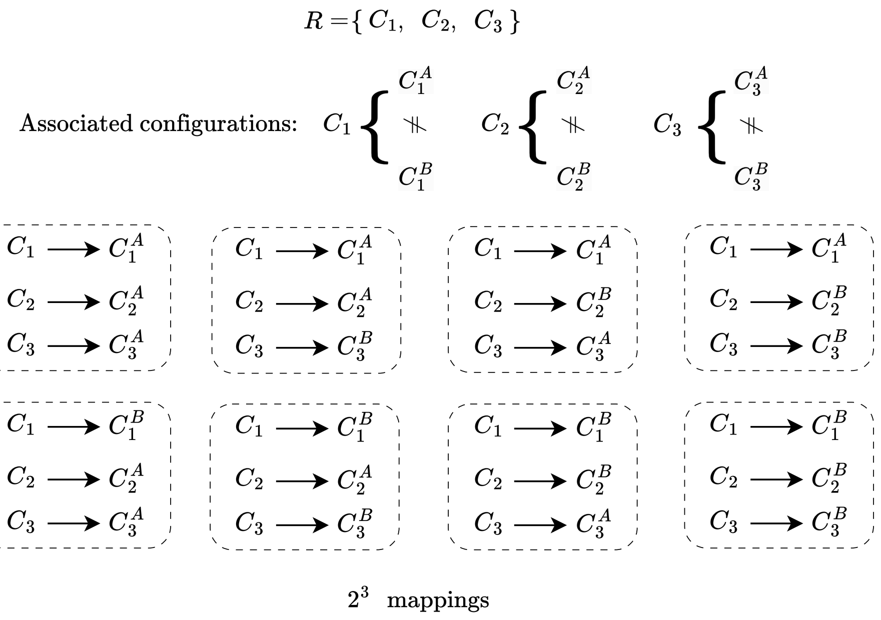
Setting $q = \lceil 1/\epsilon \cdot 1/\beta \cdot k \cdot \log(\sigma k/\delta)\rceil$, we have $1 - \sigma k \cdot (1-(\epsilon\beta)/k)^q \geq 1-\delta$. ■

6.3 Additional Material for Section 4

We first revisit some definitions.

Definition 6.1 (**Shattering**)**.** Given a hypothesis class $\mathcal{H}$, a set $\mathcal{R} \subseteq \mathcal{X}$ is **shattered** by $\mathcal{H}$ if there exist two functions $g_1, g_2 : \mathcal{R} \to \mathcal{X}$ that satisfy both of the following conditions:

- Condition 1: For every $\mathcal{C} \in \mathcal{R}$, $g_1(\mathcal{C}) \neq g_2(\mathcal{C})$.
- Condition 2: For every subset $\mathcal{R}' \subseteq \mathcal{R}$, there exists $h \in \mathcal{H}$ such that $\forall \mathcal{C} \in \mathcal{R}'$, $h(\mathcal{C}) = f(\mathcal{C})$ and $\forall \mathcal{C} \in \mathcal{R} \setminus \mathcal{R}'$, $h(\mathcal{C}) = g(\mathcal{C})$.



$R = \{ C_1, \ C_2, \ C_3 \}$
Associated configurations:
$C_1 \{ C_1^A \nparallel C_1^B$
$C_2 \{ C_2^A \nparallel C_2^B$
$C_3 \{ C_3^A \nparallel C_3^B$
$C_1 \to C_1^A, C_2 \to C_2^A, C_3 \to C_3^A$
$C_1 \to C_1^A, C_2 \to C_2^A, C_3 \to C_3^B$
$C_1 \to C_1^A, C_2 \to C_2^B, C_3 \to C_3^A$
$C_1 \to C_1^A, C_2 \to C_2^B, C_3 \to C_3^B$
$C_1 \to C_1^B, C_2 \to C_2^A, C_3 \to C_3^A$
$C_1 \to C_1^B, C_2 \to C_2^A, C_3 \to C_3^B$
$C_1 \to C_1^B, C_2 \to C_2^B, C_3 \to C_3^A$
$C_1 \to C_1^B, C_2 \to C_2^B, C_3 \to C_3^B$
2^3 mappings

Figure 4: An alternative interpretation of shattering: associated configurations and $2^{|\mathcal{R}|}$ mappings for a set $\mathcal{R}$.

An alternative interpretation of shattering. In our context, equivalent definitions of the two conditions are as follows:

- Condition 1: Each $\mathcal{C} \in \mathcal{R}$ is associated with two configurations, denoted by $\mathcal{C}^A$ and $\mathcal{C}^B$, where $\mathcal{C}^A \neq \mathcal{C}^B$ (i.e., $\mathcal{C}^A = g_1(\mathcal{C})$ and $\mathcal{C}^B = g_2(\mathcal{C})$).
- Condition 2: Consider the $2^{|\mathcal{R}|}$ possible mappings from $\mathcal{R}$ to the associated configurations, such that in each mapping Φ, every $\mathcal{C} \in \mathcal{R}$ is mapped to one of its associated configuration (i.e., $\Phi(\mathcal{C}) = \mathcal{C}^A$ or $\Phi(\mathcal{C}) = \mathcal{C}^B$). For each such mapping Φ, there exists a system (hypothesis) $h_\Phi \in \mathcal{H}$ that produces Φ. That is, $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$ for all $\mathcal{C} \in \mathcal{R}$.

Definition 6.2 (**Contested Vertices**)**.** We call a vertex v **contested** for a $\mathcal{C} \in \mathcal{R}$ if $\mathcal{C}^A(v) \neq \mathcal{C}^B(v)$.

We use the above definition of shattering in all the proofs. An example of condition 1 and the $2^{|\mathcal{R}|}$ mappings of condition 2 for a set $\mathcal{R}$ with three configurations are shown in Fig 4.

Definition 6.3 (**Landmark Vertices**)**.** Suppose the underlying network has a single layer. Given a set $\mathcal{R} \subseteq \mathcal{X}$, a vertex $v \in \mathcal{V}'$ is a ***landmark*** vertex for a configuration $\mathcal{C} \in \mathcal{R}$ if $\Gamma[\mathcal{C}, v] \neq \Gamma[\hat{\mathcal{C}}, v]$ for all $\hat{\mathcal{C}} \in \mathcal{R} \setminus \{\mathcal{C}\}$.

Let $\mathcal{W}(\mathcal{R}) \subseteq \mathcal{V}'$ be the set vertices that are landmarks for at least one configuration in $\mathcal{R}$.

