A Walsh Hadamard Derived Linear Vector Symbolic Architecture

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Abstract

Vector Symbolic Architectures (VSAs) are one approach to developing Neurosymbolic AI, where two vectors in \mathbb{R}^d are 'bound' together to produce a new vector in the same space. VSAs support the commutativity and associativity of this binding operation, along with an inverse operation, allowing one to construct symbolicstyle manipulations over real-valued vectors. Most VSAs were developed before deep learning and automatic differentiation became popular and instead focused on efficacy in hand-designed systems. In this work, we introduce the Hadamardderived linear Binding (HLB), which is designed to have favorable computational efficiency, and efficacy in classic VSA tasks, and perform well in differentiable systems. Code is available at https://github.com/FutureComputing4AI/ Hadamard-derived-Linear-Binding.

1 Introduction

Vector Symbolic Architectures (VSAs) are a unique approach to performing symbolic style AI. Such methods use a binding operation $\mathcal{B} : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}^d$, where $\mathcal{B}(x, y) = z$ denotes that two concepts/vectors x and y are connected to each other. In VSA, any arbitrary concept is assigned to vectors in \mathbb{R}^d (usually randomly). For example, the sentence "the fat cat and happy dog" would be represented as $\mathcal{B}(fat, cat) + \mathcal{B}(happy, dog) = S$. One can then ask, "what was happy" by *unbinding* the vector for happy, which will return a noisy version of the vector bound to happy. The unbinding operation is denoted $\mathcal{B}^*(x, y)$, and so applying $\mathcal{B}^*(S, happy) \approx dog$.

Because VSAs are applied over vectors, they offer an attractive platform for neuro-symbolic methods by having natural symbolic AI-style manipulations via differentiable operations. However, current VSA methods have largely been derived for classical AI tasks or cognitive science-inspired work. Many such VSAs have shown issues in numerical stability, computational complexity, or otherwise lower-than-desired performance in the context of a differentiable system.

As noted in [39], most VSAs can be viewed as a linear operation where $\mathcal{B}(a, b) = a^{\top}Gb$ and $\mathcal{B}^*(a, b) = a^{\top}Fb$, where G and F are $d \times d$ matrices. Hypothetically, these matrices could be learned via gradient descent, but would not necessarily maintain the neuro-symbolic properties of VSAs without additional constraints. Still, the framework is useful as all popular VSAs we are aware fit within this framework. By choosing G and F with specified structure, we can change the computational complexity from $\mathcal{O}(d^2)$, down to $\mathcal{O}(d)$ for a diagonal matrix.

In this work, we derive a new VSA that has multiple desirable properties for both classical VSA tasks, and in deep-learning applications. Our method will have only O(d) complexity for the binding step, is numerically stable, and equals or improves upon previous VSAs on multiple recent deep

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learning applications. Our new VSA is derived from the Walsh Hadamard transform, and so we term our method the Hadamard-derived linear Binding (HLB) as it will avoid the $O(d \log d)$ normally associated with the Hadamard transform, and has better performance than more expensive VSA alternatives.

Related work to our own will be reviewed in Appendix A, including our baseline VSAs and their definitions. Our new HLB will be derived in section 2, showing it theoretically desirable properties. section 3 will empirically evaluate HLB in classical VSA benchmark tasks, and in two recent deep learning tasks, showing improved performance in each scenario. We then conclude in section 4.

2 Methodology

In this section we review the Hadamard transform, its properties, and how we derive our new HLB via these properties. It follows a similar intuition to the original HRR [32], followed by a projection step as suggested by [10]. However, by choosing the Hadamard transform, we obtain a closed-form solution that requires only linear operations, making HLB fast to apply in practice. Hadamard H_d is a square matrix of size $d \times d$ of orthogonal rows consisting of only +1s and -1s given in Equation 1 where $d = 2^n \forall n \in \mathbb{N} : n \ge 0$.

$$H_1 = \begin{bmatrix} 1 \end{bmatrix} \qquad H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad \cdots \qquad H_{2^n} = \begin{bmatrix} H_{2^{n-1}} & H_{2^{n-1}} \\ H_{2^{n-1}} & -H_{2^{n-1}} \end{bmatrix}$$
(1)

Vector symbolic architectures (VSA), such as Holographic Reduced Representations (HRR) employs circular convolution to represent compositional structure which is computed using the Fast Fourier Transform (FFT) [32]. However, it can be numerically unstable due to irrational multiplications of complex numbers. Prior work [10] devised a projection step to mitigate the numerical instability of the FFT and it's inverse, but we instead ask if re-deriving the binding/unbinding operations may yield better results if we use the favorable properties of the Hadamard transform as given in Lemma 2.1.

