IMPLICIT BIAS AND INVARIANCE: HOW HOPFIELD NETWORKS EFFICIENTLY LEARN GRAPH ORBITS

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ABSTRACT

Many learning problems involve symmetries, and while invariance can be built into neural architectures, it can also emerge implicitly when training on group-structured data. We study this phenomenon in classical Hopfield networks and show they can infer the full isomorphism class of a graph from a small random sample. Our results reveal that: (i) graph isomorphism classes can be represented within a three-dimensional invariant subspace, (ii) using gradient descent to minimize energy flow (MEF) has an implicit bias toward norm-efficient solutions, which underpins a polynomial sample complexity bound for learning isomorphism classes, and (iii) across multiple learning rules, parameters converge toward the invariant subspace as sample sizes grow. Together, these findings highlight a unifying mechanism for generalization in Hopfield networks: a bias toward norm efficiency in learning drives the emergence of approximate invariance under group-structured data.

1 INTRODUCTION

Here, we analyze the emergence of invariance arising implicitly during training in Hopfield networks (HNs) (Hopfield, 1982), which represent arguably the simplest example of an Associative Memory. Building on classical ideas Rosenblatt (1958); Willshaw et al. (1969); Amari (1972); Little (1974); Pastur & Figotin (1977), HNs are recurrent neural networks consisting of n linear-threshold McCulloch–Pitts neurons McCulloch & Pitts (1943) that can store binary patterns as distributed memories in the form of fixed-point attractors of its recurrent dynamics. In the literature, HNs are usually associated with a particular Hebbian learning scheme called the "Outer-Product Rule", but for the purposes of this work we also consider other standard training methods. This setting is intentionally minimal so that we can focus on developing novel mathematical tools for understanding generalization in a classical architecture. As data symmetry is not made explicit in this model, any invariance must arise from the interplay of the group structure in the data and the implicit bias of the learning rule in question. More specifically, and inspired by Hillar & Tran (2018); Hillar et al. (2021), this paper studies whether or not standard learning rules and objectives, notably minimization of the energy flow (MEF) Hillar et al. (2012), a tractable convex loss, *can learn the isomorphism class of a graph from a small, random subset*. Our key findings are as follows.

1. **HNs can memorize any graph isomorphism class.** We characterize the subspace of parameters invariant to edge-adjacency–preserving permutations (of which graph isomorphisms are a subset) (Lemma 4.2) and observe that this subspace aligns well with the parameters of successfully trained models (Fig. 3). Moreover, for any graph we give an explicit construction within this space that memorizes it (Lemma 4.3) as well as its isomorphism class.
2. **Implicit bias towards norm efficient solutions.** We reparameterize the MEF objective and show that gradient descent on it is directionally biased towards the solution to a hard-margin support vector machine (HSVM) problem on an induced linear representation (Theorem 3.1).
3. **Polynomial sample complexity suffices for orbit generalization.** Suppose $D \subset \{0,1\}^n$ is strictly memorizable with min-norm parameter $\boldsymbol{\theta}^*$, $\|\boldsymbol{x}\|_0 \leq m$ for all $\boldsymbol{x} \in D$, and let $\mathcal{D}$ be a distribution supported on D. We prove $N = \tilde{\Omega}\big(n\|\boldsymbol{\theta}^*\|^2 m\epsilon^{-2}\big)$ random samples suffices for both HSVM and MEF to memorize new samples with probability at least $1-\epsilon$ (Theorem 3.2). These theoretical results corroborate the empirical "few-shot-to-orbit" phenomenon we observe (Figs. 1, 2). Moreover, specializing to isomorphism classes this result implies a polynomial sample complexity in the number of vertices v, supporting a conjecture in Hillar et al. (2021).

4. **Emergence of invariance.** We observe that as the sample size N grows the learned parameters concentrate near the invariant subspace (Fig. 3). For a simplified average HSVM surrogate, we prove the sample solution converges to the invariant set at rate $\tilde{O}(v^{3/2}/\sqrt{N})$ (Lemma 4.6).

1.1 Related work

Capacity of Hopfield networks. The capacity of a Hopfield network depends on the learning rule and the structure of the data. For dense, uncorrelated random patterns under Hebbian learning, the statistical–mechanics analysis of (Amit et al., 1985) gives the classic linear law: reliable retrieval up to approximately 0.138 patterns per neuron with subsequent refinements via replica methods (Gardner, 1988; Krauth & Mézard, 1989). Coding-theoretic analyses further show that, for Hebbian constructions and exact recovery of randomly chosen patterns, one typically cannot exceed $n/(4 \ln n)$ (McEliece et al., 1987) memories. More generally, Cover's classical bound Cover (1965) restricts the capacity for exact storage of dense, random data to only $2n$. Nonetheless, superlinear capacity is achievable for certain structured datasets. For example, sparse data having few active neurons can yield an increase of capacity to nearly quadratic in n (Tsodyks & Feigel'man, 1988; Amari, 1989). Additionally, robust exponential memory has been observed for particular examples of group structured data (Hillar & Tran, 2018; Hillar et al., 2021); in particular, for storing all k-clique graphs and their hypergraph analogues. Our work builds on the observations of (Hillar & Tran, 2018; Hillar et al., 2021) by proving that all graph isomorphism classes are memorizable.

Modern Hopfield Networks. A line of recent investigation has sought to increase the capacity and retrieval properties of Hopfield networks by changing the energy function. Dense Associative Memories (DAMs) replace the classical quadratic energy with higher-order polynomial interactions, resulting in a capacity that scales polynomially with neuron count (Krotov & Hopfield, 2016; Horn & Usher, 1988). Building on this, Modern Hopfield Networks (MHNs) introduced a log-sum-exp energy function that allows the capacity to grow exponentially (Ramsauer et al., 2020; Demircigil et al., 2017). Our work provides a complementary perspective to these advancements by showing classical HNs can achieve exponential capacity capturing the symmetry of the data in its parameters.

Generalization beyond the training set for HNs. Theoretical study of classical HNs primarily focuses on storage limits, basins of attraction, and noise robustness around memorized patterns, rather than sample–complexity guarantees for generalization to patterns outside the training set. Earlier analyses of concept generalization in classical HNs investigate when networks capture latent data regularities (Fontanari, 1990). More recently, Random-Features Hopfield Models (RFHMs) exhibit learning phase transitions and even retrieval of previously unseen examples (Negri et al., 2023; Kalaj et al., 2024). These results complement but are distinct from our own; in particular, they do not provide sample–complexity bounds or analyze the emergence of invariance induced by a symmetry present in the data. In addition, while these results primarily use techniques from statistical physics, here we leverage tools from statistical learning theory.

Emergent invariance through data augmentation and feature averaging. One perspective on data augmentation is as orbit averaging over a symmetry group; in particular, empirical risk minimization on augmented data is equivalent to averaging features or predictions along group orbits. This has been shown to induce approximate invariance and reduces estimator variance (Chen et al., 2020). From a kernel perspective, augmentation decomposes into first-order invariant feature averaging plus a second-order variance regularizer (Dao et al., 2019). Enforcing invariance through this averaging method yields provable generalization benefits in the context of invariant kernel regression (Elesedy & Zaidi, 2021). Beyond static estimators, recent results show that with full group augmentation deep ensembles become equivariant in expectation at all training times in the infinite-width limit (Gerken & Kessel, 2024) and that the expected predictions of group-convolutional networks match those of data-augmented conventional networks throughout training (Marthaler et al., 2024). While these results assume explicit invariance, either through architectural design or by averaging over the full group orbit, here we ask whether simple learning rules can implicitly recover approximate invariance from small random sample of elements.

Implicit bias. A large body of work shows that, even without explicit regularization, certain learning dynamics have a preference for particular solutions. In particular, for classification using the logistic loss, gradient descent drives the parameter norm to infinity while the parameter direction converges to the max–margin classifier (Soudry et al., 2018; Ji & Telgarsky, 2018; Nacson et al., 2019). Our work

leverages these results in order to show that standard learning rules for HNs are implicitly biased towards learning invariant representations when trained on group data.

2 PRELIMINARIES

Notation: we use capitalized boldface characters to denote matrices, bold lowercase characters to denote vectors and non-bold lowercase characters to denote scalar values. If $\boldsymbol{x} \in \mathbb{R}^n$ is a vector then x_i denotes the ith entry of $\boldsymbol{x}$. If $\boldsymbol{X} \in \mathbb{R}^{N \times n}$ then $\boldsymbol{x}_i \in \mathbb{R}^n$ denotes the ith row of $\boldsymbol{X}$ and to access individual entries of $\boldsymbol{X}$ we use the notation x_{ij} or $[\boldsymbol{X}]_{ij}$, whichever is clearer in context. Whether a matrix, vector or scalar is deterministic or random is also inferred from context. We use Π_a to denote the set of permutations on $[a]$ and $\mathcal{P}_a$ to denote the set of $a \times a$ permutation matrices. Overloading our notation, we also refer to $\mathcal{P}_a$ as the group of permutation matrices. Finally, if $\mathcal{H}$ is a group that acts on a set $\mathcal{A}$, then the orbit of $a \in \mathcal{A}$ under $\mathcal{H}$ is denoted $\text{Orb}(a, \mathcal{H}) = \{ha \in A : h \in \mathcal{H}\}$.

Associative Memory: we consider a Hopfield network Hopfield (1982) with asynchronous dynamics but do not restrict ourselves to Hebbian learning. To this end, let $\text{Sym}_0^n \subset \mathbb{R}^{n \times n}$ denote the set of symmetric, real, $n \times n$ matrices whose diagonal entries are zero, and let $\Theta = \text{Sym}_0^n \times \mathbb{R}^n$. Clearly Θ is a convex vector subspace. We introduce the energy function $E : \{0,1\}^n \times \boldsymbol{\Theta} \to \mathbb{R}$ defined as

$$E(\boldsymbol{x}; \boldsymbol{\theta}) = \frac{1}{2} \boldsymbol{x}^T \boldsymbol{W} \boldsymbol{x} + \boldsymbol{b}^T \boldsymbol{x}, \tag{1}$$

where $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) \in \boldsymbol{\Theta}$. Given an input binary vector $\boldsymbol{x} \in \{0,1\}^n$, the Hopfield network generates a sequence of binary vectors $(\boldsymbol{x}(t))_{t \geq 0}$ through the following recurrent dynamics: with $\boldsymbol{x}(0) = \boldsymbol{x}$ then

$$x_j(t) = \begin{cases} \mathbb{1}(-\boldsymbol{w}_j^T \boldsymbol{x}(t-1) > b_j) & t \equiv j \pmod{n}, \\ x_j(t-1) & \text{otherwise} \end{cases} \tag{2}$$

for all $t \geq 1$ and $j \in [n]$. For any input $\boldsymbol{x} \in \{0,1\}^n$, this sequence converges in finite time to a fixed point Bruck (1990). We define the input-output map of the Hopfield network, denoted $H_\theta : \{0,1\}^n \to \{0,1\}^n$ as follows: given an input $\boldsymbol{x}$, the output $H_\theta(\boldsymbol{x})$ is the attractor or fixed point of 2 reached when initialized with $\boldsymbol{x}(0) = \boldsymbol{x}$. If $H_\theta(\boldsymbol{x}) = \boldsymbol{x}$, then $\boldsymbol{x}$ is a fixed point of the recurrent dynamics, and furthermore, we say that H_θ has *memorized* $\boldsymbol{x}$. A sufficient condition for H_θ to memorize $\boldsymbol{x}$ is $E(\boldsymbol{x}; \boldsymbol{\theta}) < E(\boldsymbol{x}'; \boldsymbol{\theta})$ for all $\boldsymbol{x}' \in \mathcal{N}(\boldsymbol{x})$, where here $\mathcal{N}(\boldsymbol{x})$ denotes the set of all binary vectors a Hamming distance of exactly one from $\boldsymbol{x}$. If $\boldsymbol{\theta}$ satisfies this property, we say that H_θ *strictly memorizes* $\boldsymbol{x}$. We also denote the action of a permutation matrix $\boldsymbol{P} \in \mathcal{P}_n$ on the parameters of a Hopfield network as $\boldsymbol{P}\boldsymbol{\theta} \coloneqq (\boldsymbol{P}^T \boldsymbol{W} \boldsymbol{P}, \boldsymbol{P}^T \boldsymbol{b})$.

Training and memorization: let $\mathcal{S} \subset \{0,1\}^n$, we say that H_θ memorizes $\mathcal{S}$ if it memorizes all $\boldsymbol{x} \in \mathcal{S}$. There are many methods Hertz et al. (1991) that have been proposed to *train* networks to memorize a set $\mathcal{S}$, including Hebbian learning Hebb (1949); Hopfield (1982), the projection rule Personnaz et al. (1985; 1986), Delta learning Widrow & Hoff (1960), and Storkey's learning rule Storkey (1999), among several others Tolmachev & Manton (2020). In this work, we focus on minimization of the energy flow (MEF) Hillar et al. (2012); Hillar & Tran (2018); Hillar et al. (2021) and study its implicit bias. If $\boldsymbol{x} \in \{0,1\}^n$ and $j \in [n]$, let $\boldsymbol{x}^{(j)} \in \{0,1\}^n$ satisfy $x_l \neq x_l^{(j)}$ iff $l = j$. We define the energy flow loss as

$$L(\boldsymbol{\theta}; \mathcal{S}) = \sum_{\boldsymbol{x} \in \mathcal{S}} \sum_{j=1}^{n} \exp\left(E(\boldsymbol{x}; \boldsymbol{\theta}) - E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) \right). \tag{3}$$

For any given set of points $\mathcal{S}$, note that L is nonnegative, infinitely differentiable, and is convex in Θ. As a result, minimizing L is a convex problem to which a wide variety of numerical techniques can be applied, including but not limited to variants of gradient descent (GD) as well as (approximate) second order methods such as L-BFGS Liu & Nocedal (1989). As long as $\mathcal{S}$ can be memorized, then sufficiently minimizing 3 will result in a network which memorizes $\mathcal{S}$. For further details on MEF, we refer the reader to Hillar et al. (2021) and its inspiration from the theory of density estimation Sohl-Dickstein et al. (2011).

3 IMPLICIT BIAS, MINIMUM NORM MEMORIZERS AND GENERALIZATION

In this section, and prior to specializing to the study datasets drawn from isomorphism classes of graphs, we connect memorization to solving a linear program and identify the implicit bias of MEF. This enables us to provide generalization guarantees for memorization in Hopfield networks as per Theorem 3.2. Given $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) \in \Theta$, for any $j \in [n]$ we define the vector $\boldsymbol{\theta}_j = [\boldsymbol{w}_j, b_j] \in \mathbb{R}^{n+1}$. Overloading our notation, we also use $\boldsymbol{\theta} = [\boldsymbol{\theta}_1, \boldsymbol{\theta}_2 ... \boldsymbol{\theta}_n] \in \mathbb{R}^{n,n+1}$ to refer to the flattened vector of all the network parameters $(\boldsymbol{W}, \boldsymbol{b})$. For any $\boldsymbol{x} \in \{0,1\}^n$ let $\boldsymbol{z}(\boldsymbol{x}) = [\boldsymbol{x}, 1] \in \{0,1\}^{n+1}$ and $y_j(\boldsymbol{x}) = 1 - 2x_j \in \{\pm 1\}$. Using this notation it is well known that the energy difference between a point and one of its neighbors is

$$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) = y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle, \tag{4}$$

see Appendix A.1 for further details. As a consequence, parameters which strictly memorize a set $\mathcal{S} \subseteq \{0,1\}^n$ must satisfy a system of linear inequalities: in particular, there must exists some $\epsilon > 0$, referred to as the functional margin, such that $y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle \geq \epsilon$ for all $\boldsymbol{x} \in \mathcal{S}$ and $j \in [n]$. Clearly the energy function (1) is quadratic in the inputs $\boldsymbol{x}$ but linear in the parameters, $E(\boldsymbol{x}; a\boldsymbol{\theta}) = aE(\boldsymbol{x}, \boldsymbol{\theta})$. Moreover, this implies the energy is positively homogeneous of degree 1 in the parameters and as a result the set of attractors of a Hopfield network is invariant under positive rescaling of the parameters. Without loss of generality, we therefore select a functional margin of one and define the feasible set of parameters up to positive rescaling as

$$\mathcal{F}_\theta(\mathcal{S}) = \{\boldsymbol{\theta} \in \Theta : y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle \geq 1 \ \ \forall \boldsymbol{x} \in \mathcal{S}, \forall j \in [n]\} \tag{5}$$

In addition, the inequality constraints that define $\mathcal{F}(\mathcal{S})$ can be written with respect to a single vector of unique parameters, which we denote $\boldsymbol{\omega}$. Let $p = \frac{n(n-1)}{2}$ and $q = \frac{n(n+1)}{2}$. There exists a $\boldsymbol{V} \in \{0, 1, 1/\sqrt{2}\}^{n(n+1) \times q}$ such that for any $\boldsymbol{\theta} \in \Theta$ there exists a $\boldsymbol{a} \in \mathbb{R}^p$ with $\boldsymbol{\omega} = [\sqrt{2}\boldsymbol{a}, \boldsymbol{b}] \in \mathbb{R}^q$, such that $\boldsymbol{\theta} = \boldsymbol{V}\omega$. In short, $\boldsymbol{V}$ copies the unique elements, i.e., the upper triangular elements of $\boldsymbol{W}$ and the biases $\boldsymbol{b}$, into their appropriate locations in the flattened vector $\boldsymbol{\theta}$. For any $j \in [n]$ let $\boldsymbol{V}_j \in \mathbb{R}^{(n+1) \times q}$ denote the submatrix of rows of $\boldsymbol{V}$ such that $\boldsymbol{\theta}_j = \boldsymbol{V}_j \boldsymbol{\omega}$. For any $\boldsymbol{x} \in \{0,1\}^n$ and $j \in [n]$ let $\boldsymbol{u}_j(\boldsymbol{x}) = y_j(\boldsymbol{x}) \boldsymbol{V}_j^T \boldsymbol{z}(\boldsymbol{x})$. Then each constraints can be re-written as $y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle = \langle \boldsymbol{u}_j(\boldsymbol{x}), \boldsymbol{\omega} \rangle$ and thus we can equivalently define the feasible set as

$$\mathcal{F}_\omega(\mathcal{S}) = \{\boldsymbol{\omega} \in \mathbb{R}^q : \langle \boldsymbol{u}_j(\boldsymbol{x}), \boldsymbol{\omega} \rangle \geq 1 \ \ \forall \boldsymbol{x} \in \mathcal{S}, \forall j \in [n]\} \tag{6}$$

Inspecting (6), clearly memorization of a dataset is equivalent to solving a linear program (LP) and therefore any algorithm which successfully memorizes $\mathcal{S}$ is implicitly solving an LP. Moreover, these algorithms may have an *implicit bias* towards feasible points or solutions which satisfy other conditions or criterion. A popular and well studied example is the feasible point with the smallest norm: identifying this requires solving a quadratic program (QP) or, more specifically, a hard margin support vector machine (HSVM) problem. In particular, note that if $\boldsymbol{\theta} = \boldsymbol{V}\boldsymbol{\omega}$ where $\boldsymbol{\omega} = [\sqrt{2}\boldsymbol{a}, \boldsymbol{b}]$ then $\|\boldsymbol{\theta}\|^2 = \|\boldsymbol{W}\|_F^2 + \|\boldsymbol{b}\|^2 = \|\sqrt{2}\boldsymbol{a}\|^2 + \|\boldsymbol{b}\|^2 = \|\boldsymbol{\omega}\|^2$. As a result, finding the minimum norm feasible point for a set $\mathcal{S} \subset \{0,1\}^n$ is equivalent to solving

$$\text{HSVM}(\mathcal{S}) = \underset{\boldsymbol{\omega} \in \mathbb{R}^q}{\arg\min} \|\boldsymbol{\omega}\|^2 \ \ s.t. \ \ \boldsymbol{\omega} \in \mathcal{F}_\omega(\mathcal{S}). \tag{7}$$

The key takeaway of this section is that minimizing (3) with gradient descent (GD) is implicitly biased in direction towards the solution of (7), i.e., norm-minimization. To this end, first observe that (3) can be re-parameterized as:

$$L(\boldsymbol{\theta}; \mathcal{S}) = \sum_{\boldsymbol{x} \in \mathcal{S}} \sum_{j=1}^{n} \exp\Big(E(\boldsymbol{x}; \boldsymbol{\theta}) - E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta})\Big) = \sum_{\boldsymbol{x} \in \mathcal{S}} \sum_{j=1}^{n} \exp\left(-\langle \boldsymbol{u}_j(\boldsymbol{x}), \boldsymbol{\omega} \rangle\right) =: L(\boldsymbol{\omega}; \mathcal{S}).$$

Consider now updates to the parameters of the Hopfield network using GD: in particular, given initial parameters $\boldsymbol{\omega}^{(0)}$ and step-size $\eta > 0$, for all $t \geq 0$ let

$$\boldsymbol{\omega}(t+1) = \boldsymbol{\omega}(t) + \eta \sum_{i=1}^{N} \sum_{j=1}^{n} \exp\left(-\boldsymbol{u}_j(\boldsymbol{x}_i)^T \boldsymbol{\omega}\right) \boldsymbol{u}_j(\boldsymbol{x}_i). \tag{8}$$

Applying (Soudry et al., 2018, Thm.3) it can be proved that this sequence of GD iterates converges in direction to the solution of (7).