Definition 6.4 (**Canonical Sets**)**.** Suppose the underlying network has a single layer. A set $\mathcal{R} \subseteq \mathcal{X}$ is ***canonical*** w.r.t. $\mathcal{H}$ if there exists an injective mapping from $\mathcal{R}$ to $\mathcal{W}(\mathcal{R})$ s.t. each $\mathcal{C} \in \mathcal{R}$ is mapped to a landmark vertex of $\mathcal{C}$.

Detailed Proofs in Section 4

Lemma 4.4. *When the underlying network has a single-layer, a set $\mathcal{R} \subseteq \mathcal{X}$ can be shattered by $\mathcal{H}$* ***if and only if*** *$\mathcal{R}$ is canonical w.r.t. $\mathcal{H}$*

Proof.

($\Rightarrow$) Suppose $\mathcal{H}$ shatters $\mathcal{R}$. We want to show that $\mathcal{R}$ is canonical. For each configuration $\mathcal{C} \in \mathcal{R}$, let $\mathcal{C}^A$ and $\mathcal{C}^B$ be the two associated configurations, where $\mathcal{C}^A \neq \mathcal{C}^B$ (i.e., they disagree on the state of at least one vertex). Consider the $2^{|\mathcal{R}|}$ possible mappings from $\mathcal{R}$ to the associated configurations, where in each mapping Φ, each $\mathcal{C} \in \mathcal{R}$ is mapped to one of its associated configuration (i.e., $\Phi(\mathcal{C}) = \mathcal{C}^A$ or $\Phi(\mathcal{C}) = \mathcal{C}^B$). The *second condition* of shattering implies that for each of the mapping Φ defined above, there exists a system $h_\Phi \in \mathcal{H}$ such that $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$ for all $\mathcal{C} \in \mathcal{R}$.

Recall that a vertex v **contested** for a configuration $\mathcal{C} \in \mathcal{R}$ if the state of v in $\mathcal{C}^A$ is different from its state in $\mathcal{C}^B$. An example of a contested vertex is given in Fig 5.

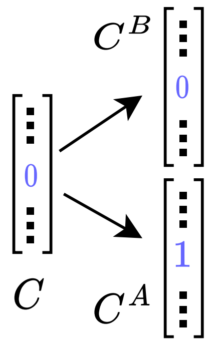


Figure 5: An example of a contested vertex v for a configuration $\mathcal{C}$. In particular, $\mathcal{C}^A$ and $\mathcal{C}^B$ are the two associated configurations of $\mathcal{C}$. The state of v is highlighted in blue.

Since $\mathcal{C}^A \neq \mathcal{C}^B$, each $\mathcal{C} \in \mathcal{R}$ has at least one contested vertex. We argue that contexted vertices can only be in $\mathcal{V}'$.

Claim 6.4.1. If $\mathcal{H}$ shatters $\mathcal{R}$, then contested vertices can only be in the set $\mathcal{V}'$; that is, only vertices with unknown thresholds can be contested.

For purposes of contradiction, suppose there exists a vertex $v \in \mathcal{V} \setminus \mathcal{V}'$ whose threshold is known, and v is contested for a configuration $\mathcal{C} \in \mathcal{R}$. The second condition of shattering implies that there exist two systems $h, h' \in \mathcal{H}$ such that the state of v is 1 in $h(\mathcal{C})$, and is 0 under $h'(\mathcal{C})$. However, since the threshold of v is fixed, for the same configuration $\mathcal{C}$, the state of v is always the same in the successor of $\mathcal{C}$ regardless of the underlying system in $\mathcal{H}$. Therefore, such $h, h' \in \mathcal{H}$ cannot coexist, which contradicts the fact that $\mathcal{H}$ shatters $\mathcal{R}$. This establishes the claim.

Our argument of $\mathcal{R}$ being canonical is developed based on this notion of contested vertices. Overall, we want to show the following two claims: (i) configurations in $\mathcal{R}$ do not share contested vertices, and (ii) a contested vertex for a $\mathcal{C} \in \mathcal{R}$ is also a landmark vertex for $\mathcal{C}$. Then since each $\mathcal{C} \in \mathcal{R}$ has at least one contested vertex, it immediately follows that there exists an injective (i.e., one-to-one) mapping from $\mathcal{R}$ to $\mathcal{W}(\mathcal{R})$ where $\mathcal{W}(\mathcal{R}) \subseteq \mathcal{V}'$ is the set of vertices that are landmarks for at least one configuration in $\mathcal{R}$. Then by definition, $\mathcal{R}$ is canonical.

We now establish the above two claims. Recall that for a configuration $\mathcal{C}$ and a vertex v, $\Gamma[\mathcal{C}, v]$ is the **score** of v in $\mathcal{C}$, that is, the number of 1's in the input provided by $\mathcal{C}$ to the interaction function.

Claim 6.4.2. If $\mathcal{H}$ shatters $\mathcal{R}$, then no two configurations in $\mathcal{R}$ can have any common contested vertices.

For purposes of contradiction, suppose $v \in \mathcal{V}'$ is a contested vertex for at least two configurations in $\mathcal{R}$; let $\mathcal{C}_a$ and $\mathcal{C}_b$ be two such configurations. We now show that $\mathcal{H}$ cannot shatter $\mathcal{R}$. Recall that $h(\mathcal{C}_a)(v)$ is the state of v in the successor $h(\mathcal{C}_a)$ of $\mathcal{C}_a$ under a system $h \in \mathcal{H}$. By the second condition of shattering, there exists a $h \in \mathcal{H}$ such that $h(\mathcal{C}_a)(v) \neq h(\mathcal{C}_b)(v)$ (i.e., $h(\mathcal{C}_a)(v) = 1$ and $h(\mathcal{C}_b)(v) = 0$, or $h(\mathcal{C}_a)(v) = 0$ and $h(\mathcal{C}_b)(v) = 1$).

If $\Gamma[\mathcal{C}_a, v] = \Gamma[\mathcal{C}_b, v]$, then there cannot exist such a system $h \in \mathcal{H}$ where $h(\mathcal{C}_a)(v) \neq h(\mathcal{C}_b)(v)$ since the threshold condition of v cannot be both satisfied and unsatisfied under the same input to the interaction function. This violates the second condition of shattering; thus, $\mathcal{H}$ fails to shatter $\mathcal{R}$ under this case. Now suppose $\Gamma[\mathcal{C}_a, v] < \Gamma[\mathcal{C}_b, v]$. Then there cannot exist an $h \in \mathcal{H}$ such that $h(\mathcal{C}_a)(v) = 1$ but $h(\mathcal{C}_b)(v) = 0$ since if the threshold condition is satisfied under the smaller score (i.e., $\Gamma[\mathcal{C}_a, v]$), it must also be satisfied under the larger score (i.e., $\Gamma[\mathcal{C}_b, v]$). Thus, $\mathcal{H}$ fails to shatter $\mathcal{R}$. The argument for the case where $\Gamma[\mathcal{C}_a, v] > \Gamma[\mathcal{C}_b, v]$ follows analogously. This concludes the Claim 6.4.2.