Lemma 2.1 (Hadamard Properties). Let H be the Hadamard matrix of size $d \times d$ that holds the following properties for $x, y \in \mathbb{R}^d$. First, H(Hx) = dx, and second H(x + y) = Hx + Hy.

The bound composition of two vectors into a single vector space is referred to as BINDING (\mathcal{B}). The knowledge retrieval from a bound representation is known as UNBINDING (\mathcal{B}^*). We define the binding function by replacing the Fourier transform in circular convolution with the Hadamard transform given in Definition 2.1.

Definition 2.1 (Binding and Unbinding). The binding of vectors $x, y \in \mathbb{R}^d$ in the Hadamard domain is defined in Equation 2 where \odot is elementwise multiplication. The unbinding function is defined in a similar fashion, i.e., $\mathcal{B} = \mathcal{B}^*$.

$$\mathcal{B}(x,y) = \frac{1}{d} \cdot H(Hx \odot Hy) \tag{2}$$

Composite representation in vector symbolic architectures is defined by the summation of the bound vectors. We define a parameter $\rho \in \mathbb{N} : \rho \ge 1$ that denotes the number of vector pairs bundled in a composite representation. Given vectors $x_i, y_i \in \mathbb{R}^d$ and $\forall i \in \mathbb{N} : 1 \le i \le \rho$, we can define the composite representation χ as

$$\chi_{\rho=1} = \mathcal{B}(x_1, y_1) \qquad \chi_{\rho=2} = \mathcal{B}(x_1, y_1) + \mathcal{B}(x_2, y_2) \qquad \cdots \qquad \chi_{\rho} = \sum_{i=1}^{\rho} \mathcal{B}(x_i, y_i)$$
(3)

Next, we require the unbinding operation, which is defined via an inverse function in the following theorem. This will give a symbolic form of our unbinding step that retrieves the original component x being searched for, as well as a necessary noise component η° , which must exist whenever $\rho \ge 2$ items are bound together without expanding the dimension d.

Theorem 2.1 (Inverse Theorem). Given the identity function $Hx \cdot Hx^{\dagger} = 1$ where x^{\dagger} is the inverse of x in the Hadamard domain, then $\mathcal{B}^*(\mathcal{B}(x_1, y_1) + \dots + \mathcal{B}(x_{\rho}, y_{\rho}), y_i^{\dagger}) = \begin{cases} x_i & \text{if } \rho = 1 \\ x_i + \eta_i^{\circ} & \text{else } \rho > 1 \end{cases}$ where $x_i, y_i \in \mathbb{R}^d$ and η_i° is the noise component.

Proof of Theorem 2.1. We start from the identity function $Hx \cdot Hx^{\dagger} = 1$ and thus $Hx^{\dagger} = \frac{1}{Hx}$. Now using Equation 2 we get,

$$\begin{aligned} \mathcal{B}^*(\mathcal{B}(x_1, y_1) + \dots + \mathcal{B}(x_{\rho}, y_{\rho}), y_i^{\dagger}) &= \frac{1}{d} \cdot H((Hx_1 \odot Hy_1 + \dots + Hx_{\rho} \odot Hy_{\rho}) \odot \frac{1}{Hy_i}) \\ &= \frac{1}{d} \cdot H(Hx_i + \frac{1}{Hy_i} \odot \sum_{\substack{j=1\\j \neq i}}^{\rho} (Hx_j \odot Hy_j)) = x_i + \frac{1}{d} \cdot H(\frac{1}{Hy_i} \odot \sum_{\substack{j=1\\j \neq i}}^{\rho} (Hx_j \odot Hy_j)) \quad Lemma \ 2.1 \\ &= \begin{cases} x_i & \text{if } \rho = 1\\ x_i + \eta_i^{\circ} & \text{else } \rho > 1 \end{cases} \end{aligned}$$

 \square

To reduce the noise component and improve retrieval accuracy, [10, 32] proposes a projection step to the input vectors by normalizing them by the absolute value in the Fourier domain. While such identical normalization is not useful in the Hadamard domain since it will only transform the elements to +1s and -1s, we will define a projection step with only the Hadamard transformation without normalization given in Definition 2.2.