Theorem 3.1. ***((Soudry et al., 2018, Thm.3) adapted to our setting)*** *Assume $\mathcal{S}$ can be strictly memorized, let $\boldsymbol{\omega}^* = \text{HSVM}(\mathcal{S}_N)$, $\boldsymbol{\omega}(0) \in \mathbb{R}^q$ be arbitrary and $\boldsymbol{\omega}(t)$ be generated for all $t \in \mathbb{N}_{\geq 1}$ as per* (8)*. There exists a choice of step size η such that $\boldsymbol{\omega}(t) = \boldsymbol{\omega}^* \log(t) + \rho(t)$ for all $t \in \mathbb{N}_{\geq 1}$, where $\rho(t)$ grows as $\|\rho(t)\| = O(\log(\log(t)))$. Moreover, $\lim_{t\to\infty} \frac{\boldsymbol{\omega}(t)}{\|\boldsymbol{\omega}(t)\|} = \frac{\boldsymbol{\omega}^*}{\|\boldsymbol{\omega}^*\|}$.*

Informally, Theorem 3.1 states that the solution returned by minimizing the energy flow with gradient descent (MEF-GD) after exponentially many iterations is a close approximation directionally to the solution returned by solving the HSVM problem (7). We now derive generalization bounds both for the HSVM solution and MEF with GD.

Theorem 3.2. *Let $D \subset \{0,1\}^n$ be a set which can be strictly memorized and assume $\|\boldsymbol{x}\|_0 \leq m \in \mathbb{N}_{\geq 1}$ for all $\boldsymbol{x} \in D$. Let $\mathcal{D}$ be a probability distribution on D, and consider a random sample $\mathcal{S}_N = (\boldsymbol{x}_i)_{i\in[N]}$, where $\boldsymbol{x}_i \sim \mathcal{D}$ are mutually i.i.d. Let $\hat{\boldsymbol{\omega}} = \text{HSVM}(\mathcal{S}_N)$, $\boldsymbol{\omega}^* = \text{HSVM}(D)$, $\boldsymbol{\omega}(0) \in \mathbb{R}^q$ be arbitrary and $\boldsymbol{\omega}(t)$ be generated for all $t \in \mathbb{N}_{\geq 1}$ as per* (8)*, $\delta, \epsilon \in (0,1)$ and assume $\boldsymbol{x} \sim \mathcal{D}$ is sampled independent of $\mathcal{S}_N$. If $N \gtrsim \epsilon^{-2} n \|\boldsymbol{\omega}^*\|^2 m \log(1/\delta)$ then*

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\hat{\boldsymbol{\omega}}) \neq \boldsymbol{x}) \leq \epsilon \quad \textit{and} \quad \mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}(t)) \neq \boldsymbol{x}) = O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\|}{\log(t)}\right) + \epsilon$$

hold with probability at least $1 - \delta$ over the sample $\mathcal{S}_N$.

To prove Theorem 3.2 we combine a vector contraction inequality (Maurer, 2016, Corollary 1) with Rademacher bounds, see e.g., (Mohri et al., 2018, Theorem 3.3), we refer the reader to Appendix B.1 for a full proof. It is worth emphasizing that Theorem 3.2 implies any dataset D which can be strictly memorized, can be at least *nearly* strictly memorized using only a polynomial number of samples. In Section 4.3 we take preliminary steps towards relaxing this statement, from memorizing samples drawn from $\mathcal{D}$ with high probability, to memorizing the set D itself with high probability. Finally, we remark that the MEF bound implies gradient descent may require exponentially many iterations to converge directionally to the max-margin solution. We hypothesize that this is a tail phenomenon: once the weights are approximately aligned, all points are classified with a significant margin and their loss contributions become exponentially small.

4 Storing isomorphism classes of graphs and invariance

4.1 Encoding Simple, Undirected Graphs as Binary Vectors

Let $\mathcal{G}_v$ denote the set of all simple, undirected graphs on $v \in \mathbb{N}$ vertices. Recall two graphs $G = (V, E)$, $G' = (V', E')$ are isomorphic, which we denote $G \cong G'$, if there exists a bijection $\phi : V \to V'$ such that $(\phi(\nu_1), \phi(\nu_2)) \in E'$ if and only if $(\nu_1, \nu_2) \in E$. We refer to such a ϕ as an isomorphism between G and G'. Note when $V = V'$, as is the case here since $V = V' = [v]$, then ϕ is a permutation. The *isomorphism class* of a graph $G \in \mathcal{G}_v$ is defined as $\mathcal{I}(G) \coloneqq \{G' \in \mathcal{G}_v : G' \cong G\}$. Let $\mathcal{V}_2$ denote the set of unordered pairs of $[v]$, $n \coloneqq |\mathcal{V}_2| = \binom{v}{2}$ and $\text{Ind} : \mathcal{V}_2 \to [n]$ be a bijection which indexes the elements of $\mathcal{V}_2$.

Definition 1 (Edge representation of a graph)**.** *Let $\mathcal{E}_{rep} : \mathcal{G}_v \to \{0,1\}^n$ be defined as follows: if $G = ([v], E) \in \mathcal{G}_v$ and $\boldsymbol{x} = \mathcal{E}_{rep}(G)$ then, for all $j \in [n]$, $x_j \coloneqq \mathbb{1}(\text{Ind}^{-1}(j) \in E)$. We refer to $\boldsymbol{x}$ as the edge representation of G.*

To be clear, $\mathcal{E}_{rep}$ is a bijection which assigns each graph to a binary vector of dimension n whose support defines the vertex pairs present in the edge set of the graph in question. Any vertex permutation induces an edge permutation.

Definition 2 (Edge permutation induced by a vertex permutation)**.** *Let $\phi : [v] \to [v]$ be a permutation. The edge permutation $\pi_\phi : [n] \to [n]$ induced by ϕ is defined as follows: if $\text{Ind}^{-1}(j) = (\nu_1, \nu_2)$ then $\pi_\phi(j) = \text{Ind}((\phi(\nu_1), \phi(\nu_2)))$. We denote the subset of these edge permutations as Π_n^Φ and the corresponding subset of permutation matrices as Φ_n.*

We now claim the following: first Φ_n is a subgroup of Π_n, second if two graphs $G, G' \in \mathcal{G}_v$ are isomorphic then there is a vertex induced edge permutation which maps between their edge representations, and third, for any $G \in \mathcal{G}_v$ we have $\mathcal{E}_{rep}(\mathcal{I}(G)) = \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$. For proofs of

these claims we refer the reader to Appendix A.3. Two edges are said to be *adjacent* if they share a vertex in common: more specifically, if $j, l \in [n]$ then j and l are *adjacent*, which we denote $j \sim l$, if and only if $|\text{Ind}^{-1}(j) \cap \text{Ind}^{-1}(l)| = 1$, otherwise we say j and l are not adjacent, which we denote $j \nsim l$. We now identify a subset of edge permutations which are characterized by preserving edge adjacency.

Definition 3 (Edge adjacency preserving permutation)**.** *A permutation $\pi : [n] \to [n]$ preserves edge adjacency if $\pi(j) \sim \pi(l)$ if and only if $j \sim l$. We denote such permutations as $\Pi_n^{\mathcal{Q}}$ and the corresponding set of permutation matrices as $\mathcal{Q}_n$.*

Similar to Φ_n, this subset forms a subgroup of $\mathcal{P}_n$. Moreover Φ_n is a subgroup of $\mathcal{Q}_n$ and as a result $\mathcal{E}_{rep}(\mathcal{I}(G)) \subset \text{Orb}(\mathcal{E}_{rep}(G), \mathcal{Q}_n)$. Again we refer the reader to Appendix A.3 for further details. As a result, the edge representations of the isomorphism class of a graph are a subset of the orbit of the edge representation of the graph in question under edge adjacency preserving permutations.

4.2 Experiments on graph data

To experimentally assess storage across isomorphism classes we study three classes of graphs: namely cliques, bipartite and Paley graphs. Bipartite graphs split the v vertices into two equally sized groups with all possible inter-group edges present and no intra-group edges. Paley graphs connect vertices l and j when $(l - j)$ is a quadratic residue mod v, as per NetworkX Developers; cf. Bollobás (2001). Clique graphs, or more specifically k-cliques, contain a fully connected subset of k vertices while the remaining $v - k$ vertices are isolated. We remark that extensive experiments for cliques are already provided in Hillar & Tran (2018); Hillar et al. (2021), we include them here again for comparison and completeness. We remark that we selected these three classes due to the ease with which we are able to sample from them and emphasize that these families are representative rather than special. Indeed, we observe similar behavior for many other graph isomorphism classes, including random graphs.

Figure 1 shows test accuracy versus training sample size, with mean and min–max over 10 trials, for Hopfield networks trained by MEF, Perceptron, and Delta (the latter two used only as baselines; see Appendix A.2). For small graphs ($v = 8$) we enumerate the full isomorphism class and report the true accuracy, i.e., the fraction of the class memorized. For larger graphs ($v = 20$), accuracy is estimated on an independent random sample of 1000 graphs. We highlight two observations: (i) MEF appears to reach higher test accuracy with fewer samples relative to the other methods, despite all methods perfectly memorizing the training set. This suggests differing implicit biases or implicit bias strengths. (ii) For MEF and Delta, the sample size needed to memorize an isomorphism class is tiny relative to the class size, aligning with the findings in Hillar & Tran (2018); Hillar et al. (2021). Furthermore, the number of iterations was capped at 1000, suggesting that the exponential dependency in Theorem 3.2 is highly pessimistic. Finally, within our hyperparameter range, the Delta rule using Adam failed on the k-clique class, whereas MEF learned all classes and was insensitive to optimizer choice.

Figure 2 estimates and compares the specific polynomial sample complexity of learning k-cliques versus Paley graphs. We do this in order to highlight that different isomorphism classes may be harder or easier to learn depending on their connectivity structure. For each graph size v we record s_{50}, which we define as the smallest training sample size for which MEF attains $\geq 50\%$ average test accuracy on test samples of size 1000 averaged over 10 trials. The left subplot shows s_{50} vs. v. The right subplot shows a log-log fit. Assuming $s_{50} = Cv^p$ for some constant $C \in \mathbb{R}_{>0}$, this allows us to estimate p via linear regression. While Paley graphs need $N = \tilde{\Omega}(v^{2+\epsilon})$, cliques require $N = \tilde{\Omega}(v^{1+\epsilon})$ (note here we use $\epsilon \in (0, 1)$ to denote a small error term). Thus, although Hopfield networks can memorize all classes (Lemma 4.3), the specific sample complexity appears to vary with graph connectivity. We leave a full study of this to future work.

Figure 3 shows weight heatmaps for networks trained on clique data using MEF for sample sizes 10, 50 and 600. It is apparent that as the sample size grows the parameters returned by the optimizer converge onto a distinct subspace: we identify this subspace as the parameters invariant to the underlying group action of the data in Lemma 4.2 below. In particular, weights w_{lj} are approximately the same between all pairs $l \nsim j$ (purple in color) and all pairs for $l \sim j$ (purple in color), and this approximation improves rapidly for larger samples sizes. An extension of Figure 3 is provided in Figure 4, Appendix C.1, and shows heatmaps for both MEF and Delta on clique and Payley graphs.

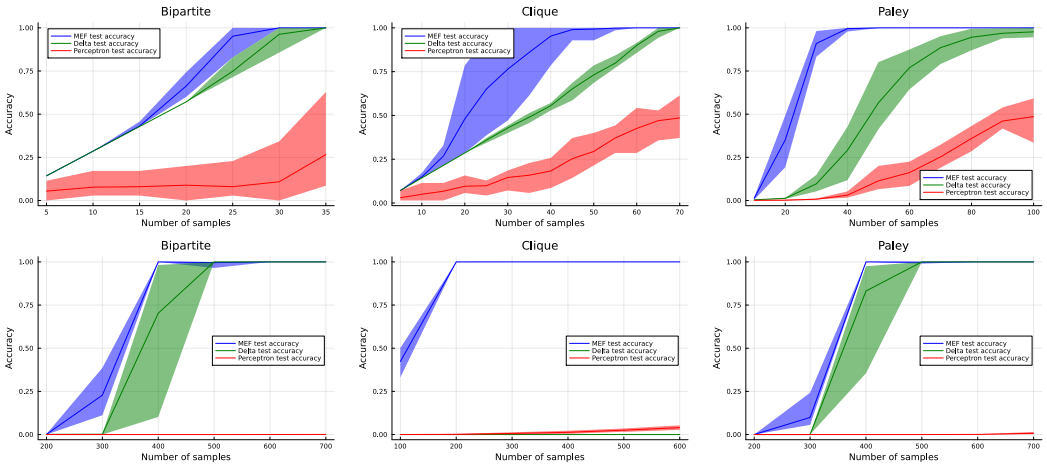

Figure 1: **Test accuracy vs. training sample size for isomorphism classes at two scales.** Top row: $v = 8$ (isomorphism class sizes: bipartite 35, Paley 2520). Bottom row: $v = 20$ (for reference class size for bipartite is 92,378). Curves show mean and min-max over 10 trials. Networks are trained with Perceptron, Delta (MSE), and MEF learning rules.

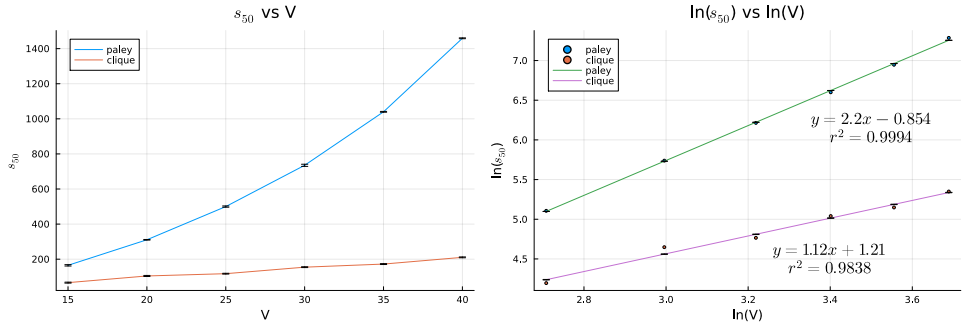

Figure 2: **Sample complexity scaling.** Plots showing the number of samples s_{50} required for a Hopfield network trained via MEF using accelerated gradient descent to memorize 50% of a random sample of 1000 graphs drawn from bipartite and Paley graph isomorphism classes on v vertices. On the right we plot $\ln(s_{50})$ vs $\ln(v)$ and compute the lines of best fit.

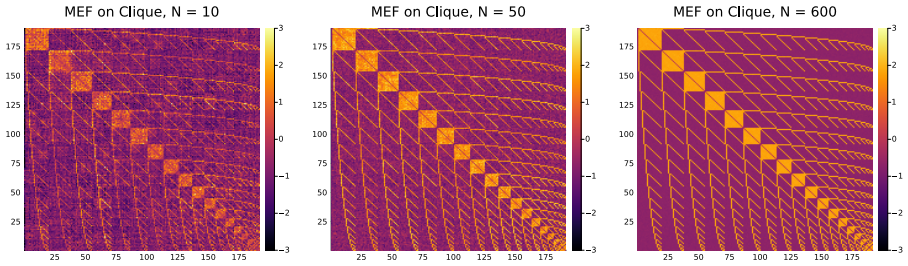

Figure 3: **Weights found by MEF on clique data varying N:** samples from isomorphism class of 10-cliques on $v = 20$ vertices with sample size ranging from 10 to 600.

4.3 Invariant Parameters

In what follows let Γ_n denote an arbitrary subgroup of $\mathcal{P}_n$. For any $\boldsymbol{Q} \in \mathcal{P}_n$ and $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) \in \boldsymbol{\Theta}$ recall that we define the action of $\boldsymbol{Q}$ on the parameter $\boldsymbol{\theta}$ as $\boldsymbol{Q}\boldsymbol{\theta} := (\boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q}, \boldsymbol{Q}^T\boldsymbol{b})$. Let $\boldsymbol{Q} \in \mathcal{P}_n$, $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) \in \Theta$ and $\boldsymbol{\theta}' = \boldsymbol{Q}\boldsymbol{\theta} = (\boldsymbol{W}', \boldsymbol{b}')$. Note $\boldsymbol{W}'^T = (\boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q})^T = \boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q} = \boldsymbol{W}'$ and for all $j \in [n]$ we have $W'_{jj} = \boldsymbol{e}_{\pi(j)}^T\boldsymbol{W}\boldsymbol{e}_{\pi(j)} = W_{\pi(j)\pi(j)} = 0$. As a result $\boldsymbol{W}' \in \mathrm{Sym}_0^n$, in addition

trivially $\boldsymbol{b}' \in \mathbb{R}^n$ and therefore $\boldsymbol{\theta}' \in \Theta$. As a result, the action of $\mathcal{P}_n$, or any subgroup Γ_n of $\mathcal{P}_n$, on Θ is closed.