Claim 6.4.3. If $\mathcal{H}$ shatters $\mathcal{R}$, then a contested vertex for a configuration $\mathcal{C} \in \mathcal{R}$ is also a landmark vertex for $\mathcal{C}$.

We want to show that if $v \in \mathcal{V}'$ is contested for $\mathcal{C} \in \mathcal{R}$, then $\Gamma[\mathcal{C}, v] \neq \Gamma[\hat{\mathcal{C}}, v]$ for all $\hat{\mathcal{C}} \in \mathcal{R} \setminus \{\mathcal{C}\}$. Suppose there exists such a $\hat{\mathcal{C}} \in \mathcal{R}$ where $\Gamma[\mathcal{C}, v] = \Gamma[\hat{\mathcal{C}}, v]$. Claim 6.4.2 implies that v cannot be contested for $\hat{\mathcal{C}}$, that is, the state of v is the same in the two associated configurations of $\hat{\mathcal{C}}$; let s_v denote this state value. Given that v is contested for $\mathcal{C}$, the state of v in one of $\mathcal{C}$'s associated configurations must be different from s_v. Since $\Gamma[\mathcal{C}_a, v] = \Gamma[\mathcal{C}_b, v]$, however, there cannot exist an $h \in \mathcal{H}$ where $h(\mathcal{C}_a)(v) \neq s_v$ because the threshold condition of v cannot be both satisfied and unsatisfied under the same input to the interaction function, contradicting the second condition of shattering. This concludes the proof of Claim 6.4.3.

Overall, we have shown that configurations in $\mathcal{R}$ do not share common contested vertices, and that every contested vertex for a configuration is also a landmark vertex. it follows that there exists an injective mapping where each $\mathcal{C} \in \mathcal{R}$ is mapped to a landmark vertex of $\mathcal{C}$. Then by definition, $\mathcal{R}$ is canonical.

($\Leftarrow$) Suppose that $\mathcal{R} \subseteq \mathcal{X}$ is canonical w.r.t $\mathcal{H}$. To show that $\mathcal{H}$ shatters $\mathcal{R}$, we first discuss how the two associated configurations, $\mathcal{C}^A$ and $\mathcal{C}^B$, of each $\mathcal{C} \in \mathcal{R}$ should be chosen. We then establish that for each of the $2^{|\mathcal{R}|}$ possible mappings from $\mathcal{R}$ to the associated configurations (where $\mathcal{C} \in \mathcal{R}$ is mapped to one of its associated configurations), there exists a system in $\mathcal{H}$ that produces this mapping.

Given that $\mathcal{R}$ is canonical, let $\Upsilon : \mathcal{R} \to \mathcal{W}(\mathcal{R})$ be a corresponding *injective* mapping from $\mathcal{R}$ to the set $\mathcal{W}(\mathcal{R})$ such that each $\mathcal{C} \in \mathcal{R}$ is mapped to a landmark vertex of $\mathcal{C}$. For each $\mathcal{C} \in \mathcal{R}$, we construct two associated configuration $\mathcal{C}^A$ and $\mathcal{C}^B$ by specifying states of each vertex $v \in \mathcal{V}$ as follows:

- **Case 1**: Suppose $v \in \mathcal{V} \setminus \mathcal{V}'$, that is, the threshold of v, denoted by $\tau^{h^*}(v)$, is known. Then the state of v in $\mathcal{C}^A$ and $\mathcal{C}^B$ is the same, which is determined by $\tau^{h^*}(v)$ and $\Gamma[v, \mathcal{C}]$. That is, $\mathcal{C}^A(v) = \mathcal{C}^B(v) = 1$ if $\Gamma[v, \mathcal{C}] \geq \tau^{h^*}(v)$, and $\mathcal{C}^A(v) = \mathcal{C}^B(v) = 0$ otherwise.
- **Case 2**: $v \in \mathcal{V}'$.
  - Subcase 2.1: Suppose $v = \Upsilon(\mathcal{C})$. Then we set $\mathcal{C}^A(v) = 0$ and $\mathcal{C}^B(v) = 1$. That is, v is contested for $\mathcal{C}$.
  - Subcase 2.2: Suppose $v \neq \Upsilon(\mathcal{C})$, and $v = \Upsilon(\hat{\mathcal{C}})$ for some other $\hat{\mathcal{C}} \in \mathcal{R}$. Note that the case where $\Gamma[\mathcal{C}, v] = \Gamma[\hat{\mathcal{C}}, v]$ cannot arise since v is a landmark vertex for $\hat{\mathcal{C}}$. If $\Gamma[\mathcal{C}, v] < \Gamma[\hat{\mathcal{C}}, v]$, then $\mathcal{C}^A(v) = \mathcal{C}^B(v) = 0$. On the other hand, if $\Gamma[\mathcal{C}, v] > \Gamma[\hat{\mathcal{C}}, v]$, then $\mathcal{C}^A(v) = \mathcal{C}^B(v) = 1$.
  - Subcase 2.3: Suppose $v \neq \Upsilon(\mathcal{C})$, and also $v \neq \Upsilon(\hat{\mathcal{C}})$ for any other $\hat{\mathcal{C}} \in \mathcal{R}$, then $\mathcal{C}^A(v) = \mathcal{C}^B(v) = 1$.

This completes the construction of the two associated configurations $\mathcal{C}^A$ and $\mathcal{C}^B$ for each $\mathcal{C} \in \mathcal{R}$. We now show that $\mathcal{H}$ shatters $\mathcal{R}$ under the defined associations.

To begin with, observe that $\mathcal{C}^A \neq \mathcal{C}^B$ for all $\mathcal{C} \in \mathcal{R}$, as the states of $\Upsilon(\mathcal{C})$ are different in $\mathcal{C}^A$ and $\mathcal{C}^B$. Thus, the first condition of shattering is satisfied.