Definition 2.2 (Projection). The projection function of x is defined by $\pi(x) = \frac{1}{d} \cdot Hx$.

If we apply the Definition 2.2 to the inputs in Theorem 2.1 then we get

$$\mathcal{B}^*(\mathcal{B}(\pi(x_1),\pi(y_1)) + \dots + \mathcal{B}(\pi(x_{\rho}),\pi(y_{\rho})),\pi(y_i)^{\dagger}) = \mathcal{B}^*(\frac{1}{d} \cdot H(x_1 \odot y_1 + \dots + x_{\rho} \odot y_{\rho}),\frac{1}{y_i})$$
$$= \frac{1}{d} \cdot H(\frac{1}{y_i} \odot (x_1 \odot y_1 + \dots + x_{\rho} \odot y_{\rho}))$$
(4)

The retrieved value is projected onto the Hadamard domain, and to recover the original data we apply the reverse projection. Since the Hadamard matrix is its own inverse, in the reverse projection step we just apply the Hadamard transformation again which derives the output to

$$H(\frac{1}{d} \cdot H(\frac{1}{y_i} \odot (x_1 \odot y_1 + \dots + x_\rho \odot y_\rho))) = \frac{1}{y_i} \odot (x_1 \odot y_1 + \dots + x_\rho \odot y_\rho)$$

$$= \begin{cases} x_i & \text{if } \rho = 1\\ x_i + \sum_{j=1, \ j \neq i}^{\rho} \frac{x_j y_j}{y_i} & \text{else } \rho > 1 \end{cases} = \begin{cases} x_i & \text{if } \rho = 1\\ x_i + \eta_i^{\pi} & \text{else } \rho > 1 \end{cases}$$

$$(5)$$

where η_i^{π} is the noise component due to the projection step. In expectation, $\eta_i^{\pi} < \eta_i^{\circ}$ (see Appendix C). Thus, the projection step diminishes the accumulated noise. More interestingly, the retrieved output term does not contain any Hadamard matrix. Therefore, we can recast the initial binding definition by multiplying the query vector y_i to the output of Equation 5, i.e, the binding function becomes $\mathcal{B}'(x,y) = x \odot y$. ρ bundle of the vector pairs is $\chi'_{\rho} = \sum_{i=1}^{\rho} (x_i \odot y_i)$ and the unbinding would be $\mathcal{B}^{*'}(x,y) = x \odot \frac{1}{y}$.

2.1 Initialization of HLB

For binding and unbinding operations to work, vectors need an expected value of zero. However, dividing the bound vector by the query during unbinding can cause instability if values are too close to zero. Thus, we define a Mixture of Normal Distribution (MiND) with a zero expected value but a non-zero absolute mean, as given in Equation 6, where \mathcal{U} is the Uniform distribution. Half the elements are sampled from a normal distribution with mean $-\mu$, and the other half from a distribution with mean μ , yielding a vector with a zero mean and absolute mean of μ . The properties of the vectors sampled from a MiND distribution are given in Properties 2.1.

$$\Omega(\mu, 1/d) = \begin{cases} \mathcal{N}(-\mu, 1/d) & \text{if } \mathcal{U}(0, 1) > 0.5\\ \mathcal{N}(\mu, 1/d) & \text{else } \mathcal{U}(0, 1) \le 0.5 \end{cases}$$
(6)

Properties 2.1 (Initialization Properties). Let $x \in \mathbb{R}^d$ sampled from $\Omega(\mu, 1/d)$ holds the following properties. $\mathbb{E}[x] = 0$, $\mathbb{E}[|x|] = \mu$, and $||x||_2 = \sqrt{\mu^2 d}$

2.2 Similarity Augmentation

In VSAs, it is common to measure the similarity with an extracted embedding \hat{x} with some other vector x using the cosine similarity. For our HLB, we devise a correction term leveraging Theorem 2.2.

Theorem 2.2 ($\phi - \rho$ Relationship). Given $x_i, y_i \sim \Omega(\mu, 1/d) \forall i \in \mathbb{N} : 1 \leq i \leq \rho$, the cosine similarity ϕ between the original x_i and retrieved vector \hat{x}_i is approximately equal to the inverse square root of the number of vector pairs in a composite representation ρ given by $\phi \approx \frac{1}{\sqrt{\rho}}$.