Definition 4 (Parameter invariance to the action of a subgroup)**.** *A parameter $\boldsymbol{\theta} \in \Theta$ is invariant with respect to Γ_n iff for all $\boldsymbol{Q} \in \Gamma_n$ then $\boldsymbol{Q}\boldsymbol{\theta} = \boldsymbol{\theta}$. We denote the set of these parameters as $\Psi(\Gamma_n)$.*

Recall $E(\boldsymbol{Q}\boldsymbol{x}; \boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{x}^T(\boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q})\boldsymbol{x} + (\boldsymbol{Q}^T\boldsymbol{b})^T\boldsymbol{x}$, if $\boldsymbol{\theta} \in \Psi(\Gamma_n)$, then for any $\boldsymbol{x} \in \{0,1\}^n$ and $\boldsymbol{Q} \in \Gamma_n$ we have

$$E(\boldsymbol{Q}\boldsymbol{x}; \boldsymbol{\theta}) = E(\boldsymbol{x}; \boldsymbol{Q}\boldsymbol{\theta}) = E(\boldsymbol{x}; \boldsymbol{\theta}). \tag{9}$$

We refer to (9) as the intertwining property of the energy function. Using this property, the following lemma extends energy difference bounds between neighbors from a point to an orbit.

Lemma 4.1. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$ and $\boldsymbol{\theta} \in \Psi(\Gamma_n)$. For $\delta \in \mathbb{R}$, if $E(\boldsymbol{x}_0^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}_0; \boldsymbol{\theta}) \geq 1 - \delta$ for all $j \in [n]$, then for all $\boldsymbol{x} \in \mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ it follows that $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1 - \delta$ for all $j \in [n]$.*

For a proof of this lemma, as well as the other results presented in this section, we refer the reader to Appendix B.2. A key implication of Lemma 4.1 is if $\boldsymbol{\theta} \in \Psi(\Gamma_n)$ strictly memorizes $\boldsymbol{x}_0 \in \{0,1\}^n$ then $\boldsymbol{\theta}$ also strictly memorizes $\mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$. We now show that invariance with respect to edge adjacency preserving permutations, of which graph isomorphisms are a subset, corresponds to a particular rank three subspace of the parameters.

Lemma 4.2. *Let $F : \mathbb{R}^3 \to \boldsymbol{\Theta}$ denote the linear map defined as follows: if $(\boldsymbol{W}, \boldsymbol{b}) = F(\boldsymbol{\beta})$ then for all $i, j \in [n]$ we have $w_{ij} = 0$ if $i = j$, $w_{ij} = \beta_1$ if $i \sim j$, $w_{ij} = \beta_2$ if $i \nsim j$ and $b_j = \beta_3$. Then $\Psi(\mathcal{Q}_n) = F(\mathbb{R}^3)$ where $F(\mathbb{R}^3)$ denotes the image of F.*

By inspection, the parameter patterns observed in Figure 3 for MEF appear to approximately lie on the invariant subspace identified in Lemma 4.2. This suggests, given a sufficiently large training sample, that there is an implicit bias not just towards small norm solutions, but also those that are at least approximately invariant. Following this observation, a natural question to ask is whether or not parameters lying on this subspace can memorize any graph.

Lemma 4.3. *For $m \in [0, n]$, let $\boldsymbol{\beta} = [2, 2, 1 - 2m] \in \mathbb{R}^3$ and $\boldsymbol{\theta} = F(\boldsymbol{\beta})$. Then $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1$ for all $j \in [n]$ and for all $\boldsymbol{x} \in \{0,1\}^n$ satisfying $\|\boldsymbol{x}\|_0 = m$.*

Combining Lemmas 4.3 and 4.1 we conclude that any graph isomorphism class can be strictly memorized by a Hopfield network. We also note that the only statistic used by the construction in Lemma 4.3 is the sparsity of the representation: in fact, this construction memorizes $\boldsymbol{x} \in \{0,1\}^n$ iff $\|\boldsymbol{x}\|_0 = m$. As a result, this is a poor parameter candidate if our goal is to memorize an isomorphism class while avoiding spurious memories. In addition, assuming $m = \Theta(n)$, the norm of this construction grows as $\Theta(n)$. For specific graph isomorphism classes we observe solutions with a far smaller norm exist. As an example we consider k-cliques: for typographical ease we denote the set of binary representations of k-cliques on v vertices as $\mathcal{C}_{v,k}$.

Lemma 4.4. *If $\boldsymbol{\beta} = [-5/k, 14/k^2, 0] \in \mathbb{R}^3$, $\boldsymbol{\theta} = F(\boldsymbol{\beta})$, and $k \geq 5$, then the following hold.*

1. *$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1$ for all $\boldsymbol{x} \in \mathcal{C}_{v,k}$ and $j \in [n]$.*
2. *If $k = cv$ for some constant $c \in (0, 1]$, then there exists a constant $C > 0$ such that $\|\boldsymbol{\theta}\|^2 \leq Cv$.*

Lemma 4.4 shows that a parameter exists which strictly memorizes $\mathcal{C}_{v,k}$ with norm only $O(\sqrt{v})$ rather than $\Theta(v^2)$. The construction in 4.4 also does not memorize all m-sparse binary vectors. For example and fixing some $j \in [n]$, suppose $\boldsymbol{x}$ is such that $\|\boldsymbol{x}\|_0 = m \leq 2(v-2)$ and for all $l \in \mathrm{supp}(\boldsymbol{x})$ we have $l \sim j$. Then $\boldsymbol{u}_j(\boldsymbol{x})^T\boldsymbol{\theta} = -5m/k$ and as a result $\boldsymbol{x}$ is not strictly memorized. We speculate that perhaps a correlation between the size of the norm and the number of spurious memories exists, but we leave a proper investigation to future work.

Before proceeding we pause to reflect on the implications of our results with respect to (Hillar et al., 2021, Conjecture 1). Together, Theorem 3.2, Lemma 4.3 and Lemma 4.4 imply that k-cliques on v vertices can be strictly memorized with high probability as long as $N = \tilde{\Omega}(v^3k^2)$. If $k = \alpha v$, where $\alpha \in (0,1)$ is a constant and we assume αv is an integer, then using Stirling's approximation the critical ratio satisfies $\tilde{O}(v^5)/\binom{v}{\alpha v} = \tilde{O}\left(2^{-vH(\alpha)}v^{5.5}\right)$ where here H denotes the binary entropy

function. Clearly the critical ratio decays to zero at a rate which as $v \to \infty$ is dominated by the exponential term. Our experiments and results thus far suggest that memorization of a graph isomorphism class occurs when the training sample is sufficiently large that the optimizer is forced to return a solution lying close to the invariant set $\Psi(\Phi_n) \subset F(\mathbb{R}^3)$. The following lemma establishes that the HSVM solution on the full isomorphism class, which as $N \to \infty$ is equivalent to the training sample with probability one, must be graph isomorphism invariant.

Lemma 4.5. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$ and Γ_n denote a subgroup of $\mathcal{P}_n$ and assume $\text{Orb}(\boldsymbol{x}_0, \Gamma_n)$ can be strictly memorized. If $\boldsymbol{\theta}^* = \boldsymbol{V}\boldsymbol{\omega}^*$ where $\boldsymbol{\omega}^* = \text{HSVM}_\Theta(\text{Orb}(\boldsymbol{x}_0, \Gamma_n))$ then $\boldsymbol{\theta}^* \in \Psi(\Gamma_n)$.*

Following Lemma 4.5, we ask how many samples do we require in order to achieve at least approximate invariance? Deriving a sample complexity result is challenging, primarily due to the fact that the feasible set of the HSVM problem changes non-smoothly with respect to the training sample. Instead and to gain intuition, we conclude this section by analyzing a related but simpler problem, which we refer to as the average hard-margin support vector machine (AHSVM) problem. To this end, we define the following,

$$\mathcal{F}_A(\mathcal{S}) = \{\boldsymbol{\omega} \in \mathbb{R}^q : \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{x}\in\mathcal{S}} \langle \bar{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\omega}\rangle \geq 1\}, \quad \text{AHSVM}(\mathcal{S}) = \underset{\boldsymbol{\omega}\in\mathbb{R}^q}{\arg\min} \frac{1}{2}\|\boldsymbol{\omega}\|^2 \; s.t. \; \boldsymbol{\omega} \in \mathcal{F}_A(\mathcal{S}).$$

The following lemma bounds the difference between the sample AHSVM solution and the population AHSVM solution in the the context of a uniform distribution over an arbitrary $\mathcal{O} \subseteq \{0,1\}^n$.

Lemma 4.6. *Let $\mathcal{O} \subseteq \{0,1\}^n$ satisfy $\|\boldsymbol{x}\|_0 \leq m \in \mathbb{N}_{\geq 2}$ and assume $\boldsymbol{\omega}^* = \text{HSVM}(\mathcal{O})$ is feasible. Consider a random sample $\mathcal{S} = (\boldsymbol{x}_i)_{i=1}^N$ where $\boldsymbol{x}_i \sim U(\mathcal{O})$ are mutually i.i.d. and define $\boldsymbol{\omega}_\mathcal{O} = \text{AHSVM}(\mathcal{O})$ and $\boldsymbol{\omega}_\mathcal{S} = \text{AHSVM}(\mathcal{S})$. For $\delta \in (0,1]$ and $\epsilon \in \mathbb{R}_{>0}$, if $N \gtrsim \epsilon^{-2}\|\boldsymbol{\omega}^*\|^2 m \log(1/\delta)$ then $\|\boldsymbol{\omega}_\mathcal{S} - \boldsymbol{\omega}_\mathcal{O}\| \leq \epsilon$ with probability at least $1-\delta$.*

Now let $\text{Proj}^\perp_{\Psi(\Phi_n)}(\boldsymbol{\theta})$ denote the projection onto the subspace orthogonal to $\Psi(\Phi_n)$. Together, Lemmas 4.4, 4.6 and B.6 characterize proximity of the AHSVM solution for a k-clique sample to the invariant subspace.

Corollary 4.0.1. *Assume $k = cv \geq 3$ for some constant $c \in (0,1)$ and let $\mathcal{S}_N = (\boldsymbol{x}_i)_{i\in[n]}$, where $\boldsymbol{x}_i \sim U(\mathcal{C}_{v,k})$ are mutually i.i.d. Let $\boldsymbol{\omega} = \text{AHSVM}(\mathcal{S}_N)$ and $\boldsymbol{\theta} = \boldsymbol{V}\boldsymbol{\omega}$. For $\delta \in (0,1)$, if $N \gtrsim \epsilon^{-2}v^3\log(1/\delta))$ then $\|\text{Proj}^\perp_{\Psi(\Phi_n)}(\boldsymbol{\omega})\| \leq \epsilon$ with probability at least $1-\delta$.*

Corollary 4.0.1 illustrates that, at least for the AHSVM problem, we can get arbitrarily close to the invariant subspace with high probability using a sample size cubic in the number of vertices. We emphasize that even in the AHSVM setting bounding the distance from the learned parameters to the invariant subspace is challenging. We leave further refinement of these results as well as a derivation of an analogous one for the HSVM problem to future work.

5 Limitations and Future Work

This work has limits: we do not prove convergence of the full HSVM/ MEF solutions to the invariant subspace (although we observe it empirically), and we do not yet explain why some isomorphism classes appear to be easier to learn than others. Future work should quantify spurious fixed points and basin robustness, treat other subgroups and unions of orbits, handle noisy or non-uniform group data, extend the analysis to hypergraphs, and involve continuous and modern HNs. Towards achieving these goals, we highlight preliminary experimental findings around the two themes outlined below. In addition, we highlight preliminary experiments detailed in Appendix C concerning robust generalization, the hidden clique problem and isomorphic graph checking.

Reproducibility Statement: To ensure reproducibility, we make the code public `https://github.com/hopnetorbit/HopfieldNetworksIsomorphism`.

Ethics Statement: This work uses only synthetic, non-sensitive data, involves no human or animal subjects, carries minimal dual-use or environmental risks (modest compute), and we release reproducible code while noting limitations.

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APPENDIX A BACKGROUND

A.1 ENERGY GAP FOR BINARY VECTORS A HAMMING DISTANCE ONE APART

As discussed in Section 2, memorization is equivalent of a point is equivalent to ensuring an energy gap between it and its neighbors. Recall we define $\boldsymbol{x}^{(j)} \in \{0,1\}^n$ as the vector that differs from $\boldsymbol{x} \in \{0,1\}^n$ only at the jth location, and $\boldsymbol{z}(\boldsymbol{x}) = [\boldsymbol{x}, 1] \in \mathbb{R}^{n+1}$.

Lemma A.1. $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) = y_j(\boldsymbol{x})\langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle$.

Proof. By definition $x_l^{(j)} \neq x_l$ iff $l = j$. In addition, $x_j^{(j)} - x_j = 1 - 2x_j$ and, if $r \neq l$, then $x_l x_r \neq x_l^{(j)} x_r^{(j)}$ iff either $l = j$ and $r \neq j$, or $l \neq j$ and $r = j$. Furthermore, recall $\boldsymbol{W}$ is symmetric and $W_{jj} = 0$ for all $j \in [n]$. As a result,

$$
\begin{aligned}
E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) &= \frac{1}{2} \sum_{l,r \in [n]} W_{rl}(x_r^{(j)} x_l^{(j)} - x_r x_l) + \sum_{l=1}^{n} b_l (x_l^{(j)} - x_l) \\
&= \frac{1}{2} \sum_{r \in [n], r \neq j} W_{rj}(x_r^{(j)} x_j^{(j)} - x_r x_j) + \frac{1}{2} \sum_{l \in [n], l \neq j} W_{jl}(x_j^{(j)} x_l^{(j)} - x_j x_l) + b_j(1 - 2x_j) \\
&= \sum_{l \in [n], l \neq j} W_{jl}(x_j^{(j)} x_l^{(j)} - x_j x_l) + b_j(1 - 2x_j) \\
&= \sum_{l \in [n], l \neq j} W_{jl}(x_j^{(j)} - x_j) x_l + b_j(1 - 2x_j) \\
&= (1 - 2x_j) \left(\sum_{l \in [n]} W_{jl} x_l + b_j \right) \\
&= y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle.
\end{aligned}
$$

as claimed. □

A.2 LEARNING ALGORITHMS FOR HOPFIELD NETWORKS

We briefly describe several classical learning rules Hertz et al. (1991) that can be applied to find parameters in Hopfield networks. These methods typically trade off between biological plausibility and performance. We remark that this list is far from exhaustive; see Tolmachev & Manton (2020) for a recent summary.

- **Outer-Product Rule** (Hebb, 1949; Nakano, 1972; Amari, 1972; Hopfield, 1982). In the attractor neural network case Hopfield (1982), this Hebbian rule constructs weights as the normalized sum of training pattern outer products. This rule is simple, biologically motivated, and local in nature, but it is often observed to suffer from spurious attractors, shallow basins of attraction, and overall limited capacity.
- **Perceptron Rule** (Rosenblatt, 1958). The difference between the desired response – that the network dynamics should fix a training sample – and the actual linear-threshold response of a neuron gives a learning signal to update parameters.
- **Delta** (Hoff & Widrow, 1960; Rescorla, 1972). The delta rule, also called the Mean Squared Error (MSE) or Least Mean Square (LMS) rule, considers a relaxation and follows a gradient to minimize the squared error between the linear output activations of neurons and the training pattern to memorize.
- **Projection Rule** (Personnaz et al., 1985; 1986). The weight matrix is obtained by projecting onto the span of the training data and then zeroing the diagonal entries.
- **Storkey Rule** (Storkey, 1997; Storkey & Valabregue, 1999). A modification of the Hebbian update that reduces interference between patterns by accounting for previously stored ones. This rule achieves higher storage capacity than Hebbian learning and reduces spurious minima.

A.3 Encoding simple, undirected graphs as binary vectors

First we recap some of our notation. Let $\mathcal{G}_v$ denote the the set of all simple, undirected graphs on $v \in \mathbb{N}$ vertices. Recall two graphs $G = (V, E)$, $G' = (V', E')$ are isomorphic, which we denote $G \cong G'$, if there exists a bijection $\phi : V \to V'$ such that $(\phi(\nu_1), \phi(\nu_2)) \in E'$ if and only if $(\nu_1, \nu_2) \in E$. We refer to such a ϕ as an isomorphism between G and G'. Furthermore, ϕ is a permutation when $V = V'$: in our setting we consider $V = V' = [v]$ and therefore we shall discuss only permutations moving forward. The *isomorphism class* of a graph $G \in \mathcal{G}_v$ is defined as $\mathcal{I}(G) \coloneqq \{G' \in \mathcal{G}_v : G' \cong G\}$. An automorphism of a graph $G = (V, E)$ is a permutation $\phi : V \to V$ such that $(\nu_1, \nu_2) \in E$ implies $(\phi(\nu_1), \phi(\nu_2)) \in E$. In short, while an isomorphism preserves the vertex adjacency structure of a graph an automorphism preserves not just the vertex adjacency structure but also the vertex labels. Recall that $\Phi_n \subset \mathcal{P}_n$ refers to the set of edge permutation matrices induced by permutations of the vertices, see Definition 2.

Lemma A.2. *Φ_n is a subgroup of $\mathcal{P}_n$.*

Proof. Clearly this is equivalent to showing that Π_n^Φ is a subgroup of Π_n. It is easy to check that $I \in \Pi_n^\Phi$, $\pi_\phi \in \Pi_n^\Phi$ implies $\pi_\phi^{-1} \in \Pi_n^\Phi$ and $\pi_\phi, \pi_{\phi'} \in \Pi_n^\Phi$ implies $\pi_\phi \circ \pi_{\phi'} \in \Pi_n^\Phi$, therefore Π_n^Φ is a subgroup of Π_n. □

The following lemmas establish a straightforward equivalence between isomorphism classes of graphs and certain orbits of binary vectors. First, Lemma A.3 shows that if two graphs $G, G' \in \mathcal{G}_v$ are isomorphic then there is a vertex induced edge permutation which maps between their edge representations.