Now consider the $2^{|\mathcal{R}|}$ possible mappings from $\mathcal{R}$ to the associated configurations, where in each mapping Φ, each $\mathcal{C} \in \mathcal{R}$ is mapped to one of its associated configuration (i.e., $\Phi(\mathcal{C}) = \mathcal{C}^A$ or $\Phi(\mathcal{C}) = \mathcal{C}^B$). To prove the second condition of shattering, we want to show that for each Φ defined above, there exists a system $h_\Phi \in \mathcal{H}$ such that $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$ for all $\mathcal{C} \in \mathcal{R}$. Given a mapping Φ, we characterize h_Φ by presenting how the threshold of each vertex is determined:

- **Case 1**: Suppose $v \in \mathcal{V} \setminus \mathcal{V}'$, then its threshold is already known.
- **Case 2**: Suppose $v \in \mathcal{V}'$.
  - Subcase 2.1: If $v \neq \Upsilon(\mathcal{C})$ for any $\mathcal{C} \in \mathcal{R}$, then we set v's threshold to be 0.
  - Subcase 2.2: If $v = \Upsilon(\mathcal{C})$ for a $\mathcal{C} \in \mathcal{R}$. Then set v's threshold to be $\Gamma[\mathcal{C}, v]$ if $\Phi(\mathcal{C})(v) = 1$. On the other hand, $\Phi(\mathcal{C})(v) = 0$, then set v's threshold to be $\Gamma[\mathcal{C}, v] + 1$.

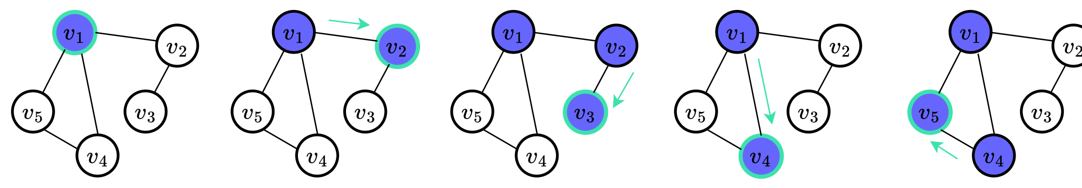
This completes the specification of h_Φ. One can easily verify that $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$ for all $\mathcal{C} \in \mathcal{R}$; that is, the second condition of shattering is satisfied. Overall, we have shown that $\mathcal{H}$ shatters $\mathcal{R}$. This concludes the proof. ■

Theorem 4.5. *When the underlying network has a single layer, a shatterable set of size σ can be constructed. Thus, we have $Ndim(\mathcal{H}) = \sigma$.*

Proof. We show how a canonical set of size σ can be constructed. Then the theorem follows from the equivalence between a canonical set and a shatterable set. In particular, given *any* underlying single-layer network $\mathcal{G}$, we present an algorithm to construct a canonical set $\mathcal{R} \subset \mathcal{X}$ that consists of σ configurations.

Let $\mathcal{G}' = \mathcal{G}[\mathcal{V}']$ be the subgraph induced on $\mathcal{V}'$; $\mathcal{G}'$ could be disconnected. The algorithm involves a depth-first traversal over $\mathcal{G}'$, starting from any initial vertex. During the traversal, when a vertex $v \in \mathcal{V}'$ is visited for the first time, a configuration $\mathcal{C}_v$ is constructed. In particular, our algorithm enforces v to be the landmark vertex to which $\mathcal{C}_v$ is mapped under the injective mapping defined for a canonical set.

We now describe the algorithm. The set $\mathcal{R}$ is initially empty. Starting from any vertex $v_1 \in \mathcal{V}'$, we proceed with a depth-first traversal on $\mathcal{G}'$, while maintaining a stack $\mathcal{K} \subseteq \mathcal{V}'$ of vertices that are currently being visited. Let v_i, $i \in [\sigma]$, denote the ith vertex that is visited for the first time in the traversal. When v_i is visited for the first time, a configuration $\mathcal{C}_{v_i}$ is constructed and added to the set $\mathcal{R}$ where $\mathcal{C}_{v_i}(v) = 1$ if $v \in \mathcal{K}$ and $\mathcal{C}_{v_i}(v) = 0$ otherwise. Note that the states of vertices in $\mathcal{V} \setminus \mathcal{V}'$ are always 0 in $\mathcal{C}_{v_i}$. The algorithm terminates when all vertices in $\mathcal{V}'$ are visited (and thus $\mathcal{K}$ is empty), and returns $\mathcal{R}$. A pictorial example of the algorithm is given in Fig 6.



$$R = \left\{ C_{v_1} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad C_{v_2} = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad C_{v_3} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad C_{v_4} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad C_{v_5} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \right\}$$

Figure 6: A pictorial example of the algorithm running on a graph of 5 vertices. Vertices in the stack $\mathcal{K}$ are highlighted in blue.

Given the resulting set $\mathcal{R}$, Since $\mathcal{G}'$ has σ vertices, $|\mathcal{R}| = \sigma$. We now show that each $v_i \in \mathcal{V}'$ is a landmark vertex of $\mathcal{C}_{v_i} \in \mathcal{R}$, thereby establishing that $\mathcal{R}$ is canonical. For a $v_i \in \mathcal{V}'$, recall that the score v_i in a configuration $\mathcal{C}$, denoted by $\Gamma[\mathcal{C}, v_i]$, is the number of state-1 vertices in v's closed neighborhood in $\mathcal{G}$.

The proof of v_i being a landmark vertex for $\mathcal{C}_{v_i}$ proceeds in two steps. First, consider the subset $\mathcal{R}_1 = \{C_{v_1}, ..., \mathcal{C}_{v_{i-1}}\} \subset \mathcal{R}$ of configurations constructed by the algorithm *before* v_i was visited for the first time. (If $v_i = v_1$, then $\mathcal{R}_1$ is empty.) We argue that the score of v_i in any of the configurations in $\mathcal{R}_1$ is different from the score of v_i in $\mathcal{C}_{v_i}$. That is, $\Gamma[\mathcal{C}, v_i] \neq \Gamma[\mathcal{C}_{v_i}, v_i]$, $\forall \mathcal{C} \in \mathcal{R}_1$. Next, consider the subset $\mathcal{R}_2 = \{C_{v_i+1}, ..., \mathcal{C}_{v_\sigma}\} \subset \mathcal{R}$ of configurations constructed by the algorithm *after* v_i was visited for the first time; if $v_i = v_\sigma$, then $\mathcal{R}_2$ is empty. Similarly, we argue that the scores of v_i in configurations in $\mathcal{R}_2$ are different from the score of v_i in $\mathcal{C}_{v_i}$.