The proof of the theorem is provided in Appendix B. The experimental result of the $\phi - \rho$ relationship closely follows the theoretical expectation provided in Appendix E which also indicates that the approximation is valid. We know from Theorem 2.2 that the similarity score ϕ drops by the inverse square root of the number of vector pairs in a composite representation ρ . Therefore, in places where ρ is known or can be estimated from $\|\chi_{\rho}\|_2 \approx \mu^2 \sqrt{\rho \cdot d}$ (proof in Appendix D), it can be used to update the cosine similarity multiplying the scores by $\sqrt{\rho}$. Equation 7 shows the updated similarity score where in a positive case (+), ϕ would be close to $1/\sqrt{\rho}$ and in a negative case (-), ϕ would be close to zero.

$$\phi' = \phi \times \sqrt{\rho} \qquad \phi'_{(+)} = \phi_{\rightarrow \frac{1}{\sqrt{\rho}}} \times \sqrt{\rho} \approx 1 \qquad \phi'_{(-)} = \phi_{\rightarrow 0} \times \sqrt{\rho} \quad \approx 0 \tag{7}$$

3 Empirical Results

3.1 Classical VSA Tasks

A common VSA task is, given a bundle (addition) of ρ pairs of bound vectors $\boldsymbol{s} = \sum_{i=1}^{\rho} \mathcal{B}(\boldsymbol{x}_i, \boldsymbol{y}_i)$, given a query $\boldsymbol{x}_q \in \boldsymbol{s}$, can the corresponding vector \boldsymbol{y}_q be correctly retrieved from the bundle. To test this, we perform an experiment similar to one in [37]. We first create a pool P of N = 1000 random vectors, then sample (with replacement) p pairs of vectors for $p \in \{1, 2, \dots, 25\}$. The pairs are bound together and added to create a composite representation \boldsymbol{s} . Then, we iterate through all left pairs \boldsymbol{x}_q in the composite representation and attempt to retrieve the corresponding $\boldsymbol{y}_q, \forall q \in [1, p]$. A retrieval is considered correct if $\mathcal{B}^*(\boldsymbol{s}, \boldsymbol{x}_q)^\top \boldsymbol{y}_q > \mathcal{B}^*(\boldsymbol{s}, \boldsymbol{x}_q)^\top \boldsymbol{y}_j, \forall j \neq q$. The total accuracy score for the bundle is recorded, and the experiment is repeated for 50 trials. Experiments are performed to compare HRR [32], VTB [13], MAP [11], and our HLB VSAs. For each VSA, the area under the curve (AUC) of the accuracy vs. the number of bound terms plot is computed, and the results are shown in Figure 5. In general, HLB has comparable performance to HRR and VTB, and performs better than MAP.

The scenario we just considered looked at bindings of only two items together, summed of many pairs of bindings. [13] proposed addition evaluations over sequential bindings that we now consider. In the *random* case we have an initial vector b_0 , and for p rounds, we will modify it by a random vector x_t such that $b_{t+1} = \mathcal{B}(b_t, x_t)$, after which we unbind each x_t to see how well the previous b_t is recovered. In the *auto binding* case, we use a single random vector x for all p rounds. Figure 6 shows that HLB maintains a stable magnitude regardless of the number of bound vectors in both cases. This property arises due to the properties of the distribution shown in Properties 2.1. As all components have an expected absolute value of 1, the product of all components also has an expected absolute value of 1. Thus, the norm of the binding is simply \sqrt{d} . Combined with Figure 1 that shows the scores are near-zero when an item is not present, HLB has significant advantages in consistency for designing VSA solutions.

3.2 Deep Learning with Hadamard-derived Linear Binding

Two recent methods that integrate HRR with deep learning are tested to further validate our approach. The details of each method are provided in Appendix G and Appendix H. In each case, we run all four VSAs and see that HLB either matches or exceeds the performance of other VSAs. In every experiment, the standard method of sampling vectors from each VSA is followed as outlined in Table 3. All the experiments are performed on a single NVIDIA TESLA PH402 GPU with 32GB memory.

3.2.1 Connectionist Symbolic Pseudo Secrets

Connectionist Symbolic Pseudo Secrets (CSPS) [3] is a pseudo-encryption method used to deploy convolutional networks on untrusted platforms by binding secrets to the inputs. More details are available in Appendix G. Experiments are performed with 5 datasets: MNIST, SVHN, CIFAR-10 (CR10), CIFAR-100 (CR100), and Mini-ImageNet (MIN). First, we look at the accuracy of each method, which is lower due to the noise of the random vector *s* added at test time since no secret VSA is ever reused. The results are shown in Table 1, where HLB outperforms all prior methods significantly. Notably, the MAP VSA is second best despite being one of the older VSAs, indicating its similarity to HLB in using a simple binding procedure, and thus simple gradient may be an important factor in this scenario.