Lemma A.3. *Suppose $G = ([v], E), G' = ([v], E') \in \mathcal{G}_v$ and $\boldsymbol{x} = \mathcal{E}_{rep}(G)$, $\boldsymbol{x}' = \mathcal{E}_{rep}(G')$. Then $G \cong G'$ iff there exists a $\boldsymbol{P} \in \Phi_n$ such that $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{x}'$.*

Proof. Assume $G \cong G'$. Then there exists a permutation $\phi : [v] \to [v]$ such that $(\nu_1, \nu_2) \in E$ implies $(\phi(\nu_1), \phi(\nu_2)) \in E'$. Let $\pi_\phi : [n] \to [n]$ be the edge permutation induced by ϕ and $\boldsymbol{P} \in \Phi_n$ the corresponding permutation matrix. By construction $x_j = x'_{\pi_\phi(j)}$ for all $j \in [n]$, equivalently, if $\boldsymbol{P} \in \Phi_n$ is the permutation matrix associated with π_ϕ then $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{x}'$. Now suppose there exists a $\boldsymbol{P} \in \Phi_n$ such that $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{x}'$. Then there exists a vertex permutation $\phi : [v] \to [v]$ which induces an edge permutation $\pi_\phi : [n] \to [n]$ such that $x_j = x'_{\pi_\phi(j)}$. By construction, if $j = \text{Ind}((\nu_1, \nu_2))$ then this implies $\pi_\phi(j) = \text{Ind}((\phi(\nu_1), \phi(\nu_2)))$. Therefore, by the definition of $\mathcal{E}_{rep}$ we have $\phi(\nu_1), \phi(\nu_2)) \in E'$ iff $(\nu_1, \nu_2) \in E$. Therefore ϕ is an isomorphism between G and G' and $G \cong G'$. □

Building on Lemma A.3, the following lemma characterizes the isomorphism class of a graph in terms of the orbit of its edge representation under vertex induced edge permutations.

Lemma A.4. *For any $G \in \mathcal{G}_v$ we have $\mathcal{E}_{rep}(\mathcal{I}(G)) = \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$.*

Proof. Let $\boldsymbol{x} = \mathcal{E}_{rep}(G)$, then

$$\text{Orb}(\mathcal{E}_{rep}(G), \Phi_n) = \{\boldsymbol{P}\boldsymbol{x} : \boldsymbol{P} \in \Phi_n\}.$$

Suppose $\mathcal{E}_{rep}(\mathcal{I}(G)) \not\subset \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$. Then there exists a $G' \in \mathcal{I}(G)$ such that $\boldsymbol{x}' \coloneqq \mathcal{E}_{rep}(G') \notin \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$. Therefore there does not exist a $\boldsymbol{P} \in \Phi_n$ such that $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{x}'$. However, $G \cong G'$ which implies a contradiction by Lemma A.3, therefore $\mathcal{E}_{rep}(\mathcal{I}(G)) \subset \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$. Now suppose $\text{Orb}(\mathcal{E}_{rep}(G), \Phi_n) \not\subset \mathcal{E}_{rep}(\mathcal{I}(G))$, then there exists a $\boldsymbol{x}' \in \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$ such that $G' = \mathcal{E}_{rep}^{-1}(\boldsymbol{x}') \notin \mathcal{I}(G)$. However, as $\boldsymbol{x}' \in \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$ then there exists a $\boldsymbol{P} \in \Phi_n$ such that $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{x}'$, but using Lemma A.3 this implies $G \cong G'$ which is a contradiction. Therefore $\text{Orb}(\mathcal{E}_{rep}(G), \Phi_n) \subset \mathcal{E}_{rep}(\mathcal{I}(G))$. Combining these two observations we conclude that $\mathcal{E}_{rep}(\mathcal{I}(G)) = \text{Orb}(\mathcal{E}_{rep}(G), \Phi_n)$. □

Lemma A.5. *$\boldsymbol{Q}_n$ is a subgroup of $\mathcal{P}_n$.*

Proof. Trivially it suffices to show that $\Pi_n^\mathcal{Q}$ is a subgroup of Π_n. It is easy to check that $I \in \Pi_n^\mathcal{Q}$, $\pi \in \Pi_n^\mathcal{Q}$ implies $\pi^{-1} \in \Pi_n^\mathcal{Q}$ and $\pi, \pi' \in \Pi_n^\mathcal{Q}$ implies $\pi \circ \pi' \in \Pi_n^\mathcal{Q}$. Therefore $\Pi_n^\mathcal{Q}$ is a subgroup of Π_n. □

The following lemma states that the vertex induced edge permutations form a subgroup of the edge adjacency preserving subgroup of permutations. As a result, the edge representations of the isomorphism class of a graph are a subset of the orbit of the edge representation of the graph in question under edge adjacency preserving permutations.

Lemma A.6. *Φ_n is a subgroup of $\mathcal{Q}_n$ and $\mathcal{E}_{rep}(\mathcal{I}(G)) \subset \text{Orb}(\mathcal{E}_{rep}(G), \mathcal{Q}_n)$.*

Proof. Trivially it suffices to show that Π_n^{ϕ} is a subgroup of $\Pi_n^{\mathcal{Q}}$, we proceed to show that any vertex induced permutation is an edge adjacency preserving permutation. Consider two edge indices $i, j \in [n]$ and let $\nu_1, \nu_2, \nu_3, \nu_4 \in [v]$ be distinct. Suppose $i \sim j$, then without loss of generality let $\text{Ind}^{-1}(i) = (\nu_1, \nu_2)$ and $\text{Ind}^{-1}(j) = (\nu_2, \nu_3)$. Then $\text{Ind}^{-1}(\pi_\phi(i)) = (\phi(\nu_1), \phi(\nu_2))$ and $\text{Ind}^{-1}(\pi_\phi(j)) = (\phi(\nu_2), \phi(\nu_3))$, therefore $i \sim j$ implies $\pi_\phi(i) \sim \pi_\phi(j)$. Suppose now $i \nsim j$, if $i = j$ then trivially $\pi_\phi(i) = \pi_\phi(j)$ and therefore $i = j$ implies $\pi_\phi(i) \nsim \pi_\phi(i)$. Otherwise, and again without loss of generality, let $\text{Ind}^{-1}(i) = (\nu_1, \nu_2)$ and $\text{Ind}^{-1}(j) = (\nu_3, \nu_4)$. Then $\text{Ind}^{-1}(\pi_\phi(i)) = (\phi(\nu_1), \phi(\nu_2))$ and $\text{Ind}^{-1}(\pi_\phi(j)) = (\phi(\nu_3), \phi(\nu_4))$, as ϕ is bijection then this implies $\pi_\phi(i) \nsim \pi_\phi(j)$. As a result, $\pi_\phi(i) \sim \pi_\phi(i)$ if and only if $i \sim j$. Finally as Φ_n is a group and it is a subset of $\mathcal{Q}_n$ the it must be a subgroup of $\mathcal{Q}_n$. As a result $\text{Orb}(\mathcal{E}_{rep}(G), \Phi_n) \subset \text{Orb}(\mathcal{E}_{rep}(G), \mathcal{Q}_n)$ □

A.4 Bounded representations

In order to establish the connection between Hopfield networks and SVMs discussed in Section 3, we identified and defined a certain feature map for the inputs to the underlying linear classification problem. Recall there exists a matrix $\boldsymbol{V} \in \{0, 1, 1/\sqrt{2}\}^{n(n+1)\times q}$ such that for any $\boldsymbol{\theta} \in \Theta$ there exists a $\boldsymbol{a} \in \mathbb{R}^p$, $\boldsymbol{\omega} = [\sqrt{2}\boldsymbol{a}, \boldsymbol{b}]$ such that $\boldsymbol{\theta} = \boldsymbol{V}\boldsymbol{\omega}$. Recall also that we define $\boldsymbol{V}_j \in \{0, 1, 1/\sqrt{2}\}^n$ as the matrix which satisfies $\boldsymbol{\theta}_j = \boldsymbol{V}_j\boldsymbol{\omega}$, where $\boldsymbol{\theta}_j = [\boldsymbol{w}_j, b_j] \in \mathbb{R}^{n+1}$. In addition, for any $\boldsymbol{x} \in \{0, 1\}$ then we let $\boldsymbol{z}(\boldsymbol{x}) = [\boldsymbol{x}, 1] \in \mathbb{R}^{n+1}$, $\boldsymbol{u}_j(\boldsymbol{x}) = \boldsymbol{V}_j^T\boldsymbol{z}(\boldsymbol{x})$ for all $j \in [n]$ and $\bar{\boldsymbol{u}}(\boldsymbol{x}) = \frac{1}{n}\sum_{j=1}^n \boldsymbol{u}_j(\boldsymbol{x})$. The following lemma bounds the norm of these representations.

Lemma A.7. *For any $\boldsymbol{x} \in \{0, 1\}^n$ then*

$$\|\bar{\boldsymbol{u}}(\boldsymbol{x})\|^2 \leq \|\boldsymbol{u}_j(\boldsymbol{x})\|^2 = \frac{1}{2}\left(\|\boldsymbol{x}\|_0 - x_j\right) + 1$$

for all $j \in [n]$.

Proof. Let $\delta_n(j) \in \{0, 1\}^n$ denote the one hot vector such that $\text{supp}(\delta_n(j)) = j$. In addition, let $\phi_j : [q] \to [n]$ denote the injective mapping between the indices of $\boldsymbol{a}$ and their respective positions in $\boldsymbol{w}_j$, and let $\boldsymbol{B}_j \in \{0, 1\}^{n\times p}$ be the associated matrix which copies the elements of $\boldsymbol{a}$ into their positions in $\boldsymbol{\theta}_j$. Therefore, we can write

$$\boldsymbol{\theta}_j = \begin{bmatrix} \boldsymbol{w}_j \\ b_j \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}}\boldsymbol{B}_j & \boldsymbol{0}_{n\times n} \\ \boldsymbol{0}_{1\times n} & \delta_n(j)^T \end{bmatrix} \begin{bmatrix} \sqrt{2}\boldsymbol{a} \\ \boldsymbol{b} \end{bmatrix} = \boldsymbol{V}_j\boldsymbol{\omega}.$$

By definition

$$\boldsymbol{u}_j(\boldsymbol{x}) = \boldsymbol{V}_j^T\boldsymbol{z}(\boldsymbol{x}) = \begin{bmatrix} \frac{1}{\sqrt{2}}\boldsymbol{B}_j^T & \boldsymbol{0}_{n\times 1} \\ \boldsymbol{0}_{n\times n} & \delta_n(j) \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}}\boldsymbol{B}_j^T\boldsymbol{x} \\ \delta_n(j) \end{bmatrix},$$

therefore

$$\|\boldsymbol{u}_j(\boldsymbol{x})\|^2 = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{B}_j\boldsymbol{B}_j^T\boldsymbol{x} + 1.$$

Recall $W_{jj} = 0$ and each other element of $\boldsymbol{w}_j$ corresponds to exactly one element of $\boldsymbol{a}$, therefore $\boldsymbol{B}_j$ has one nonzero per row other than the jth row, which we let be zero. Moreover, by the injectivity of ϕ_j then $\boldsymbol{B}_j$ has at most one nonzero per column. As a result,

$$\boldsymbol{B}_j\boldsymbol{B}_j^T = \mathbf{I}_n - \boldsymbol{e}_j\boldsymbol{e}_j^T.$$

This implies

$$\boldsymbol{x}^T\boldsymbol{B}_j\boldsymbol{B}_j^T\boldsymbol{x} = \boldsymbol{x}^T\left(\mathbf{I}_n - \boldsymbol{e}_j\boldsymbol{e}_j^T\right)\boldsymbol{x} = \|\boldsymbol{x}\|_0 - x_j$$

for all $j \in [n]$. As

$$\|\bar{\boldsymbol{u}}(\boldsymbol{x})\| = \|\frac{1}{n}\sum_{j=1}^{n}\boldsymbol{u}_j(\boldsymbol{x})\| \leq \frac{1}{n}\sum_{j=1}^{n}\|\boldsymbol{u}_j(\boldsymbol{x})\| \leq \|\boldsymbol{u}_j(\boldsymbol{x}),\|$$

then

$$\|\bar{\boldsymbol{u}}(\boldsymbol{x})\|^2 \leq \|\boldsymbol{u}_j(\boldsymbol{x})\|^2 = \frac{1}{2}\left(\|\boldsymbol{x}\|_0 - x_j\right) + 1$$

for all $j \in [n]$ as claimed. □

A.5 Euclidean distance bounds between normalized vectors

Here we recall some basic bounds pertaining to normalized vectors.

Lemma A.8. *Define $f(\boldsymbol{x}) = \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2}$ for all $\boldsymbol{x} \in \mathbb{R}^q$. Suppose without loss of generality that $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^q$ and $\|\boldsymbol{y}\| \geq \|\boldsymbol{x}\| > 0$, then*

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| \leq \frac{3\|\boldsymbol{x} - \boldsymbol{y}\|}{\|\boldsymbol{x}\|^2}.$$

Proof. First observe

$$\begin{aligned} f(\boldsymbol{x}) - f(\boldsymbol{y}) &= \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2} - \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|^2} \\ &= \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2} - \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|^2} + \frac{\boldsymbol{y}}{\|\boldsymbol{x}\|^2} - \frac{\boldsymbol{y}}{\|\boldsymbol{x}\|^2} \\ &= \frac{\boldsymbol{x} - \boldsymbol{y}}{\|\boldsymbol{x}\|^2} + \frac{\boldsymbol{y}(\|\boldsymbol{y}\|^2 - \|\boldsymbol{x}\|^2)}{\|\boldsymbol{x}\|^2\|\boldsymbol{y}\|^2}. \end{aligned}$$

Taking the norm on both sides and applying the triangle inequality we have

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| = \frac{\|\boldsymbol{x} - \boldsymbol{y}\|}{\|\boldsymbol{x}\|^2} + \frac{\|\boldsymbol{y}\|(|\|\boldsymbol{y}\|^2 - \|\boldsymbol{x}\|^2|)}{\|\boldsymbol{x}\|^2\|\boldsymbol{y}\|^2}.$$

By assumption $\|\boldsymbol{y}\| \geq \|\boldsymbol{x}\|$, therefore

$$|\|\boldsymbol{y}\|^2 - \|\boldsymbol{x}\|^2| = |\langle \boldsymbol{y} - \boldsymbol{x}, \boldsymbol{y} + \boldsymbol{x}\rangle| \leq \|\boldsymbol{y} - \boldsymbol{x}\|\|\boldsymbol{y} + \boldsymbol{x}\| \leq \|\boldsymbol{y} - \boldsymbol{x}\|(\|\boldsymbol{y}\| + \|\boldsymbol{x}\|) \leq 2\|\boldsymbol{y}\|\|\boldsymbol{y} - \boldsymbol{x}\|.$$

This implies

$$\begin{aligned} \|f(\boldsymbol{x}) - f(\boldsymbol{y})\| &\leq \frac{\|\boldsymbol{x} - \boldsymbol{y}\|}{\|\boldsymbol{x}\|^2} + \frac{2\|\boldsymbol{y}\|^2\|\boldsymbol{y} - \boldsymbol{x}\|}{\|\boldsymbol{x}\|^2\|\boldsymbol{y}\|^2} \\ &= \frac{3\|\boldsymbol{x} - \boldsymbol{y}\|}{\|\boldsymbol{x}\|^2} \end{aligned}$$

as claimed. □

A.6 Hoeffding's inequality in Hilbert space

Lemma 4.6 rests on the application of the following concentration bound for sums of independent, mean zero, bounded random vectors. We remark that this is a specialization of more general results for martingales in 2-smooth Banach spaces.

Lemma A.9. ***[Specialization of (Pinelis, 1994, Thm. 3.5)]*** *For $i \in [N]$ and $R \in \mathbb{R}_{>0}$, let $\boldsymbol{x}_i \in \mathbb{R}^q$ be independent, mean zero random vectors which satisfy $\|\boldsymbol{x}_i\| \leq R$ almost surely. Let $S_N = \sum_{i=1}^{N}\boldsymbol{x}_i$, then for $t \in \mathbb{R}_{\geq 0}$ we have*

$$\mathbb{P}(\|S_N\| \geq t) \leq \exp\left(-\frac{t^2}{2NR^2}\right).$$

APPENDIX B PROOFS OF RESULTS

B.1 PROOF OF THEOREM 3.2

Theorem 3.2. *Let $D \subset \{0,1\}^n$ be a set which can be strictly memorized and assume $\|\boldsymbol{x}\|_0 \leq m \in \mathbb{N}_{\geq 1}$ for all $\boldsymbol{x} \in D$. Let $\mathcal{D}$ be a probability distribution on D, and consider a random sample $\mathcal{S}_N = (\boldsymbol{x}_i)_{i\in[N]}$, where $\boldsymbol{x}_i \sim \mathcal{D}$ are mutually i.i.d. Let $\hat{\boldsymbol{\omega}} = \text{HSVM}(\mathcal{S}_N)$, $\boldsymbol{\omega}^* = \text{HSVM}(D)$, $\boldsymbol{\omega}(0) \in \mathbb{R}^q$ be arbitrary and $\boldsymbol{\omega}(t)$ be generated for all $t \in \mathbb{N}_{\geq 1}$ as per (8), $\delta, \epsilon \in (0,1)$ and assume $\boldsymbol{x} \sim \mathcal{D}$ is sampled independent of $\mathcal{S}_N$. If $N \gtrsim \epsilon^{-2} n \|\boldsymbol{\omega}^*\|^2 m \log(1/\delta)$ then*

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\hat{\boldsymbol{\omega}}) \neq \boldsymbol{x}) \leq \epsilon \quad \textit{and} \quad \mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}(t)) \neq \boldsymbol{x}) = O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\|}{\log(t)}\right) + \epsilon$$

hold with probability at least $1-\delta$ over the sample $\mathcal{S}_N$.