We start with the first claim:

Claim 6.4.4. For each i, $1 \leq i \leq \sigma$, $\Gamma[\mathcal{C}, v_i] \neq \Gamma[\mathcal{C}_{v_i}, v_i]$, $\forall \mathcal{C} \in \mathcal{R}_1$ where $\mathcal{R}_1 = \{C_{v_1}, ..., \mathcal{C}_{v_{i-1}}\} \subset \mathcal{R}$.

The claim is trivially true if $v_i = v_1$ since $\mathcal{R}_1$ is empty. Suppose $i > 1$. Observe that when v_i is visited for the first time, v_i gets added to $\mathcal{K}$, and thus $\Gamma[\mathcal{C}_{v_i}, v_i] = \Gamma[\mathcal{C}_{v_{i-1}}, v_i] + 1$. We now show that before the algorithm visits v_i for the first time, the scores of v_i in the sequence of constructed configurations in $\mathcal{R}_1$ are non-decreasing. Note that when the algorithm traverses connected components that do **not** contain v_i, the score of v_i is always 0 in the resulting configurations. Now focus on the connected component containing v_i. Recall that in a depth-first traversal, a vertex remains on the stack if it has at least one unvisited neighbor. It follows that all of v_i's neighbors who were visited before v_i will remain on the stack $\mathcal{K}$ before v_i is visited. Since only vertices on the stack have state-1 in each configuration, the score of v_i is non-decreasing in $(C_{v_1}, ..., \mathcal{C}_{v_{i-1}})$, that is $\Gamma[\mathcal{C}_{v_1}, v_i] \leq ... \leq \Gamma[\mathcal{C}_{v_{i-1}}, v_i]$. Since $\Gamma[\mathcal{C}_{v_i}, v_i] = \Gamma[\mathcal{C}_{v_{i-1}}, v_i] + 1$, it follows that $\Gamma[\mathcal{C}, v_i] \neq \Gamma[\mathcal{C}_{v_i}, v_i]$, $\forall \mathcal{C} \in \mathcal{R}_1$. This concludes Claim 6.4.4.

Now, we establish the second claim:

Claim 6.4.5. For each i, $1 \leq i \leq \sigma$, $\Gamma[\mathcal{C}, v_i] \neq \Gamma[\mathcal{C}_{v_i}, v_i]$, $\forall \mathcal{C} \in \mathcal{R}_2$ where $\mathcal{R}_2 = \{C_{v_{i+1}}, ..., \mathcal{C}_{v_\sigma}\} \subset \mathcal{R}$.

The claim is trivially true if $v_i = v_\sigma$ since $\mathcal{R}_2$ is then empty. Suppose $i < \sigma$. We show that when a vertex $v_j \in \mathcal{V}'$, $i < j \leq \sigma$, is visited for the first time (and $\mathcal{C}_{v_j} \in \mathcal{R}_2$ is constructed), if v_i is on the stack (i.e., $v_i \in \mathcal{K}$), then $\Gamma[\mathcal{C}_{v_j}, v_i] > \Gamma[\mathcal{C}_{v_i}, v_i]$; if v_i is not on the stack, then $\Gamma[\mathcal{C}_{v_j}, v_i] < \Gamma[\mathcal{C}_{v_i}, v_i]$. Let $\mathcal{N}_{\text{bef}}(v)$ and $\mathcal{N}_{\text{aft}}(v)$ be the set of neighbors that were visited before and after v_i, respectively. Suppose $v_i \in \mathcal{K}$ when v_j is visited. Note that all vertices in $\mathcal{N}_{\text{bef}}(v)$ must also be on the stack $\mathcal{K}$. Further, at least one of v's neighbors in $\mathcal{N}_{\text{aft}}(v)$ must be on the stack. It follows that $\Gamma[\mathcal{C}_{v_j}, v_i] \geq \Gamma[\mathcal{C}_{v_i}, v_i] + 1 > \Gamma[\mathcal{C}_{v_i}, v_i]$. Now suppose $v_i \notin \mathcal{K}$ when v_j is visited. This means that no neighbors in $\mathcal{N}_{\text{aft}}(v)$ are on the stack. It follows that $\Gamma[\mathcal{C}_{v_j}, v_i] \leq \Gamma[\mathcal{C}_{v_i}, v_i] - 1 < \Gamma[\mathcal{C}_{v_i}, v_i]$. Consequently, $\Gamma[\mathcal{C}, v_i] \neq \Gamma[\mathcal{C}_{v_i}, v_i]$, $\forall \mathcal{C} \in \mathcal{R}_2$. This establishes the claim.

With Claims 6.4.4 and 6.4.5, we have shown that for any $\mathcal{C}_{v_i} \in \mathcal{R}$, it holds that

$$\Gamma[\mathcal{C}_{v_i}, v_i] \neq \Gamma[\mathcal{C}, v_i], \ \forall \mathcal{C} \in \mathcal{R}, \mathcal{C} \neq \mathcal{C}_{v_i} \tag{20}$$

That is, v_i is a landmark vertex of $\mathcal{C}_{v_i}$. This immediately implies the existence of an injective mapping where each $\mathcal{C}_{v_i} \in \mathcal{R}$ is mapped to v_i, $i \in [\sigma]$. Then by definition, $\mathcal{R}$ is canonical. Given the equivalence between a canonical set and a shatterable set shown in Lemma 4.4, it follows that $\mathcal{R}$ is also shatterable by $\mathcal{H}$. This concludes the proof. ∎

Lemma 4.6. *Suppose the underlying network has $k \geq 2$ layers. Then the size of any shatterable set is at most $k\sigma$.*

Proof. We first show that for any shatterable set $\mathcal{R}$, each vertex $v \in \mathcal{V}'$ is contested for at most k configurations in $\mathcal{R}$. Recall that a vertex v is **contested** for a configuration $\mathcal{C} \in \mathcal{R}$ if $\mathcal{C}^A(v) \neq \mathcal{C}^B(v)$, where $\mathcal{C}^A$ and $\mathcal{C}^B$ are the two associated configurations of $\mathcal{C}$ defined by shattering (i.e., $\mathcal{C}^A = g_1(\mathcal{C})$ and $\mathcal{C}^B = g_2(\mathcal{C})$). It is easy to see that Claim 6.4.1 in Theorem 4.5 carries over to the multilayer case. That is, contested vertices can only be in the set $\mathcal{V}'$.