Table 1: Accuracy comparison of the proposed HLB with HRR, VTB, MAP-C, and MAP-B in CSPS. The dimensions of the inputs along with the no. of classes are listed in the Dims/Labels column. The last row shows the geometric mean of the results.

DATASET	Dims/ Labels	CSPS + HRR		CSPS + VTB		CSPS + MAP-C		CSPS + MAP-B		CSPS + HLB	
		Top@1	Top@5	Top@1	Top@5	Top@1	Top@5	Top@1	Top@5	Top@1	Top@5
MNIST	$28^2/10$	98.51	_	98.44	_	98.46	_	98.40	_	98.73	_
SVHN	$32^{2}/10$	88.44	-	19.59	-	79.95	-	92.43	-	94.53	-
CR10	$32^{2}/10$	78.21	-	74.22	-	76.69	-	82.83	-	83.81	_
CR100	$32^2/100$	48.84	75.82	35.87	61.79	56.77	81.52	57.76	84.63	58.82	87.50
MIN	$84^{2}/100$	40.99	66.99	45.81	73.52	52.22	78.63	57.91	82.81	59.48	83.35
GM		67.14	71.26	47.24	67.40	70.89	80.06	75.90	83.72	77.17	85.40

However, improved accuracy is not useful in this scenario if more information is leaked. The test in this scenario, as proposed by [3], is to calculate the Adjusted Rand Index (ARI) after attempting to cluster the inputs \hat{x} and the outputs \hat{y} , which are available/visible to the snooping third-party. To be successful, the Adjusted Rand Index (ARI) must be near zero (indicating random label assignment) for both inputs and outputs. We use K-means, Gaussian Mixture Model (GMM), Birch [45], and HDBSCAN [8] as the clustering algorithms and specify the true number of classes to each method to maximize attacker success (information they would not know). The results can be found in Table 4, where the top rows indicate the clustering of the input $\mathcal{B}(x, s)$, and the bottom rows the clustering of the output \hat{y} . All the numbers are percentages (%), showing all methods do a good job at hiding information from the adversary (except on the MNIST dataset, which is routinely degenerate).

3.2.2 Xtreme Multi-Label Classification

Extreme Multi-label (XML) classification is a challenging task due to the large output space, which can be in the range of hundreds of thousands, contributing to the bulk of the size of a neural network. While many prior works focus on innovative strategies to cluster/make hierarchies/compress the penultimate layer [20, 21, 31, 19, 44, 23], a neuro-symbolic approach was proposed by [10]. Given K total possible classes, they assigned each class a vector c_k to be each class's representation, and the set of all classes $a = \sum_{k=1}^{K} c_k$. More details about the XML methodology is provided in Appendix H. The details and network sizes of [10] are followed, except we replace the original VSA with our four candidates. The network is trained on 8 datasets listed in Table 2 from [5] and evaluated using normalized discounted cumulative gain (nDCG) and propensity-scored (PS) based normalized discounted cumulative gain (PSnDCG) as suggested by [20].

The classification result in terms of nDCG and PSnDCG in all the eight datasets is presented in Table 2 where the top four datasets are comparatively easy with maximum no. of features of 5000 and no. of labels of 4000. The bottom four datasets are comparatively hard with the no. of features and labels on the scale of 100K. The proposed HLB has attained the best results in all the datasets on both metrics. In contrast to the prior CSPS results, here we see that the performance differences between HRR, VTB, and MAP are more varied, with no clear "second-place" performer.

DATASET	BIBTEX		DELICIOUS		Medi	AMILL	EURLEX-4K		
METRICS	nDCG	PSnDCG	nDCG	PSnDCG	nDCG	PSnDCG	nDCG	PSnDCG	
HRR VTB MAP-C MAP-B HLB	60.296 57.693 59.280 59.412 61.741	45.572 45.219 46.092 46.340 48.639	66.454 63.325 65.376 65.431 67.821	30.016 31.449 31.943 32.122 32.797	83.885 87.232 87.255 86.886 88.064	63.684 66.948 66.886 66.562 67.525	77.225 76.964 72.439 71.128 77.868	30.684 31.180 26.752 26.340 31.526	
DATASET	EURLE	EX-4.3K	WIKI1	0-31K	Amazo	on-13K	K DELICIOUS-20		
METRICS	nDCG	PSnDCG	nDCG	PSnDCG	nDCG	PSnDCG	nDCG	PSnDCG	
HRR VTB MAP-C MAP-B HLB	84.497 84.663 85.472 85.023 88 204	38.545 38.540 39.233 38.820 43.622	81.068 78.025 80.203 80.238 83.589	9.185 9.645 10.027 10.035 11 869	93.258 92.373 92.013 92.307 93.672	49.642 49.463 48.686 48.812 50 270	44.933 44.092 45.373 45.459 46.331	6.839 6.664 6.862 6.870 6.952	