Proof. For any $t \in \mathbb{R}$ define the margin loss $\phi : \mathbb{R} \to \mathbb{R}$ as

$$\phi(z) = \begin{cases} 0, & 1 \leq t, \\ 1-t, & 0 \leq t \leq 1, \\ 1, & t \leq 0, \end{cases}$$

and note trivially for all $t \in \mathbb{R}$ that $\mathbb{1}(t \leq 0) \leq \phi(t)$. We note on occasion we overload this notation and apply ϕ to vectors by applying it elementwise. Observe for any $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{\omega} \in \mathbb{R}^q$ with $\boldsymbol{\theta} = \boldsymbol{V}\boldsymbol{\omega}$, that

$$\mathbb{1}(H(\boldsymbol{x};\boldsymbol{\theta}) \neq \boldsymbol{x}) \leq \mathbb{1}\left(\exists j \in [n] : \boldsymbol{u}_j(\boldsymbol{x})^T \omega \leq 0\right) = \mathbb{1}\left(\min_{j\in[n]} \boldsymbol{u}_j(\boldsymbol{x})^T\boldsymbol{\omega} \leq 0\right) \leq \phi(\min_{j\in[n]} \boldsymbol{u}_j(\boldsymbol{x})^T\boldsymbol{\omega}) = \max_{j\in[n]} \phi(\boldsymbol{u}_j(\boldsymbol{x})^T\boldsymbol{\omega}).$$

For any $\boldsymbol{z} \in \mathbb{R}^n$, let $\ell(\boldsymbol{z}) = \max_{j\in[n]} \phi(z_j)$. Using the fact that ϕ is 1-Lipschitz, for any $\boldsymbol{z}, \boldsymbol{z}' \in \mathbb{R}^n$ we have

$$|\ell(\boldsymbol{z}) - \ell(\boldsymbol{z}')| \leq |\max_{j\in[n]} \left(\phi(z_j) - \phi(z'_j)\right)| = \|\phi(\boldsymbol{z}) - \phi(\boldsymbol{z}')\|_\infty \leq \|\boldsymbol{z} - \boldsymbol{z}'\|_\infty \leq \|\boldsymbol{z} - \boldsymbol{z}'\|_2.$$

Therefore ℓ is 1-Lipschitz with respect to the Euclidean norm. Let $\boldsymbol{U}(\boldsymbol{x}) \in \mathbb{R}^{n\times q}$ denote the matrix whose jth row is $\boldsymbol{u}_j(\boldsymbol{x})^T \in \mathbb{R}^{1\times q}$ for all $j \in [n]$. Furthermore, for some $\Lambda \in \mathbb{R}_{>0}$, define

$$\mathcal{H} = \{\boldsymbol{x} \mapsto \boldsymbol{U}(\boldsymbol{x})\boldsymbol{\omega} \ : \boldsymbol{\omega} \in \mathbb{R}^q, , \ \|\boldsymbol{\omega}\| \leq \Lambda\}$$

and let

$$\mathcal{G}_\Lambda = \{\boldsymbol{x} \mapsto (\ell \circ \boldsymbol{b})(\boldsymbol{x}) : h \in \mathcal{H}_\Lambda\}.$$

Note by construction that $g \in \mathcal{G}_\Lambda$ implies $g : \mathbb{R}^n \to [0,1]$. We now compute the empirical Rademacher complexity of $\mathcal{G}_\Lambda$ on a sample $\mathcal{S}_N = (\boldsymbol{x}_i)_{i\in[N]}$, to this end let $\boldsymbol{\sigma} \in \{\pm 1\}^n$ and $\boldsymbol{\epsilon} \in \{\pm\}^{N\times n}$ be a random vector and matrix respectively whose entries are mutually i.i.d. and distributed uniformly on $\{\pm 1\}$. As ℓ is 1-Lipschitz in the ℓ_2 norm, then applying a vector contraction inequality (Maurer, 2016, Corollary 1) we have

$$\begin{aligned}
\tilde{\mathfrak{R}}_{\mathcal{S}}(\mathcal{G}_\Lambda) &= \mathbb{E}_{\boldsymbol{\sigma}}\left[\sup_{\boldsymbol{b}\in\mathcal{H}_\Lambda} \frac{1}{N}\sum_{i=1}^N \sigma_i(\ell\circ\boldsymbol{b})(\boldsymbol{x}_i)\right] \\
&\leq \sqrt{2}E_{\boldsymbol{\epsilon}}\left[\sup_{\boldsymbol{\omega}\in\mathbb{R}^q} \frac{1}{N}\sum_{i=1}^N\sum_{j=1}^n \epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)^T\boldsymbol{\omega}\right] \\
&\leq \sqrt{2}\mathbb{E}_{\boldsymbol{\epsilon}}\left[\sup_{\boldsymbol{\omega}\in\mathbb{R}^q} \langle\boldsymbol{\omega}, \frac{1}{N}\sum_{i=1}^N\sum_{j=1}^n \epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)\rangle\right] \\
&\leq \frac{\sqrt{2}\Lambda}{N}\mathbb{E}_{\boldsymbol{\epsilon}}\left[\left\|\sum_{i=1}^N\sum_{j=1}^n \epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)\right\|\right].
\end{aligned}$$

Let $Z = \sum_{i=1}^{N}\sum_{j=1}^{n}\epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)$, as $t \mapsto \sqrt{t}$ is concave then $\mathbb{E}_Z[\sqrt{\|Z\|^2}] \leq \sqrt{\mathbb{E}_Z\left[\|Z\|^2\right]}$ by Jensen's inequality. As a result

$$\mathbb{E}_{\boldsymbol{\epsilon}}\left[\left\|\sum_{i=1}^{N}\sum_{j=1}^{n}\epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)\right\|\right] \leq \sqrt{\mathbb{E}_{\boldsymbol{\epsilon}}\left[\left\langle\sum_{i=1}^{N}\sum_{j=1}^{n}\epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i), \sum_{l=1}^{N}\sum_{k=1}^{n}\epsilon_{lk}\boldsymbol{u}_k(\boldsymbol{x}_l)\right\rangle\right]}$$
$$= \sqrt{\sum_{i=1}^{N}\sum_{j=1}^{n}\sum_{l=1}^{N}\sum_{k=1}^{n}\mathbb{E}_{\boldsymbol{\epsilon}}[\epsilon_{ij}\epsilon_{lk}]\boldsymbol{u}_j(\boldsymbol{x}_i)^T\boldsymbol{u}_k(\boldsymbol{x}_l)}.$$

The Rademacher random variables are mutually i.i.d., therefore

$$\mathbb{E}_{\boldsymbol{\epsilon}}[\epsilon_{ij}\epsilon_{lk}] = \begin{cases} 1, & (i=l)\wedge(j=k), \\ 0, & \text{otherwise.} \end{cases}$$

Recall also from Lemma A.7 that for any $i \in [N]$ and for all $j \in [n]$

$$\|\boldsymbol{u}_j(\boldsymbol{x}_i)\|^2 = \frac{1}{2}\left(\|\boldsymbol{x}_i\|_0 - x_{ij}\right) + 1.$$

Under the assumption $\|\boldsymbol{x}_i\|_0 \leq m$ for all $i \in [N]$, then

$$\tilde{\mathfrak{R}}_{\mathcal{S}}(\mathcal{G}_\Lambda) \leq \frac{\sqrt{2}\Lambda}{N}\mathbb{E}_{\boldsymbol{\epsilon}}\left[\left\|\sum_{i=1}^{N}\sum_{j=1}^{n}\epsilon_{ij}\boldsymbol{u}_j(\boldsymbol{x}_i)\right\|\right]$$
$$\leq \frac{\sqrt{2}\Lambda}{N}\sqrt{\sum_{i=1}^{N}\sum_{j=1}^{n}\|\boldsymbol{u}_j(\boldsymbol{x}_i)\|^2}$$
$$\leq \frac{\Lambda}{N}\sqrt{\sum_{i=1}^{N}\sum_{j=1}^{n}\left(\|\boldsymbol{x}_i\|_0 - x_{ij} + 2\right)}$$
$$\leq \Lambda\sqrt{\frac{n(m+2)}{N}}.$$

Let $\delta \in \mathbb{R}_{>0}$. Applying a Rademacher complexity bound, e.g., (Mohri et al., 2018, Thm 3.3), then with probability at least $1-\delta$ over the random sample $\mathcal{S}_N$

$$\mathbb{E}[g(\boldsymbol{x})] \leq \frac{1}{N}\sum_{i=1}^{N}g(\boldsymbol{x}_i) + 2\tilde{\mathfrak{R}}_{\mathcal{S}}(\mathcal{G}_\Lambda) + 3\sqrt{\frac{\log(2/\delta)}{2N}}$$
$$\leq \frac{1}{N}\sum_{i=1}^{N}g(\boldsymbol{x}_i) + 2\Lambda\sqrt{\frac{n(m+2)}{N}} + 3\sqrt{\frac{\log(2/\delta)}{2N}}$$

for all $g \in \mathcal{G}_\Lambda$. In what follows let $\Lambda = \|\boldsymbol{\omega}^*\|$. Then, with probability at least $1-\delta$ over the random sample $\mathcal{S}_N$, for any $\boldsymbol{\omega} \in \mathbb{R}^q$ such that $\|\boldsymbol{\omega}\| \leq \|\boldsymbol{\omega}^*\|$ we have

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}) \neq \boldsymbol{x}) \leq \frac{1}{N}\sum_{i=1}^{N}\phi(\min_{j\in[n]}\boldsymbol{u}_j(\boldsymbol{x}_i)^T\boldsymbol{\omega})) + 2\sqrt{\frac{\|\boldsymbol{\omega}^*\|^2 n(m+2)}{N}} + 3\sqrt{\frac{\log(2/\delta)}{2N}} \quad (10)$$

First we consider $\hat{\boldsymbol{\omega}}$: for any sample $\mathcal{S}_N$ trivially set$(\mathcal{S}_N) \subseteq D$, therefore $\boldsymbol{\omega}^* \in \mathcal{F}_{\boldsymbol{\omega}}(\mathcal{S}_N)$. As a result, with probability one $\|\hat{\boldsymbol{\omega}}\| \leq \|\boldsymbol{\omega}^*\|$. Conditioning on this event, observe also that $\min_{j\in[n]}\boldsymbol{u}_j(\boldsymbol{x}_i)^T\hat{\boldsymbol{\omega}} \geq 1$ for $i \in [N]$. As a result, with probability at least $1-\delta$ over $\mathcal{S}_N$ we have

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\hat{\boldsymbol{\omega}}) = \boldsymbol{x}) \leq \sqrt{\frac{4\|\boldsymbol{\omega}^*\|^2 n(m+2)}{N}} + \sqrt{\frac{9\log(2/\delta)}{2N}}.$$

As $(a+b)^2 \leq 2(a^2+b^2)$ for $a, b \in \mathbb{R}$ and assuming $m \geq 1$, then for any $\epsilon \in \mathbb{R}_{>0}$, if $N \gtrsim \epsilon^{-2}n\|\boldsymbol{\omega}^*\|^2 m\log(1/\delta)$

$$\mathbb{P}_{\boldsymbol{x}}(H(\boldsymbol{x}; \hat{\boldsymbol{\theta}}) \neq \boldsymbol{x}) \leq \epsilon$$

with probability at least $1-\delta$ over the sample $\mathcal{S}_N$.

We now turn our attention to $\boldsymbol{\omega}(t)$: recall for any $a \in \mathbb{R}_{>0}$ as $E(\boldsymbol{x}; a\boldsymbol{\theta}) = aE(\boldsymbol{x}; \boldsymbol{\theta})$ then

$$a(E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta})) \geq 0 \iff E(\boldsymbol{x}^{(j)}; a\boldsymbol{\theta}) - E(\boldsymbol{x}; a\boldsymbol{\theta}) \geq 0.$$

Indeed, this implies the set of memories in a Hopfield network is invariant under positive re-scalings of the parameters. As a consequence, for any distribution $\mathcal{D}$ on $\{0,1\}^n$, $a \in \mathbb{R}_{>0}$ and $\boldsymbol{\theta} \in \Omega$, if $\boldsymbol{x} \sim \mathcal{D}$ we have

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{\theta}) \neq \boldsymbol{x}) = \mathbb{P}(H(\boldsymbol{x}; a\boldsymbol{\theta}) \neq \boldsymbol{x}).$$

Therefore, if we define

$$\bar{\boldsymbol{\omega}}(t) = \tfrac{\|\boldsymbol{\omega}^*\|}{\|\boldsymbol{\omega}(t)\|}\boldsymbol{\omega}(t)$$

it follows that

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}(t)) \neq \boldsymbol{x}) = \mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\bar{\boldsymbol{\omega}}(t)) \neq \boldsymbol{x}).$$

From (Soudry et al., 2018, Theorem 5),

$$\left\| \frac{\bar{\boldsymbol{\omega}}(t)}{\|\boldsymbol{\omega}^*\|} - \frac{\boldsymbol{\omega}^*}{\|\boldsymbol{\omega}^*\|} \right\| = \left\| \frac{\boldsymbol{\omega}(t)}{\|\boldsymbol{\omega}(t)\|} - \frac{\boldsymbol{\omega}^*}{\|\boldsymbol{\omega}^*\|} \right\| = O\left(\frac{\log(\log(t))}{\log(t)} \right)$$

which trivially implies

$$\|\bar{\boldsymbol{\omega}}(t) - \boldsymbol{\omega}^*\| = O\left(\frac{\|\boldsymbol{\omega}^*\| \log(\log(t))}{\log(t)} \right).$$

As a result, for all $i \in [N]$ we have

$$\begin{aligned}
\min_{j\in[n]} \boldsymbol{u}_j(\boldsymbol{x})^T \bar{\boldsymbol{\omega}}(t) &= \min_{j\in[n]} \left(\boldsymbol{u}_j(\boldsymbol{x})^T \boldsymbol{\omega}^* + \boldsymbol{u}_j(\boldsymbol{x})^T (\bar{\boldsymbol{\omega}}(t) - \boldsymbol{\omega}^*) \right) \\
&\geq 1 - \max_{j\in[n]} \|\boldsymbol{u}_j(\boldsymbol{x}_i)\| \|\bar{\boldsymbol{\omega}}(t) - \boldsymbol{\omega}^*\| \\
&\geq 1 - O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\| \log(\log(t))}{\log(t)} \right),
\end{aligned}$$

where the final inequality follows from Lemma A.7 and the assumption $m \geq 2$. By the definition of ϕ it follows that

$$\phi(\min_{j\in[n]} \boldsymbol{u}_j(\boldsymbol{x})^T \bar{\boldsymbol{\omega}}(t)) = O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\| \log(\log(t))}{\log(t)} \right)$$

for all $i \in [N]$. Using (10), then, with probability at least $1-\delta$ over $\mathcal{S}_N$ we have

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}(t)) = \boldsymbol{x}) \leq O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\| \log(\log(t))}{\log(t)} \right) + \sqrt{\frac{4\|\boldsymbol{\omega}^*\|^2 nm}{N}} + \sqrt{\frac{9\log(2/\delta)}{N}}.$$

Using the inequality $\log(\log(t)) \leq \frac{1}{2}\log(t)$ for all $t > 1$, then if $N \gtrsim \epsilon^{-2} n \|\boldsymbol{\omega}^*\|^2 m \log(1/\delta)$

$$\mathbb{P}(H(\boldsymbol{x}; \boldsymbol{V}\boldsymbol{\omega}(t)) \neq \boldsymbol{x}) = O\left(\frac{\sqrt{m}\|\boldsymbol{\omega}^*\|}{\log(t)} \right) + \epsilon.$$

with probability at least $1-\delta$ over the sample $\mathcal{S}_N$ □

B.2 Properties of invariant parameters

B.2.1 Energy bounds for invariant parameters across orbits

The following result states, in the context of invariant parameters, that energy bound differences for a point in an orbit extend to the entire orbit.

Lemma 4.1. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$ and $\boldsymbol{\theta} \in \Psi(\Gamma_n)$. For $\delta \in \mathbb{R}$, if $E(\boldsymbol{x}_0^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}_0; \boldsymbol{\theta}) \geq 1 - \delta$ for all $j \in [n]$, then for all $\boldsymbol{x} \in \mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ it follows that $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1 - \delta$ for all $j \in [n]$.*

Proof. As $\boldsymbol{\theta} \in \Psi(\Gamma_n)$, recall the intertwining relation (9), for $\boldsymbol{x} \in \{0,1\}^n$ and $\boldsymbol{Q} \in \Gamma_n$ then

$$E(\boldsymbol{Q}\boldsymbol{x};\boldsymbol{\theta}) = E(\boldsymbol{x};\boldsymbol{Q}\boldsymbol{\theta}) = E(\boldsymbol{x};\boldsymbol{\theta}).$$

As for any $\boldsymbol{x} \in \text{Orb}(\boldsymbol{x}_0, \Gamma_n)$ there exists a $\boldsymbol{Q} \in \Gamma_n$, corresponding to a permutation $\pi \in \Pi_n^{\mathcal{Q}}$, such that $\boldsymbol{x}_0 = \boldsymbol{Q}\boldsymbol{x}$, this implies

$$1 - \delta \leq E(\boldsymbol{x}_0^{(j)};\boldsymbol{\theta}) - E(\boldsymbol{x}_0;\boldsymbol{\theta}) = E((\boldsymbol{Q}\boldsymbol{x})^{(j)};\boldsymbol{\theta}) - E(\boldsymbol{Q}\boldsymbol{x};\boldsymbol{\theta}) = E(\boldsymbol{x}^{\pi(j)};\boldsymbol{\theta}) - E(\boldsymbol{x};\boldsymbol{\theta}).$$

As π is a bijection then for all $j \in [n]$ this implies

$$E(\boldsymbol{x}^{(j)};\boldsymbol{\theta}) - E(\boldsymbol{x};\boldsymbol{\theta}) \geq 1 - \delta$$

as claimed. □

B.2.2 Characterizing the invariant set for edge adjacency preserving permutations

The following lemma identifies the invariant parameters with respect to the set of edge adjacency preserving permutations as a particular rank three subspace.

Lemma 4.2. *Let $F : \mathbb{R}^3 \to \boldsymbol{\Theta}$ denote the linear map defined as follows: if $(\boldsymbol{W}, \boldsymbol{b}) = F(\boldsymbol{\beta})$ then for all $i, j \in [n]$ we have $w_{ij} = 0$ if $i = j$, $w_{ij} = \beta_1$ if $i \sim j$, $w_{ij} = \beta_2$ if $i \nsim j$ and $b_j = \beta_3$. Then $\Psi(\mathcal{Q}_n) = F(\mathbb{R}^3)$ where $F(\mathbb{R}^3)$ denotes the image of F.*

Proof. First we show that $F(\mathbb{R}^3) \subseteq \Psi(\mathcal{Q}_n)$. Suppose $\boldsymbol{\theta} \in F(\mathbb{R}^3)$, then there exists $\boldsymbol{\beta} \in \mathbb{R}^3$ such that $\boldsymbol{\theta} = F(\boldsymbol{\beta})$. Let $\boldsymbol{Q} \in \mathcal{Q}_n$ and $\pi \in \Pi_n^{\mathcal{Q}}$ be the corresponding permutation. Then $b_i = b_{\pi(i)} = \beta_3$ for all $i \in [n]$ and as a result $\boldsymbol{Q}^T\boldsymbol{b} = \boldsymbol{b}$. Furthermore, if $i, j \in [n]$ then $\pi(i) \sim \pi(j)$ if and only if $i \sim j$. Therefore if $i \sim j$ then $W_{ij} = \beta_1 = W_{\pi(i)\pi(j)}$. Otherwise, if $i \nsim j$ then either $i = j$, which implies $W_{jj} = 0 = W_{\pi(j)\pi(j)}$, or $i \neq j$ and then $W_{ij} = \beta_2 = W_{\pi(i)\pi(j)}$. As a result it follows that $\boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q} = \boldsymbol{W}$, this implies $\boldsymbol{Q}\boldsymbol{\theta} = \boldsymbol{\theta}$ and so $\boldsymbol{\theta} \in \Psi(\mathcal{Q}_n)$. We therefore conclude that $F(\mathbb{R}^3) \subseteq \Psi(\mathcal{Q}_n)$.