For a $v \in \mathcal{V}'$, let $\mathcal{R}_v \subseteq \mathcal{R}$ be the subset of configurations with v being (one of) their contested vertices. W.l.o.g., suppose $\mathcal{R}_v \neq \varnothing$. We establish the claim:

Claim 6.4.6. For each $\mathcal{C} \in \mathcal{R}_v$, $\exists\, i \in [k]$ such that $\Gamma_i(\mathcal{C}, v) > \Gamma_i(\hat{\mathcal{C}}, v)$, $\forall \hat{\mathcal{C}} \in \mathcal{R}_v \setminus \{\mathcal{C}\}$.

For contradiction, suppose there exists a $\mathcal{C} \in \mathcal{R}_v$ such that for all layers $i \in [k]$, $\Gamma_i(\mathcal{C}, v) \leq \Gamma_i(\hat{\mathcal{C}}, v)$ for at least one $\hat{\mathcal{C}} \neq \mathcal{C}$, $\hat{\mathcal{C}} \in \mathcal{R}_v$. We now argue that $\mathcal{H}$ cannot shatter $\mathcal{R}_v$ (and thus, cannot shatter $\mathcal{R}$). In particular, consider a mapping Φ (among the $2^{|\mathcal{R}|}$ possible mappings from $\mathcal{R}$ to the associated configurations) such that $\Phi(\mathcal{C})(v) = 1$, and $\Phi(\hat{\mathcal{C}})(v) = 0$ for all other $\hat{\mathcal{C}} \in \mathcal{R}_v \setminus \{\mathcal{C}\}$. Suppose there exists a $h_\Phi \in \mathcal{H}$ that is consistent with such a mapping Φ, where $h_\Phi(\mathcal{C})(v) = 1$ and $h_\Phi(\hat{\mathcal{C}})(v) = 0$ for all $\hat{\mathcal{C}} \in \mathcal{R}_v \setminus \{\mathcal{C}\}$. Let $\tau_i^{h_\Phi}(v)$ denote the threshold of v in the ith layer under such an h_Φ. Since $h_\Phi(\hat{\mathcal{C}})(v) = 0$ for all $\hat{\mathcal{C}} \neq \mathcal{C}$, we have

$$\tau_i^{h_\Phi}(v) > \max_{\hat{\mathcal{C}} \in \mathcal{R}_v \setminus \{\mathcal{C}\}} \Gamma_i(\hat{\mathcal{C}}, v) \geq \Gamma_i(\mathcal{C}, v), \forall i \in [k] \tag{21}$$

However, the above inequality implies that the threshold condition of v is not satisfied on any of the k layers under $\mathcal{C}$, thereby contradicting the condition $h_\Phi(\mathcal{C})(v) = 1$. Thus, no such $h_\Phi \in \mathcal{H}$ exists, and $\mathcal{H}$ does not shatter $\mathcal{R}_v$. This establishes the claim. Overall, Claim 6.4.6 implies that for each $v \in \mathcal{V}'$, the size of $\mathcal{R}_v$ is at most k. It immediately follows that $|\mathcal{R}| \leq k\sigma$ for any shatterable set $\mathcal{R}$. This concludes the proof. ■

Lemma 4.7. *Suppose h^* is an MSyDS whose underlying network has $k \geq 2$ layers. Let $\hat{h}^*$ be a single-layer system obtained from h^* by using the network in any layer $i \in [k]$. If a set $\mathcal{R}$ is shatterable by the hypothesis class of $\hat{h}^*$, then it is also shatterable by the hypothesis class of h^*.*

Proof. Given the underlying multilayer network $\mathcal{M} = \{\mathcal{G}_i\}_{i=1}^k$ of the true system h^*, let $\hat{h}^*$ be a new system with a single-layer underlying network $\mathcal{G}_i \in \mathcal{M}$, for a layer $i \in [k]$. The vertices' thresholds on $\mathcal{G}_i$ are carried over from h^* to $\hat{h}^*$. For our learning context, the set $\mathcal{V}'$ of vertices with unknown thresholds remains the same between h^* and $\hat{h}^*$. Let $\hat{\mathcal{H}}$ be the corresponding hypothesis class of $\hat{h}^*$,.

Given a set $\mathcal{R}$ that is shatterable by $\hat{\mathcal{H}}$, for each $\mathcal{C} \in \mathcal{R}$, let $\hat{\mathcal{C}}^A$ and $\hat{\mathcal{C}}^B$ be the two associated configurations of $\mathcal{C}$. Further, for each mapping Φ from $\mathcal{R}$ to the associated configurations, let $\hat{h}_\Phi \in \hat{\mathcal{H}}$ be a system that produces Φ, that is, $\hat{h}_\Phi(\mathcal{C}) = \Phi(C)$, for all $\mathcal{C} \in \mathcal{R}$.

We show that $\mathcal{R}$ is also shatterable by $\mathcal{H}$, the hypothesis class of h^*. In particular, for each $\mathcal{C} \in \mathcal{R}$, let $\mathcal{C}^A$ and $\mathcal{C}^B$ be the two associated configurations under the shatterable condition for $\mathcal{H}$; we choose $\mathcal{C}^A = \hat{\mathcal{C}}^A$ and $\mathcal{C}^B = \hat{\mathcal{C}}^B$. Now consider any of the $2^{|\mathcal{R}|}$ mappings from $\mathcal{R}$ to the associated configurations. We argue that for each of such a mapping Φ, there exists a system $h_\Phi \in \mathcal{H}$ where $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$ for all $\mathcal{C} \in \mathcal{R}$. Specifically, in h_Φ, the thresholds of each vertex $v \in \mathcal{V}'$ on each layer $j \in [k]$, denoted by, $\tau_j^{h_\Phi}(v)$, are assigned as follows. For each layer $j \in [k]$, if $j = i$ (i.e., the layer for which $\hat{h}^*$ is defined), then $\tau_j^{h_\Phi}(v)$ equals to the threshold of v in $\hat{h}_\Phi$. Otherwise, we set $\tau_j^{h_\Phi}(v) = deg_j(v) + 2$, where $\deg_j(v)$ is the degree of v in the jth layer. Note that setting $\tau_j^{h_\Phi}(v) = \deg_j(v) + 2$ makes v's interaction function on the jth layer to be the constant-0 function. One can easily verify that $h_\Phi(\mathcal{C}) = \Phi(\mathcal{C})$, for all $\mathcal{C} \in \mathcal{R}$ and thus $\mathcal{R}$ is shatterable by $\mathcal{H}$. This concludes the proof. ■

Lemma 4.9. *Given a multilayer network $\mathcal{M}$ and a subset $\mathcal{V}'$ of vertices, for each set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$, there is a shatterable set of size $|\mathcal{Q}_{\mathcal{M},\mathcal{V}'}|$ for the corresponding hypothesis class over $\mathcal{M}$ where thresholds of vertices in $\mathcal{V}'$ are unknown.*