Now assume $\boldsymbol{\theta} \in \Psi(\mathcal{Q}_n)$, to prove there exists a $\beta_3 \in \mathbb{R}$ such that $b_i = \beta_3$ for all $i \in [n]$ it suffices to show $b_i = b_j$ for all $i, j \in [n]$. Similarly, to show there exist $\beta_1, \beta_2 \in \mathbb{R}$ as per the statement of the lemma, it suffices to show $w_{ij} = w_{ab}$ whenever either of the following hold: i) $i \sim j$ and $a \sim b$ or ii) $i \nsim j$ and $a \nsim b$. It therefore suffices to prove the following two statements.

1. For any $i, j \in [n]$ there exists a $\pi \in \Pi_n^{\mathcal{Q}}$ such that $\pi(i) = j$. Note, as $\boldsymbol{\theta} \in \Psi(\mathcal{Q}_n)$ this implies $b_i = b_{\pi(i)} = b_j$.
2. For any $i, j, a, b \in [n]$ satisfying $i \sim j$ and $a \sim b$, or $i \nsim j$ and $a \nsim b$, there exists a $\pi \in \Pi_n^{\mathcal{Q}}$ such that $\pi(i) = a$ and $\pi(j) = b$. Note, and again as $\boldsymbol{\theta} \in \Psi(\mathcal{Q}_n)$, this implies $w_{ij} = w_{\pi(i)\pi(j)} = w_{ab}$.

In all that follows, for $l \in [8]$ let $\nu_l \in [v]$. To prove the first statement, let $i, j \in [n]$ and suppose $i = \text{Ind}(\{\nu_1, \nu_2\})$ and $j = \text{Ind}(\{\nu_3, \nu_4\})$. Consider the permutation $\pi \in \Pi_n^{\Phi} \subseteq \Pi_n^{\mathcal{Q}}$ which swaps the indices of the unordered vertex pairs involving ν_1 with the corresponding pair involving ν_3, likewise for ν_2 and ν_4, and is identity otherwise. To be clear, this is the permutation satisfying for $t \in [2]$ the identities $\pi(\text{Ind}(\{\nu_t, \nu\})) = \text{Ind}(\{\nu_{t+2}, \nu\})$ and $\pi(\text{Ind}(\{\nu_{t+2}, \nu\})) = \text{Ind}(\{\nu_t, \nu\})$ for all $\nu \in [v] \backslash \{\nu_t, \nu_{t+2}\}$, and $\pi(\text{Ind}^{-1}(\{\nu, \nu'\})) = \text{Ind}^{-1}(\{\nu, \nu'\})$ for all $\nu, \nu' \in [v] \backslash \{\nu_1, ...\nu_4\}$. Note if $i \sim j$ then we can without loss of generality assume $\nu_2 = \nu_4$ and this permutation reduces to swapping a single pair and treating the rest with identity. By construction this permutation preserves adjacency, moreover $\pi(i) = j$. As a result, for all $i, j \in [n]$ there exists a $\pi \in \Pi_n^{\mathcal{Q}}$ such that $b_i = b_{\pi(i)} = b_j$.

To prove the second statement, let $i, j, a, b \in [n]$ and suppose $i = \text{Ind}(\{\nu_1, \nu_2\})$, $j = \text{Ind}(\{\nu_3, \nu_4\})$, $a = \text{Ind}(\{\nu_5, \nu_6\})$ and $j = \text{Ind}(\{\nu_7, \nu_8\})$. Now consider the permutation $\pi \in \Pi_n^{\Phi} \subseteq \Pi_n^{\mathcal{Q}}$ which swaps the indices of the unordered vertex pairs involving ν_1 with those of ν_5, ν_2 with those of ν_6, ν_3 with those of ν_7, ν_4 with those of ν_8 and acts as identity on the indices of all other edges. To be clear, this is the permutation satisfying for $t \in [4]$ the identities $\pi(\text{Ind}^{-1}(\{\nu_t, \nu\})) = \text{Ind}^{-1}(\{\nu_{t+4}, \nu\})$

and $\pi(\text{Ind}^{-1}(\{\nu_{t+4}, \nu\})) = \text{Ind}^{-1}(\{\nu_t, \nu\})$ for all $\nu \in [v] \backslash \{\nu_t, \nu_{t+4}\}$, and $\pi(\text{Ind}^{-1}(\{\nu, \nu'\})) = \text{Ind}^{-1}(\{\nu, \nu'\})$ for all $\nu, \nu' \in [v] \backslash \{\nu_1, ...\nu_8\}$. By construction this permutation preserves adjacency and $\pi(i) = a, \pi(j) = b$. Moreover as $\pi \in \Pi_n^Q$ then $i \sim j$ implies $a \sim b$ and $i \nsim j$ implies $a \nsim b$. As a result $w_{ij} = w_{ab}$ for all $i, j, a, b \in [n]$ if either $i \sim j$ and $a \sim b$ or $i \nsim j$ and $a \nsim b$.

With both statements proved we conclude $\Psi(\mathcal{Q}_n) \subseteq F(\mathbb{R}^3)$. Finally, as $\Psi(\mathcal{Q}_n) \subseteq F(\mathbb{R}^3)$ and $F(\mathbb{R}^3) \subseteq \Psi(\mathcal{Q}_n)$, then $\Psi(\mathcal{Q}_n) = F(\mathbb{R}^3)$ as claimed. □

The next lemma states that parameters invariant to edge adjacency preserving permutations can memorize any binary vector. In combination with Lemma 4.1 this implies any graph isomorphism class is strictly memorizable.

Lemma 4.3. *For $m \in [0, n]$, let $\boldsymbol{\beta} = [2, 2, 1 - 2m] \in \mathbb{R}^3$ and $\boldsymbol{\theta} = F(\boldsymbol{\beta})$. Then $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1$ for all $j \in [n]$ and for all $\boldsymbol{x} \in \{0, 1\}^n$ satisfying $\|\boldsymbol{x}\|_0 = m$.*

Proof. Let $\boldsymbol{x} \in \{0, 1\}^n$ satisfy $|supp(\boldsymbol{x})| = m \in [0, n]$. Recall from Lemma A.1 that for any $j \in [n]$

$$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) = y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle,$$

where $y_j(\boldsymbol{x}) = 1 - 2x_j$, $\boldsymbol{z}(\boldsymbol{x}) = [\boldsymbol{x}, 1]$ and $\boldsymbol{\theta}_j = [\boldsymbol{w}_j, 1]$. Furthermore,

$$\begin{aligned}
\langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle &= \boldsymbol{x}^T \boldsymbol{w}_j + \beta_3 \\
&= \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \neq j) w_{jl} + \beta_3 \\
&= \beta_1 \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \sim j) + \beta_2 \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \nsim j \wedge j \neq l) + \beta_3.
\end{aligned}$$

Let $c_j(\boldsymbol{x}) = \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \sim j)$ denote the number of edges of the graph adjacent to the jth edge. Then as

$$\begin{aligned}
m &= \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge j \neq l) + \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge j = l) \\
&= \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \sim j \wedge j \neq l) + \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \nsim j \wedge j \neq l) + \mathbb{1}(j \in supp(\boldsymbol{x})) \\
&= \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \sim j) + \sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \nsim j \wedge j \neq l) + x_j,
\end{aligned}$$

it follows that

$$\sum_{l=1}^{n} \mathbb{1}(l \in supp(\boldsymbol{x}) \wedge l \nsim j \wedge j \neq l) = m - c_j(\boldsymbol{x}) - x_j.$$

As a result, the condition that must be satisfied for all $j \in [n]$ is

$$y_j(\boldsymbol{x}) \langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{\theta}_j \rangle = (1 - 2x_j) \left(c_j(\boldsymbol{x})(\beta_1 - \beta_2) + \beta_2(m - x_j) + \beta_3 \right) \geq 1.$$

If $\beta_1 = \beta_2$ then the left-hand side simplifies to an expression which depends only on the sparsity of the representation of the graph. Under this assumption, it suffices to find a $\beta_2, \beta_3 \in \mathbb{R}$ such that

$$(1 - 2x_j) \left(\beta_2(m - x_j) + \beta_3 \right) \geq 1.$$

Let $\beta_3 = 1 - \beta_2 m$, if $x_j = 0$ then

$$(1 - 2x_j) \left(\beta_2(m - x_j) + \beta_3 \right) = \beta_2 m + \beta_3 = 1$$

while if $x_j = 1$ then

$$-(\beta_2(m - 1) + \beta_3) = 1 - \beta_2.$$

Therefore, with $\beta_1 = \beta_2 = 2$ and $\beta_3 = 1 - 2m$ we have

$$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1$$

for all $j \in [n]$. □

We now make a few remarks in regard to the the construction used in the previous lemma. First, $F(2,2,1-2m)$ memorizes $\boldsymbol{x} \in \{0,1\}^n$ iff $\|\boldsymbol{x}\|_0 = m$. Indeed, the only if aspect can be demonstrated as follows: if $\boldsymbol{x}'$ satisfies $\|\boldsymbol{x}'\| = m + \delta$ for $\delta \in \mathbb{N}_{\geq 0}$, the required inequalities become $2\delta + 1 \geq 1$ for $j \in supp(\boldsymbol{x}')$ and $-2\delta + 1 \geq 1$ for $j \notin supp(\boldsymbol{x}')$. These inequalities can only simultaneously hold if $\delta = 0$. Second

$$\|F(2,2,1-2m)\|^2 = 2v(v+1) + (1-2m)^2,$$

therefore when the sparsity m is proportional to n then the norm scales like $\Theta(n)$.

B.3 Constructing an invariant, small norm parameter which memorizes k-cliques

Our goal in this section is to show that small norm parameters exist which can memorize specific isomorphism classes. In particular, we consider the case of k-cliques: recall that a k-clique graph has a fully connected subset of k vertices while the remaining $v - k$ vertices are isolated. We denote the set of representations of k-cliques on v vertices as $\mathcal{C}_{v,k}$ and trivially note $|\mathcal{C}_{v,k}| = \binom{v}{k}$. Towards constructing low-norm invariant parameters that strictly memorize all k-cliques, the following lemma derives specific expressions for the energy difference derived in Lemma A.1. To state this result, for $\boldsymbol{x} \in \mathcal{C}_{v,k}$ let $\text{Clique}(\boldsymbol{x}) \subset [v]$ denote the subset of the vertices of the graph which are in the fully connected subset.

Lemma B.1. *Let $\boldsymbol{\beta} \in \mathbb{R}^3$ and suppose $\boldsymbol{\theta} = F(\boldsymbol{\beta}) = \boldsymbol{V}\boldsymbol{\omega}$, for some $\boldsymbol{\omega} \in \mathbb{R}^q$. For $\boldsymbol{x} \in \mathcal{C}_{v,k}$ and any $j \in [n]$, define $r = |\text{Clique}(\boldsymbol{x}) \cap \text{Ind}^{-1}(j)| \in \{0,1,2\}$ as the number of vertices in the jth vertex pair which are also in the clique of $\boldsymbol{x}$. Then for any $j \in [n]$*

$$\boldsymbol{u}_j(\boldsymbol{x})^T\boldsymbol{\omega} = y_j(\boldsymbol{x})\boldsymbol{z}(\boldsymbol{x})^T\boldsymbol{\theta}_j = \begin{cases} \frac{\beta_2}{2}k^2 + \frac{\beta_2}{2}k + \beta_3, & r = 0, \\ \frac{\beta_2}{2}k^2 + \left(\beta_1 - \frac{\beta_2}{2}\right)k + (\beta_2 + \beta_3 - \beta_1), & r = 1, \\ -\left(\frac{\beta_2}{2}k^2 + \left(2\beta_1 - \frac{3}{2}\beta_1\right)k + (3\beta_2 - 4\beta_1 + \beta_3)\right), & r = 2. \end{cases}$$

Proof. By definition

$$\begin{aligned} \boldsymbol{z}(\boldsymbol{x})^T\boldsymbol{\theta}_j &= \boldsymbol{w}_j^T\boldsymbol{x} + b_j \\ &= \sum_{l=1}^n w_{jl}\mathbb{1}(l \in \text{supp}(\boldsymbol{x})) + \beta_3 \\ &= \beta_1 \sum_{l=1}^n \mathbb{1}(l \in \text{supp}(\boldsymbol{x}) \wedge l \sim j) + \beta_2 \sum_{l=1}^n \mathbb{1}(l \in \text{supp}(\boldsymbol{x}) \wedge l \nsim j \wedge l \neq j) + \beta_3 \end{aligned}$$

Observe each $j \in [n]$ can be placed in one of three distinct categories with respect to $\boldsymbol{x}$: in particular, either both, one or neither of the vertices of j are in the k-clique of the graph represented by $\boldsymbol{x}$. Fixing an arbitrary $j \in [n]$, we denote these events in turn as Φ_r for $r \in \{0,1,2\}$, where

$$\Phi_r(\boldsymbol{x}) = \{j \in [n] \ : \ |\text{Ind}^{-1}(j) \cap \text{Clique}(\boldsymbol{x})| = r\}.$$

Note $\Phi_2(\boldsymbol{x}) = \text{supp}(\boldsymbol{x})$. If $j \in \Phi_0(\boldsymbol{x})$ then neither of the vertices of j are in the clique of $\boldsymbol{x}$, as a result the jth edge cannot be adjacent to any edge in the clique. If $j \in \Phi_1(\boldsymbol{x})$ then exactly one vertex of j is in the clique, furthermore there are $k-1$ other vertices in the clique this vertex is connected to via an edge. Finally, if $j \in \Phi_2(\boldsymbol{x})$ then both of its vertices are connected via edges to $k-2$ other vertices in the clique. As a result,

$$\sum_{l=1}^n \mathbb{1}(l \in \text{supp}(\boldsymbol{x}) \wedge l \sim j) = \begin{cases} 0, & j \in \Phi_0(\boldsymbol{x}), \\ k-1, & j \in \Phi_1(\boldsymbol{x}), \\ 2(k-2), & j \in \Phi_2(\boldsymbol{x}). \end{cases}$$

Moreover, as there are $\binom{k}{2}$ edges in total in a k-clique, and as if $l \in \text{supp}(\boldsymbol{x})$ then $j = l$ can be true only if $j \in \text{supp}(\boldsymbol{x}) \in \Phi_2(\boldsymbol{x})$, then

$$\sum_{l=1}^n \mathbb{1}(l \in \text{supp}(\boldsymbol{x}) \wedge l \nsim j \wedge l = j) = \begin{cases} \binom{k}{2}, & j \in \Phi_0(\boldsymbol{x}), \\ \binom{k}{2} - k + 1, & j \in \Phi_1(\boldsymbol{x}), \\ \binom{k}{2} - 2k + 3, & j \in \Phi_2.(\boldsymbol{x}). \end{cases}$$

As a result: if $j \in \Phi_0(\boldsymbol{x})$ then

$$\boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{\theta}_j = \left(\beta_2 \frac{k(k+1)}{2} + \beta_3\right) = \frac{\beta_2}{2}k^2 + \frac{\beta_2}{2}k + \beta_3.$$

If $j \in \Phi_1(\boldsymbol{x})$ then

$$\boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{\theta}_j = \beta_1(k-1) + \beta_2 \frac{k^2 - k + 2}{2} + \beta_3 = \frac{\beta_2}{2}k^2 + \left(\beta_1 - \frac{\beta_2}{2}\right)k + (\beta_2 + \beta_3 - \beta_1).$$

Finally, if $j \in \Phi_2(\boldsymbol{x})$ then

$$\boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{\theta}_j = \beta_1(2k-4) + \beta_2 \frac{k^2 - 3k + 6}{2} + \beta_3 = \frac{\beta_2}{2}k^2 + \left(2\beta_1 - \frac{3}{2}\beta_1\right)k + (3\beta_2 - 4\beta_1 + \beta_3).$$

To conclude, observe $y_j(\boldsymbol{x}) = (1 - 2x_{ij}) = -1$ iff $j \in \Phi_2(\boldsymbol{x})$. □

We now derive a simple bound on the norm of parameters which are invariant to edge adjacency preserving permutations.

Lemma B.2. *Let $\boldsymbol{\beta} \in \mathbb{R}^3$ and $\boldsymbol{\theta} = F(\beta^3)$. Then*

$$\|\boldsymbol{\theta}\|^2 \leq \beta_2^2 v^4 + 2\beta_1^2 v^3 + \beta_3^2 v^2.$$

Proof. For any fixed edge index $r \in [n]$, note as each vertex of this edge is a member of $v - 2$ other vertex pairs then

$$\sum_{c=1}^{n} \mathbb{1}(c \sim r) = 2(v-2)$$

Moreover, as there are $\binom{v}{2}$ unordered vertex pairs in total

$$\sum_{c=1}^{n} \mathbb{1}(c \nsim r \wedge c \neq r) = \binom{v}{2} - 2(v-2) - 1 = \frac{v^2 - 3v + 6}{2}.$$

Therefore, and also noting that $n = \binom{v}{2} \leq v^2$, we have

$$\begin{aligned}
\|\boldsymbol{\theta}\|^2 &= \|\boldsymbol{W}\|_F^2 + \|\boldsymbol{b}\|^2 \\
&= \sum_{r=1}^{n} \left(\beta_1^2 \sum_{c=1}^{n} \mathbb{1}(c \sim r) + \beta_2^2 \sum_{c=1}^{n} \mathbb{1}(c \nsim r \wedge c \neq r) + \beta_3^2\right) \\
&= n\left(\beta_1^2 2(v-2) + \beta_2^2 \left(\frac{v^2 - 3v + 6}{2}\right) + \beta_3^2\right) \\
&\leq n(\beta_2^2 v^2 + 2\beta_1^2 v + \beta_3^2) \\
&\leq \beta_2^2 v^4 + 2\beta_1^2 v^3 + \beta_3^2 v^2.
\end{aligned}$$

□

We now present a low norm construction for memorizing k-cliques: in particular, Lemma 4.4 illustrates that the k-clique graph isomorphism class can be memorized using a parameter whose norm is $O(\sqrt{n})$. This is in contrast to the general construction used in the proof of Lemma 4.3 whose norm grew as $\Theta(n)$.

Lemma 4.4. *If $\boldsymbol{\beta} = [-5/k, 14/k^2, 0] \in \mathbb{R}^3$, $\boldsymbol{\theta} = F(\boldsymbol{\beta})$, and $k \geq 5$, then the following hold.*

1. *$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq 1$ for all $\boldsymbol{x} \in \mathcal{C}_{v,k}$ and $j \in [n]$.*
2. *If $k = cv$ for some constant $c \in (0, 1]$, then there exists a constant $C > 0$ such that $\|\boldsymbol{\theta}\|^2 \leq Cv$.*

Proof. For the proof of the first statement, from Lemma B.1 there are three cases we need to check. First, if $j \in \Phi_0(\boldsymbol{x})$ then

$$y_j(\boldsymbol{x})\boldsymbol{z}(\boldsymbol{x})^T\boldsymbol{\theta}_j = \frac{\beta_2}{2}k^2 + \frac{\beta_2}{2}k + \beta_3 = 7\left(1 + \frac{1}{k}\right) \geq 1.$$

Second, if $j \in \Phi_1(\boldsymbol{x})$ then

$$\begin{aligned} y_j(\boldsymbol{x})\boldsymbol{z}(\boldsymbol{x})^T\boldsymbol{\theta}_j &= \frac{\beta_2}{2}k^2 + \left(\beta_1 - \frac{\beta_2}{2}\right)k + (\beta_2 + \beta_3 - \beta_1) \\ &= 2 - \frac{7}{k} + \frac{14}{k^2} + \frac{5}{k} \\ &\geq 2 - \frac{2}{k} \\ &\geq 1. \end{aligned}$$

Third and finally, if $j \in \Phi_2(\boldsymbol{x})$ then

$$\begin{aligned} y_j(\boldsymbol{x})\boldsymbol{z}(\boldsymbol{x})^T\boldsymbol{\theta}_j &= -\left(\frac{\beta_2}{2}k^2 + \left(2\beta_1 - \frac{3}{2}\beta_1\right)k + (3\beta_2 - 4\beta_1 + \beta_3)\right) \\ &= -\left(-3 - \frac{21}{k} + \frac{42}{k^2} + \frac{20}{k}\right) \\ &\geq 3 - \frac{42}{k^2} \\ &\geq 1. \end{aligned}$$

For the proof the second statement, using Lemma B.2 we have

$$\begin{aligned} \|\boldsymbol{\theta}\|^2 &\leq \frac{14}{k^4}v^4 + 2\frac{25}{k^2}v^3 \\ &\leq (14c^{-2})^2 + (5c^{-1})^2 v \\ &\leq 2(14c^{-2})^2 v \\ &=: Cv. \end{aligned}$$

□

B.3.1 Invariance of the full orbit HSVM solution

The following lemma states a well known result that the average orbit action of a parameter is invariant to the action of the underlying group.

Lemma B.3. *Let $\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) \in \Theta$ and Γ_n denote a subgroup of $\mathcal{P}_n$. Then* $\text{Proj}_{\Gamma_n}(\boldsymbol{\theta}) = \frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}\boldsymbol{\theta} \in \Psi(\Gamma_n)$.

Proof. For typographical ease let $\boldsymbol{\theta}' = \text{Proj}_{\Gamma_n}(\boldsymbol{\theta})$. Then

$$\boldsymbol{\theta}' = (\boldsymbol{W}', \boldsymbol{b}') := \frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}\boldsymbol{\theta} = \left(\frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q}, \frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}^T\boldsymbol{b}\right).$$

Given Γ_n is a subgroup, then for any $\boldsymbol{Q}' \in \Gamma_n$

$$\begin{aligned} \boldsymbol{Q}'\boldsymbol{\theta}' &= (\boldsymbol{Q}'^T\boldsymbol{W}'\boldsymbol{Q}', \boldsymbol{Q}'^T\boldsymbol{b}') \\ &= \left(\frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} (\boldsymbol{Q}\boldsymbol{Q}')^T\boldsymbol{W}(\boldsymbol{Q}\boldsymbol{Q}'), \frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} (\boldsymbol{Q}\boldsymbol{Q}')^T\boldsymbol{b}\right) \\ &= \left(\frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}^T\boldsymbol{W}\boldsymbol{Q}, \frac{1}{|\Gamma_n|}\sum_{\boldsymbol{Q}\in\Gamma_n} \boldsymbol{Q}^T\boldsymbol{b}\right) \\ &= \boldsymbol{\theta}', \end{aligned}$$

therefore $\boldsymbol{\theta}' \in \Psi(\Gamma_n)$. □

Using the previous lemma, we show that the full orbit HSVM solution lies in the invariant set.

Lemma 4.5. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$ and Γ_n denote a subgroup of $\mathcal{P}_n$ and assume $\mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ can be strictly memorized. If $\boldsymbol{\theta}^* = \boldsymbol{V}\boldsymbol{\omega}^*$ where $\boldsymbol{\omega}^* = \mathrm{HSVM}_\Theta(\mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n))$ then $\boldsymbol{\theta}^* \in \Psi(\Gamma_n)$.*

Proof. We use a symmetrization argument. To this end, with $\boldsymbol{\theta}^* = (\boldsymbol{W}^*, \boldsymbol{b}^*)$ let

$$\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) := \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^* = \left(\frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}^T \boldsymbol{W}^* \boldsymbol{Q}, \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}^T \boldsymbol{b}^* \right).$$

By Lemma B.3 we know that $\boldsymbol{\theta} \in \Psi(\Gamma_n)$. By the definition of $\boldsymbol{\theta}^*$ we also have

$$E(\boldsymbol{x}^{(j)}, \boldsymbol{\theta}^*) - E(\boldsymbol{x}, \boldsymbol{\theta}^*) \geq 1.$$

Therefore, using both the intertwining property (9) and Lemma A.1, for any $\boldsymbol{x} \in \mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ and $j \in [n]$, and with $\boldsymbol{z}(\boldsymbol{x}) = [\boldsymbol{x}, 1]$, we have

$$\begin{aligned}
E(\boldsymbol{x}^{(j)}, \boldsymbol{\theta}) - E(\boldsymbol{x}, \boldsymbol{\theta}) &= (2x_j - 1)\boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{\theta}_j \\
&= \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} (2x_j - 1)\boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{Q}\boldsymbol{\theta}_j^* \\
&= \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} E(\boldsymbol{x}^{(j)}, \boldsymbol{Q}\boldsymbol{\theta}^*) - E(\boldsymbol{x}, \boldsymbol{Q}\boldsymbol{\theta}^*) \\
&= \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} E(\boldsymbol{x}^{(j)}, \boldsymbol{\theta}^*) - E(\boldsymbol{x}, \boldsymbol{\theta}^*) \\
&= E(\boldsymbol{x}^{(j)}, \boldsymbol{\theta}^*) - E(\boldsymbol{x}, \boldsymbol{\theta}^*) \\
&\geq 1.
\end{aligned}$$

As a result, $\boldsymbol{\theta}$ is a feasible point of the HSVM problem (7) defined on the full orbit dataset $\mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$. Therefore, by the definition of $\boldsymbol{\theta}^*$ it must follow that $\|\boldsymbol{\theta}^*\| \leq \|\boldsymbol{\theta}\|$. On the other hand, using the triangle inequality and the fact that $\boldsymbol{Q} \in \Gamma_n$ is a permutation, we have

$$\|\boldsymbol{\theta}\| = \|\frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^*\| \leq \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \|\boldsymbol{Q}\boldsymbol{\theta}^*\| = \|\boldsymbol{\theta}^*\|.$$

This implies $\frac{1}{2}\|\boldsymbol{\theta}^*\|^2 = \frac{1}{2}\|\boldsymbol{\theta}\|^2$, as this objective is 1-strongly convex this in turn implies $\boldsymbol{\theta}^* = \boldsymbol{\theta} \in \Psi(\Gamma_n)$. □

B.4 Approximately invariant parameters

B.4.1 Approximate invariance is sufficient for generalization

The following lemma states a sufficient condition for strict memorization of an orbit dataset based on proximity to the relevant invariant space. In particular, given a graph $G \in \mathcal{G}_v$ and letting $\boldsymbol{x}_0 = \mathcal{E}_{rep}(G)$, if $\boldsymbol{\omega}^* = \mathrm{HSVM}(\mathcal{S})$, where $\mathcal{S} \subset \mathrm{Orb}(\boldsymbol{x}_0, \Phi_n)$, and $\boldsymbol{\omega}^*$ is sufficiently close to the subspace $\mathcal{Q}_n$, then $\boldsymbol{\theta}^* = \boldsymbol{E}\boldsymbol{\omega}^*$ will strictly memorize all graphs isomorphic to G.

Lemma B.4. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$ satisfy $\|\boldsymbol{x}_0\| = m \in \mathbb{N}_{\geq 2}$, $\boldsymbol{\theta} = \boldsymbol{E}\boldsymbol{\omega} \in \Theta_n$ satisfy $E(\boldsymbol{x}_0^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}_0; \boldsymbol{\theta}) \geq 1$ for all $j \in [n]$, and $\boldsymbol{\theta}' = \boldsymbol{E}\boldsymbol{\omega}' \in \Psi(\Gamma_n)$ be such that $\|\boldsymbol{\omega} - \boldsymbol{\omega}'\| \leq \frac{1}{4\sqrt{m}}$. Then $E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \geq \frac{1}{2}$ for all $\boldsymbol{x} \in \mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ and $j \in [n]$.*

Proof. Inspecting Lemma A.7, if $\|\boldsymbol{x}_0\| = m \in \mathbb{N}_{\geq 2}$ then $\|\boldsymbol{u}_j(\boldsymbol{x})\| \leq \sqrt{m}$ for all $\boldsymbol{x} \in \mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$ and $j \in [n]$. By assumption $\boldsymbol{u}_j(\boldsymbol{x}_0)^T \boldsymbol{\omega} \geq 1$ for all $j \in [n]$, therefore

$$\begin{aligned}
E(\boldsymbol{x}_0^{(j)}; \boldsymbol{\theta}') - E(\boldsymbol{x}_0; \boldsymbol{\theta}') &= y_j(\boldsymbol{x}_0)\boldsymbol{z}(\boldsymbol{x}_0)^T \boldsymbol{\theta}_j' \\
&= \boldsymbol{u}_j(\boldsymbol{x}_0)^T \boldsymbol{\omega}' \\
&= \boldsymbol{u}_j(\boldsymbol{x}_0)^T \boldsymbol{\omega} - \boldsymbol{u}_j(\boldsymbol{x}_0)^T (\boldsymbol{\omega} - \boldsymbol{\omega}') \\
&\geq 1 - \|\boldsymbol{u}_j(\boldsymbol{x}_0)\| \|\boldsymbol{\omega} - \boldsymbol{\omega}'\| \\
&\geq \tfrac{3}{4}
\end{aligned}$$

for all $j \in [n]$. As $\boldsymbol{\theta}' \in \Psi(\Gamma_n)$, then Lemma 4.1 implies for any $\boldsymbol{x} \in \text{Orb}(\boldsymbol{x}_0, \Gamma_n)$ that

$$E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}') - E(\boldsymbol{x}; \boldsymbol{\theta}') = \boldsymbol{u}_j(\boldsymbol{x})^T \boldsymbol{\omega}' \geq \tfrac{3}{4}.$$

Moreover, and using the same trick as before, we also observe for all $\boldsymbol{x} \in \text{Orb}(\boldsymbol{x}_0, \Gamma_n)$ that

$$\begin{aligned} E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) &= y_j(\boldsymbol{x}) \boldsymbol{z}(\boldsymbol{x})^T \boldsymbol{\theta}_j \\ &= \boldsymbol{u}_j(\boldsymbol{x})^T \boldsymbol{\omega} \\ &= \boldsymbol{u}_j(\boldsymbol{x})^T \boldsymbol{\omega}' - \boldsymbol{u}_j(\boldsymbol{x})^T (\boldsymbol{\omega}' - \boldsymbol{\omega}) \\ &\geq \tfrac{3}{4} - \|\boldsymbol{u}_j(\boldsymbol{x})\| \|\boldsymbol{\omega} - \boldsymbol{\omega}'\| \\ &\geq \tfrac{1}{2} \end{aligned}$$

for all $j \in [n]$. □

B.4.2 Proximity of AHSVM solution to the invariant set

Lemma B.5. *Let $\mathcal{S} \subset \{0,1\}^n$, $\boldsymbol{\mu}_{\mathcal{S}} = \frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \bar{\boldsymbol{u}}(\boldsymbol{x})$ and assume $\boldsymbol{\omega}^* = \text{AHSVM}(\mathcal{S})$ is feasible. Then $\boldsymbol{\omega}^* = \frac{\boldsymbol{\mu}_{\mathcal{S}}}{\|\boldsymbol{\mu}_{\mathcal{S}}\|^2}$.*

Proof. Note by the feasibility assumption $\frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \bar{\boldsymbol{u}}(\boldsymbol{x}) \neq \boldsymbol{0}_q$. Forming the Lagrangian with Lagrange variable α we have

$$\mathcal{L}(\boldsymbol{\omega}, \alpha) = \frac{1}{2} \|\boldsymbol{\omega}\|^2 + \alpha \left(1 - \frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \langle \bar{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\omega} \rangle \right).$$

Clearly this is a strongly convex objective with a unique minimizer $\boldsymbol{\omega}^*$. Zeroing the gradient with respect to $\boldsymbol{\omega}$ and rearranging gives the identity

$$\boldsymbol{\omega}^* = \alpha^* \frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \bar{\boldsymbol{u}}(\boldsymbol{x})$$

on the solution pair $(\boldsymbol{\omega}^*, \alpha^*)$. In addition, as there is only a single constraint and the problem is feasible then the constraint must be active, meaning

$$\frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \langle \bar{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\omega}^* \rangle = 1.$$

As a result

$$\|\boldsymbol{\omega}^*\|^2 = \alpha^* \frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \langle \bar{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\omega}^* \rangle = \alpha^*. \tag{11}$$

Therefore

$$\frac{\boldsymbol{\omega}^*}{\|\boldsymbol{\omega}^*\|^2} = \frac{1}{|\mathcal{S}|} \sum_{\boldsymbol{x} \in \mathcal{S}} \bar{\boldsymbol{u}}(\boldsymbol{x}) = \boldsymbol{\mu}_{\mathcal{S}}.$$

As $\boldsymbol{\mu}_{\mathcal{S}} \neq \boldsymbol{0}_q$ then

$$\|\boldsymbol{\mu}_{\mathcal{S}}\|^2 = \left\| \frac{\boldsymbol{\omega}^*}{\|\boldsymbol{\omega}^*\|^2} \right\|^2 = \frac{1}{\|\boldsymbol{\omega}^*\|^2},$$

giving

$$\boldsymbol{\omega}^* = \frac{\boldsymbol{\mu}_{\mathcal{S}}}{\|\boldsymbol{\mu}_{\mathcal{S}}\|^2}$$

as claimed. □

Similar to Lemma 4.5, we now show that the full orbit AHSVM solution lies on the relevant invariance space.

Lemma B.6. *Let $\boldsymbol{x}_0 \in \{0,1\}^n$, Γ_n denote a subgroup of $\mathcal{P}_n$, and assume $\mathcal{O} = \text{Orb}(\boldsymbol{x}_0, \Gamma_n)$ satisfies $|\mathcal{O}| = |\Gamma_n|$. Let $\boldsymbol{\omega}^* = \text{AHSVM}_\Theta(\text{Orb}(\boldsymbol{x}_0, \Gamma_n))$ be feasible and define $\boldsymbol{\theta}^* = \boldsymbol{V}\boldsymbol{\omega}^*$, then $\boldsymbol{\theta}^* \in \Psi(\Gamma_n)$.*

Proof. Again we use a symmetrization argument. To this end, with $\boldsymbol{\theta}^* = (\boldsymbol{W}^*, \boldsymbol{b}^*)$ let

$$\boldsymbol{\theta} = (\boldsymbol{W}, \boldsymbol{b}) := \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^* = \left(\frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}^T \boldsymbol{W}^* \boldsymbol{Q}, \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}^T \boldsymbol{b}^* \right).$$

By Lemma B.3 we know that $\boldsymbol{\theta} \in \Psi(\Gamma_n)$. Let $\boldsymbol{x} \in \mathcal{O}$ and $\boldsymbol{Q} \in \Gamma_n$ be such that $\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{x}_0$, and let π denote the permutation associated with $\boldsymbol{Q}$. As $\boldsymbol{\theta} \in \Psi(\Gamma_n)$ then using the intertwining property (9)

$$\begin{aligned}
\bar{\boldsymbol{u}}(\boldsymbol{x})^T \boldsymbol{\omega} &= \frac{1}{n} \sum_{j=1}^{n} E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \\
&= \frac{1}{n} \sum_{j=1}^{n} E(Q\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(Q\boldsymbol{x}; \boldsymbol{\theta}) \\
&= \frac{1}{n} \sum_{j=1}^{n} E((Q\boldsymbol{x})^{(\pi(j))}; \boldsymbol{\theta}) - E(Q\boldsymbol{x}; \boldsymbol{\theta}) \\
&= \frac{1}{n} \sum_{l=1}^{n} E(\boldsymbol{x}_0^{(l)}; \boldsymbol{\theta}) - E(\boldsymbol{x}_0; \boldsymbol{\theta}) \\
&= \bar{\boldsymbol{u}}(\boldsymbol{x}_0)^T \boldsymbol{\omega}.
\end{aligned}$$

As the AHSVM problem is feasible and has a single constraint then $\frac{1}{|\mathcal{O}|} \sum_{\boldsymbol{x} \in \mathcal{O}} \bar{\boldsymbol{u}}(\boldsymbol{x})^T \boldsymbol{\omega}^* = 1$. Therefore

$$\begin{aligned}
\frac{1}{|\mathcal{O}|} \sum_{\boldsymbol{x} \in \mathcal{O}} \bar{\boldsymbol{u}}(\boldsymbol{x})^T \boldsymbol{\omega} &= \bar{\boldsymbol{u}}(\boldsymbol{x}_0)^T \boldsymbol{\omega} \\
&= \frac{1}{n} \sum_{l=1}^{n} E(\boldsymbol{x}_0^{(l)}; \boldsymbol{\theta}) - E(\boldsymbol{x}_0; \boldsymbol{\theta}) \\
&= \frac{1}{n} \sum_{l=1}^{n} E\left(\boldsymbol{x}_0^{(l)}; \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^* \right) - E\left(\boldsymbol{x}_0; \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^* \right) \\
&= \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \frac{1}{n} \sum_{l=1}^{n} E(\boldsymbol{Q}\boldsymbol{x}_0^{(l)}; \boldsymbol{\theta}^*) - E(\boldsymbol{Q}\boldsymbol{x}_0; \boldsymbol{\theta}^*) \\
&= \frac{1}{|\mathcal{O}|} \sum_{\boldsymbol{x} \in \mathcal{O}} \frac{1}{n} \sum_{j=1}^{n} E(\boldsymbol{x}^{(j)}; \boldsymbol{\theta}) - E(\boldsymbol{x}; \boldsymbol{\theta}) \\
&= \frac{1}{|\mathcal{O}|} \sum_{\boldsymbol{x} \in \mathcal{O}} \bar{\boldsymbol{u}}(\boldsymbol{x})^T \boldsymbol{\omega}^* \\
&= 1.
\end{aligned}$$

As a result, $\boldsymbol{\theta}$ is a feasible point of the AHSVM problem defined on the full orbit dataset $\mathrm{Orb}(\boldsymbol{x}_0, \Gamma_n)$. Therefore, by the definition of $\boldsymbol{\theta}^*$ it must follow that $\|\boldsymbol{\theta}^*\| \leq \|\boldsymbol{\theta}\|$. On the other hand, using the triangle inequality and the fact that $\boldsymbol{Q} \in \Gamma_n$ is a permutation, we have

$$\|\boldsymbol{\theta}\| = \|\frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \boldsymbol{Q}\boldsymbol{\theta}^*\| \leq \frac{1}{|\Gamma_n|} \sum_{\boldsymbol{Q} \in \Gamma_n} \|\boldsymbol{Q}\boldsymbol{\theta}^*\| = \|\boldsymbol{\theta}^*\|.$$

This implies $\frac{1}{2}\|\boldsymbol{\theta}^*\|^2 = \frac{1}{2}\|\boldsymbol{\theta}\|^2$, as this objective is 1-strongly convex this in turn implies $\boldsymbol{\theta}^* = \boldsymbol{\theta} \in \Psi(\Gamma_n)$. □

The lemma below bounds the difference between the sample AHSVM solution and the population AHSVM solution, leveraging only the boundedness of the data.