Proof. Given a k-layer network $\mathcal{M}$ with n vertices, let $\mathcal{V}'$ be any subset of vertices in $\mathcal{M}$. Let $\mathcal{H}$ be the threshold dynamical system over $\mathcal{M}$ where the threshold functions of vertices in $\mathcal{V}'$ are unknown. For a subset $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ of vertex-layer pairs, we present a method to construct a shatterable set $\mathcal{R}$ of size $|\mathcal{Q}_{\mathcal{M},\mathcal{V}'}|$. In particular, for each $(v, i) \in \mathcal{Q}_{\mathcal{M}}$, there is a corresponding configuration $\mathcal{C}_{(v,i)} \in \mathcal{R}$, defined as follows:

$$\begin{cases} \mathcal{C}_{(v,i)}(v') = 1 & \text{If } v' \in N[v,i] \\ \mathcal{C}_{(v,i)}(v') = 0 & \text{Otherwise} \end{cases}$$

where $N[v, i]$ is the closed neighborhood of v on the ith layer in $\mathcal{M}$.

It is easy to see that $|\mathcal{R}| = |\mathcal{Q}_{\mathcal{M},\mathcal{V}'}|$. We now show that the resulting set $\mathcal{R}$ is shatterable by $\mathcal{H}$. Recall that $\Gamma_i[\mathcal{C}, v]$ is the score (i.e., the number of state-1 vertices in v's closed neighborhood) of v in the ith layer under $\mathcal{C}$. We first observe the following:

Observation 6.5. $\Gamma_i[\mathcal{C}_{(v,i)}, v] = deg(v,i) + 1$, for all $(v,i) \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}$.

Observation 6.6. $\Gamma_{i'}[\mathcal{C}_{(v,i)}, v'] < deg(v',i') + 1$, for all $(v,i),(v',i') \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}$, $(v,i) \neq (v',i')$.

The first observation holds by the construction of $\mathcal{C}_{(v,i)}$. To see the second observation, recall that $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ is defined where $N_{\mathcal{M}}[v',i'] \setminus N_{\mathcal{M}}[v,i] \neq \varnothing, \forall (v',i'),(v,i) \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}, (v',i') \neq (v,i)$. This implies that given a $\mathcal{C}_{(v,i)} \in \mathcal{R}$ and a pair $(v',i') \in \mathcal{Q}$, at least one vertex in $N[v',i']$ is in state 0 under $\mathcal{C}_{(v,i)}$. The second observation follows immediately.

The key conclusion from the above two observations is that:

$$\Gamma_i[\mathcal{C}_{(v,i)}, v] > \Gamma_i[\mathcal{C}_{(v,i')}, v], \forall i' \neq i, i' \in [k] \tag{22}$$

This allows us to choose v as the contested vertex for $\mathcal{C}_{(v,i)}$, $i \in [k]$, under the shattering of $\mathcal{R}$. For each $(v,i) \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}$, we now discuss how the two associated configurations of $\mathcal{C}_{(v,i)}$, denoted by $\mathcal{C}^A_{(v,i)}$ and $\mathcal{C}^B_{(v,i)}$, can be chosen to satisfy the shattering conditions. In $\mathcal{C}^A_{(v,i)}$, the state of v is 1, where the states of all other vertices are 0. On the other hand, $\mathcal{C}^B_{(v,i)}$ is the zero vector. It is clear that $\mathcal{C}^A_{(v,i)} \neq \mathcal{C}^B_{(v,i)}$, that is, the first shattering condition is satisfied.

We now show that the second shattering condition also holds. In particular, for each mapping Φ from $\mathcal{R}$ to the associated configurations, by choosing the thresholds of vertices, we prove the existence of a system h_Φ that produces the mapping Φ. For each $\mathcal{C}_{(v,i)} \in \mathcal{R}$, if $\mathcal{C}^A_{(v,i)}(v) = 0$, then the threshold of v in the ith layer is set to $deg(v,i) + 2$ in h_Φ. On the other hand, if $\mathcal{C}^A_{(v,i)}(v) = 1$, then then the threshold of v in the ith layer is set to $deg(v,i) + 1$. By Ineq (22), one can easily verify that $h_\Phi(\mathcal{C}_{(v,i)}) = \Phi(\mathcal{C}_{(v,i)})$, for all $\mathcal{C}_{(v,i)} \in \mathcal{R}$. This concludes the proof. ∎

Lemma 4.10. *Given $n \geq 1$, $k \geq 2$, and $\mathcal{V}' \subseteq [n]$, let $\mathcal{M}$ be a graph chosen uniformly at random from the space of all k-layer graphs with n vertices. With probability at least $1 - 4 \cdot (\sigma k)^2 \cdot (\frac{3}{4})^n$, $\mathcal{M}$ admits a set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ of size $k\sigma$, $\sigma = |\mathcal{V}'|$.*

Proof. Recall that $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ is a set of vertex-layer pairs $(v,i), v \in \mathcal{V}', i \in [k]$, such that every $(v,i) \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ satisfies:

$$N_{\mathcal{M}}[v,i] \setminus N_{\mathcal{M}}[v',i'] \neq \varnothing, \forall (v',i') \in \mathcal{Q}_{\mathcal{M},\mathcal{V}'}, (v',i') \neq (v,i) \tag{23}$$

where $N_{\mathcal{M}}[v,i]$ is the closed neighborhood of v in the ith layer in $\mathcal{M}$.

We use $\mathcal{G}_{n,k,1/2}$ to denote the space of k-layer graphs with n vertices. Let $\mathcal{M}$ be a graph chosen uniformly at random from $\mathcal{G}_{n,k,1/2}$, denoted by $\mathcal{M} \sim \mathcal{G}_{n,k,1/2}$. Equivalently, $\mathcal{M}$ is a random k-layer graph with n vertices where *each edge in each layer is realized with probability* $p = 1/2$. We will use this equivalent definition in the proof.

Fix two vertex-layer pairs, (v,i) and (v',i'), $v' \in \mathcal{V}'$, $i \in [k]$, $(v,i) \neq (v',i')$. Let $A \subseteq \mathcal{V}', \{v,v'\} \subseteq A$, be a subset of vertices that includes v and v'. Let $d = A$. Recall that $N[v,i]$ denotes the closed neighborhood of v on the ith layer in $\mathcal{M}$. Suppose $v \neq v'$. The probability (over $\mathcal{M} \sim \mathcal{G}_{n,k,1/2}$) that

$N[v,i] = A$ and $A \subseteq N[v',i']$ (i.e., condition (23) is violated) is of the form

$$\begin{aligned}
&\Pr_{\mathcal{M}\sim\mathcal{G}_{n,k,1/2}}[N[v,i] = A \text{ and } A \subseteq N[v',i']] \\
&= \underbrace{\frac{1}{2}}_{\text{Edge}(v,v')} \cdot \underbrace{(\frac{1}{2})^{d-2}\cdot(\frac{1}{2})^{n-d}}_{\text{Other neighbors and non-neighbors of } v} \underbrace{\cdot (\frac{1}{2})^{d-2}\cdot\left(\sum_{j=0}^{n-d}\binom{n-d}{j}(\frac{1}{2})^{j}(\frac{1}{2})^{n-d-j}\right)}_{\text{Other neighbors and non-neighbors of } v'} \\
&= (\frac{1}{2})^{n+d-3}
\end{aligned}$$

If $v = v'$, then one can verify that $\Pr_{\mathcal{M}\sim\mathcal{G}_{n,k,1/2}}[N[v,i] = A \text{ and } A \subseteq N[v',i']] = (1/2)^{n+d-2}$.

Extending the argument to any such subset A, we then have

$$\begin{aligned}
&\Pr_{\mathcal{M}\sim\mathcal{G}_{n,k,1/2}}[N[v,i] \subseteq N[v',i']] \le \sum_{d=1}^{n}\binom{n}{d}(\frac{1}{2})^{n+d-2} \\
&< (\frac{1}{2})^{n-2}\cdot(\frac{3}{2})^{n} \\
&= 4\cdot(\frac{3}{4})^{n}
\end{aligned}$$

Combining all pairs, the probability (over $\mathcal{M} \sim \mathcal{G}_{n,k,1/2}$) that there exists a (v,i) and (v',i'), $v \in \mathcal{V}', i \in [k]$ such that $N[v,i] \subseteq N[v',i']$ is at most:

$$8\cdot\binom{\sigma k}{2}\cdot(\frac{3}{4})^{n} \le 4\cdot(\sigma k)^2\cdot(\frac{3}{4})^{n}$$

Lastly, with probability at least $1 - 4\cdot(\sigma k)^2\cdot(\frac{3}{4})^n$, condition (23) holds for all pairs $(v,i), v \in \mathcal{V}'$, $i \in [k]$, that is, there exists a set $\mathcal{Q}_{\mathcal{M},\mathcal{V}'}$ of size $k\sigma$. This concludes the proof. ■

6.4 Additional Experiments

Resources. All experiments were performed on Intel Xeon(R) Linux machines with 64GB of RAM. Our source code (in `C++` and `Python`), documentation, and selected datasets are available in the code appendix.

Additional Results on the Nararajan Dimension

Lemma 4.9 in Section 4.3 can be used to estimate the Natarajan dimension of a given graph in the following manner. Two vertex-layer pairs (v,i) and (v',i') satisfy the *pairwise non-nested neighborhood* (PNN) property if $N[v,i] \nsubseteq N[v',i']$ and $N[v',i'] \nsubseteq N[v,i]$. We recall that the Natarajan dimension is lower bounded by the cardinality of any set of vertex-layer pairs satisfying the PNN property. Therefore, our objective here is to find a large set of such pairs. To this end, we construct a graph over vertex-layer pairs, called the PNN graph. We draw an edge between two pairs if they violate the PNN property, i.e., if one of the closed neighborhoods is a subset of another. We apply a greedy vertex coloring algorithm and then choose the largest subset of vertex-layer pairs assigned the same color. By definition of vertex coloring, the chosen vertex-layer pairs form an independent set in the PNN graph, which in turn implies that any vertex-layer pairs in this set satisfy the PNN property. Hence, the cardinality of this set is a lower bound on the Natarajan dimension.

The results are shown in Figure 7. Recall that the theoretical results show that with very high probability, every vertex-layer pair satisfies the PNN property, and therefore, the Natarajan dimension is $k\sigma$ w.h.p, even for the case where $\sigma = n$ for suitably large n. Our experiments suggest that this holds for even smaller graphs, say of size $n = 1000$. Secondly, our results indicate that the Natarajan dimension is close to $k\sigma$ for a large range of edge densities. In the left panel of Figure 7, we note that only for very small or very large values of edge probabilities, the set size reduces. For the extreme cases where the graph is an independent set or is a complete graph in all layers, it can be easily shown that the Natarajan dimension is σ. We observe the same behavior for increasing k. In the right panel of Figure 7, we plot separately for very small edge probabilities to observe the evolution of the lower bound from n to nk. We note that the standard deviation across replicates is very low as well (< 50).

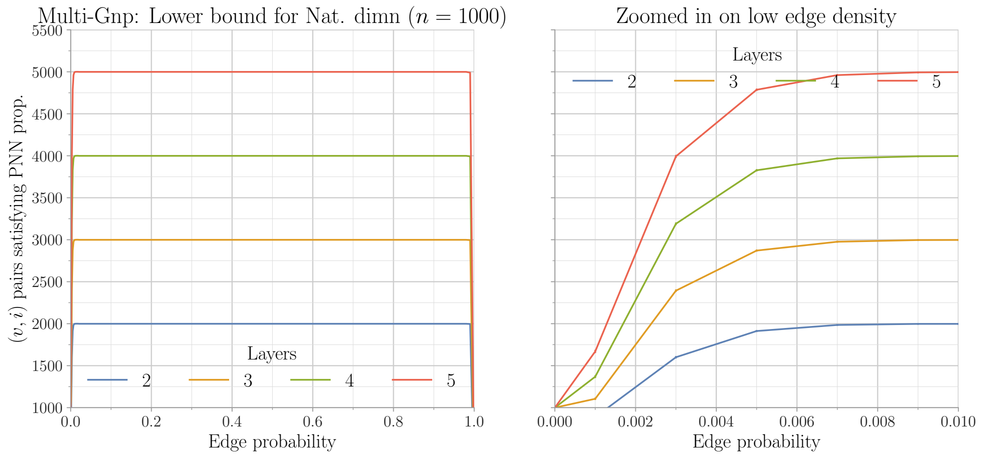


Figure 7: Experimental estimates for Natarajan dimension for Multi-Gnp graphs with varying number of layers k and edge probability. Each graph has 1000 vertices. For each value of k and edge probability, 100 replicates were used. The maximum standard deviation across replicates is less than 50.