Lemma 4.6. *Let $\mathcal{O} \subseteq \{0,1\}^n$ satisfy $\|\boldsymbol{x}\|_0 \leq m \in \mathbb{N}_{\geq 2}$ and assume $\boldsymbol{\omega}^* = \mathrm{HSVM}(\mathcal{O})$ is feasible. Consider a random sample $\mathcal{S} = (\boldsymbol{x}_i)_{i=1}^N$ where $\boldsymbol{x}_i \sim U(\mathcal{O})$ are mutually i.i.d. and define $\boldsymbol{\omega}_{\mathcal{O}} = \mathrm{AHSVM}(\mathcal{O})$ and $\boldsymbol{\omega}_{\mathcal{S}} = \mathrm{AHSVM}(\mathcal{S})$. For $\delta \in (0,1]$ and $\epsilon \in \mathbb{R}_{>0}$, if $N \gtrsim \epsilon^{-2}\|\boldsymbol{\omega}^*\|^2 m \log(1/\delta)$ then $\|\boldsymbol{\omega}_{\mathcal{S}} - \boldsymbol{\omega}_{\mathcal{O}}\| \leq \epsilon$ with probability at least $1 - \delta$.*

Proof. Let $\boldsymbol{\mu} = \mathbb{E}[\bar{\boldsymbol{u}}(\boldsymbol{x})]$ where $\boldsymbol{x} \sim U(\mathcal{O})$, then $\boldsymbol{\mu} = \frac{1}{|\mathcal{O}|}\sum_{\boldsymbol{x}\in\mathcal{O}} \bar{\boldsymbol{u}}(\boldsymbol{x})$. In addition, let $\hat{\boldsymbol{\mu}}_{\mathcal{S}} = \frac{1}{|\mathcal{S}|}\sum_{\boldsymbol{x}\in\mathcal{S}} \bar{\boldsymbol{u}}(\boldsymbol{x})$. Then using Lemma B.5 we have

$$\boldsymbol{\omega}_{\mathcal{O}} = \frac{\boldsymbol{\mu}}{\|\boldsymbol{\mu}\|^2}, \;\; \boldsymbol{\omega}_{\mathcal{S}} = \frac{\hat{\boldsymbol{\mu}}_{\mathcal{S}}}{\|\hat{\boldsymbol{\mu}}_{\mathcal{S}}\|^2}.$$

Taking norms this clearly also implies

$$\|\boldsymbol{\mu}\| = \frac{1}{\|\boldsymbol{\omega}_{\mathcal{O}}\|}, \; \|\hat{\boldsymbol{\mu}}_{\mathcal{S}}\| = \frac{1}{\|\boldsymbol{\omega}_{\mathcal{S}}\|},$$

Observe by definition that $\boldsymbol{\omega}^*$ satisfies $E(\boldsymbol{x}^{(j)};\boldsymbol{\theta}^*) - E(\boldsymbol{x};\boldsymbol{\theta}^*) = \langle \boldsymbol{u}_j(\boldsymbol{x}), \boldsymbol{\omega}^*\rangle \geq 1$, therefore for any $S \subseteq \mathcal{O}$ we have

$$\frac{1}{|S|}\sum_{\boldsymbol{x}\in S}\langle \bar{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\omega}^*\rangle = \frac{1}{n|S|}\sum_{\boldsymbol{x}\in S}\sum_{j=1}^{n}\langle \boldsymbol{u}_j(\boldsymbol{x}), \boldsymbol{\omega}^*\rangle \geq 1.$$

As a result we have both $\boldsymbol{\omega}^* \in \mathcal{F}_A(\mathcal{S})$ and $\boldsymbol{\omega}^* \in \mathcal{F}_A(\mathcal{O})$, which in turn implies $\|\boldsymbol{\omega}^*\| \geq \|\boldsymbol{\omega}_{\mathcal{S}}\|$ and $\|\boldsymbol{\omega}^*\| \geq \|\boldsymbol{\omega}_{\mathcal{O}}\|$. Defining $f(\boldsymbol{x}) = \boldsymbol{x}/\|\boldsymbol{x}\|^2$ for any $\boldsymbol{x} \in \mathbb{R}^q$, then applying Lemma A.8 this gives

$$\|\boldsymbol{\omega}_{\mathcal{S}} - \boldsymbol{\omega}_{\mathcal{O}}\| = \|f(\hat{\boldsymbol{\mu}}_{\mathcal{S}}) - f(\boldsymbol{\mu})\| \leq \frac{\|\hat{\boldsymbol{\mu}}_{\mathcal{S}} - \boldsymbol{\mu}\|}{\min\{\|\boldsymbol{\omega}_{\mathcal{O}}\|^{-2}, \|\boldsymbol{\omega}_{\mathcal{S}}\|^{-2}\}} \leq 3\|\boldsymbol{\omega}^*\|^2\|\hat{\boldsymbol{\mu}}_{\mathcal{S}} - \boldsymbol{\mu}\|.$$

Observe

$$\|\hat{\boldsymbol{\mu}}_{\mathcal{S}} - \boldsymbol{\mu}\| = \|\frac{1}{N}\sum_{i=1}^{N}(\bar{\boldsymbol{u}}(\boldsymbol{x}) - \boldsymbol{\mu})\|,$$

clearly $\bar{\boldsymbol{u}}(\boldsymbol{x}) - \mu$ is a centered random vector, moreover for any $\boldsymbol{x} \in \{0,1\}$

$$\begin{aligned}
\|\bar{\boldsymbol{u}}(\boldsymbol{x}) - \mu\| &\leq \|\bar{\boldsymbol{u}}(\boldsymbol{x})\| + \|\boldsymbol{\mu}\| \\
&= \|\bar{\boldsymbol{u}}(\boldsymbol{x})\| + \left\|\frac{1}{|\mathcal{O}|}\sum_{\boldsymbol{x}'\in\mathcal{O}}\bar{\boldsymbol{u}}(\boldsymbol{x}')\right\| \\
&\leq \|\bar{\boldsymbol{u}}(\boldsymbol{x})\| + \frac{1}{|\mathcal{O}|}\sum_{\boldsymbol{x}'\in\mathcal{O}}\|\bar{\boldsymbol{u}}(\boldsymbol{x}')\| \\
&\leq 2\sqrt{m},
\end{aligned}$$

where the last inequality follows from Lemma A.7 and the assumption $m \geq 2$. We now deploy Lemma A.9, a specialization of (Pinelis, 1994, Th, 3.5). In particular, given some $\epsilon \in \mathbb{R}_{\geq 0}$ and letting $S_N = \sum_{i=1}^{N}(\bar{\boldsymbol{u}}(\boldsymbol{x}) - \boldsymbol{\mu})$ then

$$\mathbb{P}\left(\|\hat{\boldsymbol{\mu}}_{\mathcal{S}} - \boldsymbol{\mu}\| \geq \epsilon\right) = \mathbb{P}(\|S_N\| \geq N\epsilon) \leq \exp\left(-\frac{N\epsilon^2}{4m}\right)$$

As a result, for $\delta \in (0,1]$, if $N \geq \frac{m}{4\epsilon^2}\log(1/\delta)$ then

$$\|\boldsymbol{\omega}_{\mathcal{S}} - \boldsymbol{\omega}_{\mathcal{O}}\| \leq 3\|\boldsymbol{\omega}^*\|\epsilon$$

with probability at least $1-\delta$. To arrive at the claimed result we substitute ϵ for $\frac{\epsilon}{3\|\boldsymbol{\omega}^*\|}$. □

APPENDIX C ADDITIONAL EXPERIMENTS AND PRELIMINARY RESULTS

C.1 FURTHER PARAMETER HEATMAPS

Figure 4 is an extension of Figure 3, and shows the weight matrices for MEF and Delta on clique and Payley graph data. We observe that the Delta rule also returns solutions which approach the invariant space as the sample size N increases.

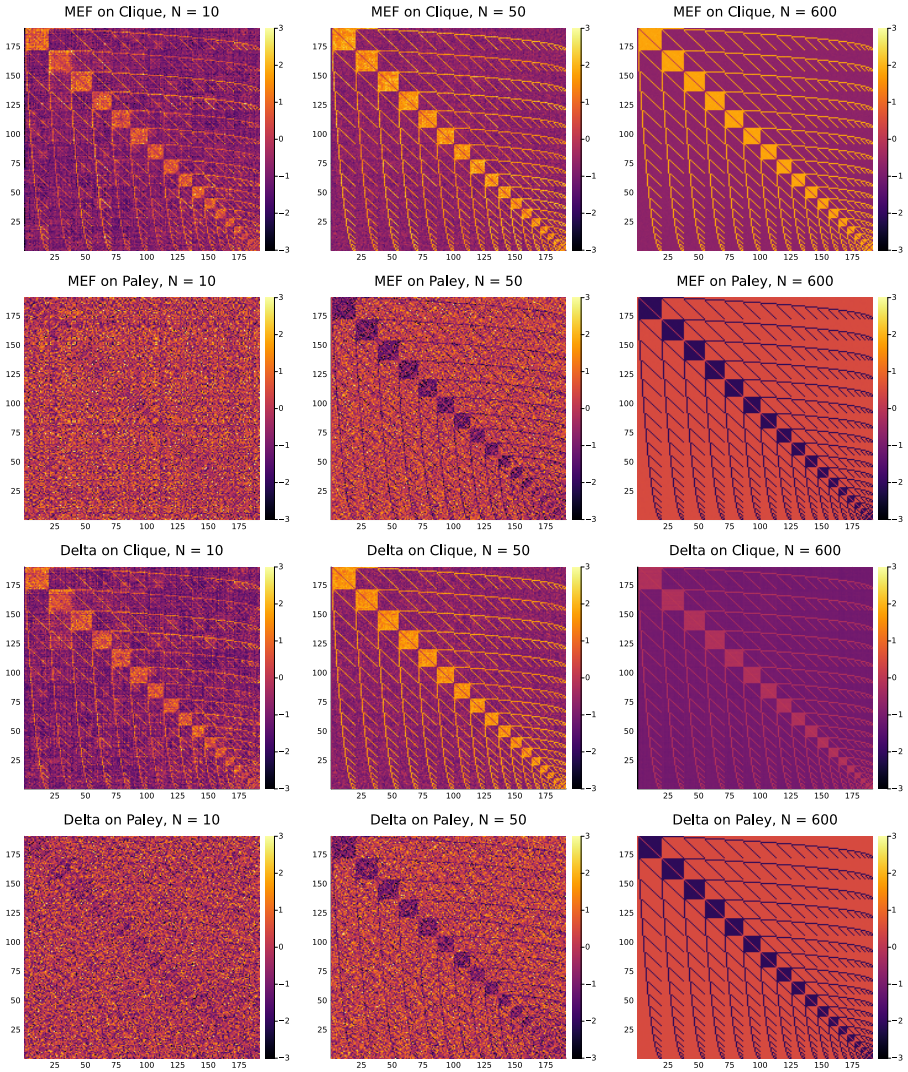

Figure 4: **Weights found by MEF and Delta on clique and Payley graph data while varying N:** networks where trained on samples from isomorphism class of 10-cliques and Payley graphs on $v = 20$ vertices with sample size ranging from 10 to 600.

C.2 HIDDEN CLIQUE PROBLEM

An equivalent interpretation of robust exponential memory Hillar & Tran (2018) in Hopfield networks is that of error-correcting codes Hillar et al. (2021). In particular, a network trained on sufficiently many cliques will not only generalize its memorization abilities to all cliques but will also have all cliques with non-trivial basins of attraction (e.g., 5% noise tolerance). For an example of this robust generalization, see Fig. 5, which plots over sample count both the generalization and denoising accuracy of HNs trained with MEF. These networks appear to learn to solve the Hidden Clique

Problem in computer science Dekel et al. (2014) with only a polynomial number of samples. Proving this observation rigorously will be the focus of future work.

C.3 Clique generalization in DAMs

We conducted experiments testing generalization performance in DAMs when presented with increasing numbers of cliques as training data. We used the architecture and algorithm described in Krotov & Hopfield (2016) for polynomial degrees 4 and 6 in the energy function. The results in Fig. 6 show that these networks have very different generalization behaviors depending on degree. In particular, in our experiments, they are not able to store all cliques when the degree is 4, and when they do for degree 6, it is when the training set contains nearly all cliques. Our preliminary investigations suggest that DAMs have challenges generalizing in the setting of cliques, but much more work is needed to understand their behavior.

C.4 The Hopfield Network Not Graph Isomorphic Check (HNNGIC)

Lemma 4.3 implies any isomorphism class of a graph can be stored in a Hopfield network. This prompts investigation into the potential for using Hopfield networks to check for graph isomorphisms,

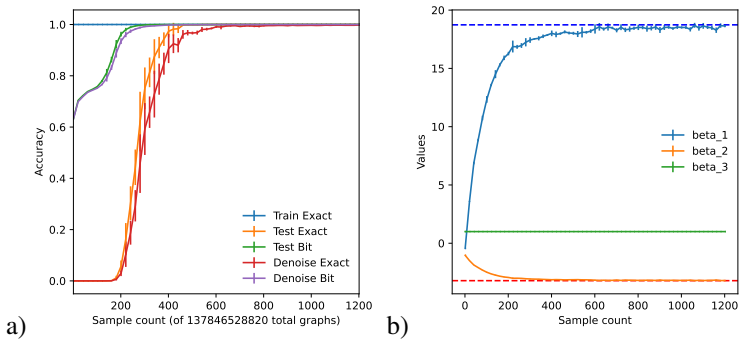

Figure 5: **Generalization solves the Hidden Clique Problem.** a) Generalization and denoising accuracy (exact / average bits) are plotted as a function of number of 20-clique samples (in 40-vertex graphs; $n = 780$) for MEF-trained HNs. Accuracy for generalization was computed using 10000 novel graphs as Test set. Denoising accuracy was computed by corrupting 5% bits in these 10000 and evaluating correctness of the attractor when dynamics is initialized at the noisy patterns (5 trials, standard deviation error bars). b) For each type of parameter (adjacent edges, non-adjacent, or thresholds), we plot their average over number of training samples (normalized so that thresholds are mean 1).

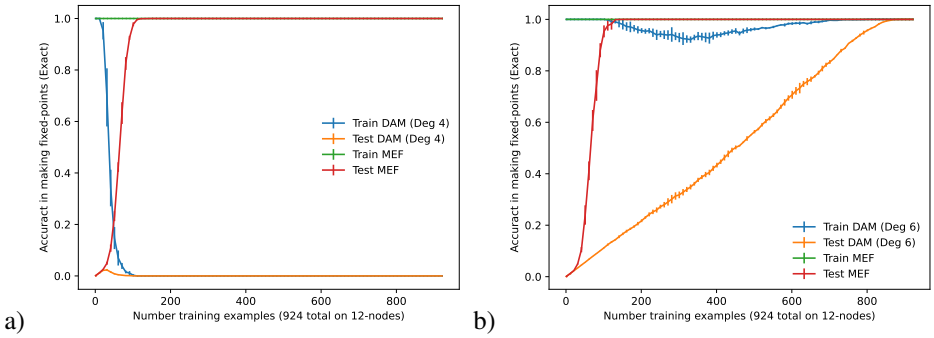

Figure 6: **DAM models trained on cliques.** We compare the generalization performance between DAMs of different degrees a) 4 and b) 6, and MEF-trained HNs for the 6-clique problem on graphs with $v = 12$ vertices. The Train (resp. Test) accuracy is the percentage of 6-clique training samples (resp. all 6-cliques) that are neural network attractors. Averaged over four trials, with standard deviation error bars.

a fundamental and important problem in computer science. To this end we propose Algorithm 1, which we refer to as the *Hopfield Network Not Graph Isomorphic Check* (HNNGIC). As the name suggests, this algorithm provides a check if two graphs are not graph isomorphic, returning true in certain cases when they are not graph isomorphic and unknown, otherwise.

Algorithm 1: Hopfield Network Not Graph Isomorphic Check (HNNGIC)

Input: two graphs $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \{0,1\}^n$ and computational budget B
Output: True or Unknown

Step 1: minimize $L(F(\boldsymbol{\beta}); \boldsymbol{x}_1)$ within computational budget B, return $\boldsymbol{\beta}^* \in \mathbb{R}^3$;
Step 2: **if** $H(\boldsymbol{x}_1; F(\boldsymbol{\beta}^*)) = \boldsymbol{x}_1$ **then**
  if $H(\boldsymbol{x}_2; F(\boldsymbol{\beta}^*)) \neq \boldsymbol{x}_2$ **then**
    return True
  end
else
  return Unknown
end

The idea behind this algorithm is simple: given two graphs, we pick one, i.e., $\boldsymbol{x}_1$, arbitrarily at random. We then attempt to train the Hopfield network by minimizing the energy flow defined on this single graph, but restrict the parameters to lie on the edge adjacency invariant subspace $\Psi(\mathcal{Q}_n)$. If the resulting invariant parameters $F(\boldsymbol{\beta}^*)$ strictly memorize $\boldsymbol{x}_1$ then this implies every point in the orbit of $\boldsymbol{x}_1$ under graph isomorphism is also strictly memorized. Therefore, if $\boldsymbol{x}_2$ is graph isomorphic to $\boldsymbol{x}_1$, then it must be a fixed point. As a result, $\boldsymbol{x}_2$ and $\boldsymbol{x}_1$ cannot be graph isomorphic if $\boldsymbol{x}_2$ is not a fixed point of an invariant Hopfield network which stores $\boldsymbol{x}_1$. Note, that if $\boldsymbol{x}_2$ is a fixed point, it does not follow that $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ are isomorphic. Indeed, there may be other fixed points, i.e., "spurious states", in the landscape, not related to the orbit of $\boldsymbol{x}_1$. Also note that Lemmas 4.3 and 4.1 imply that there is always a 3-parameter network storing any graph; in particular, given enough computation, we are guaranteed to find an approximation of $\boldsymbol{\beta}^*$ that is sufficient to store x_1.

Statement on the use of LLMs. Large language models (LLMs) were used to assist with literature search, checking and refining the clarity of writing, high level ideation and planning as well as organizing related work.