Table 2: XML classification results in dense label representation with HRR, VTB, MAP, and HLB in terms of nDCG and PSnDCG. The proposed HLB has attained the best nDCG and PSnDCG scores on all the datasets setting a new SOTA.

4 Conclusion

In this paper, a novel linear vector symbolic architecture named HLB is presented derived from Hadamard transform. Along with an initialization condition named MiND distribution is proposed for which we proved the cosine similarity ϕ is approximately equal to the inverse square root of the no. of bundled vector pairs ρ which matches with the experimental results. The proposed HLB showed superior performance in classical VSA tasks and deep learning compared to other VSAs such as HRR, VTB, and MAP. In learning tasks, HLB is applied to CSPS and XML classification tasks. In both of the tasks, HLB has achieved the best results in terms of respective metrics in all the datasets showing a diverse potential of HLB in Neuro-symbolic AI.

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A Related Work

Smolensky [38] started the VSA approach with the Tensor Product Representation (TPR), where d dimensional vectors (each representing some concept) were bound by computing an outer product. Showing distributivity ($\mathcal{B}(x, y + z) = \mathcal{B}(x, y) + \mathcal{B}(x, z)$) and associativity, this allowed specifying logical statements/structures [14]. However, for ρ total items to be bound together, it was impractical due to the $\mathcal{O}(d^{\rho})$ complexity. [36, 26, 25] have surveyed many of the VSAs available today, but our work will focus on three specific alternatives, as outlined in Table 3. The Vector-Derived Transformation Binding (VTB) will be a primary comparison because it is one of the most recently developed VSAs, which has shown improvements in what we will call "classic" tasks, where the VSA's symbolic like properties are used to manually construct a series of binding/unbinding operations that accomplish a desired task. Note, that the VTB is unique in it is non-symmetric ($\mathcal{B}(x, y) \neq \mathcal{B}(y, x)$). Ours, and most others, are symmetric.

Table 3: The binding and initialization mechanisms for our new HLB with baseline methods. HLB is related to the HRR in being derived via a similar approach, but replacing the Fourier transform $\mathcal{F}(\cdot)$ with the Hadamard transform (which simplifies out). The MAP is most similar to our approach in mechanics, but the difference in derived unbinding steps leads to dramatically different performance. The VTB is the most recently developed VSA in modern use. The matrix V_y of VTB is a block-diagonal matrix composed from the values of the y vector, which we refer the reader to [13] for details. The TorchHD library [16] is used for implementations of prior methods.

Method	BIND $\mathcal{B}(x,y)$	Unbind $\mathcal{B}^*(x,y)$	INIT x
HRR	$\mathcal{F}^{-1}(\mathcal{F}(\boldsymbol{x}) \odot \mathcal{F}(\boldsymbol{y}))$	$\mathcal{F}^{-1}(\mathcal{F}(\boldsymbol{x}) \oplus \mathcal{F}(\boldsymbol{y}))$	$x_i \sim \mathcal{N}(0, 1/d)$
VTB	$V_y x$	$V_u^{\dagger} x$	$\tilde{x}_i \sim \mathcal{N}(0, 1) \rightarrow x = \tilde{x} / \ \tilde{x}\ _2$
MAP-C	$x \circ y$	$x \odot y$	$x_i \sim \mathcal{U}(-1, 1)$
MAP-B	$x \odot y$	$x \odot y$	$x_i \sim \{-1, 1\}$
HLB	$x \odot y$	$x \oplus y$	$x_u \sim \{\mathcal{N}(-\mu, 1/d), \ \mathcal{N}(\mu, 1/d)\}$

Next is the Holographic Reduced Representation (HRR) [32], which can be defined via the Fourier transform $\mathcal{F}(\cdot)$. One derives the inverse operation of the HRR by defining the one vector $\vec{1}$ as the identity vector and then solving $\mathcal{F}(a^*)_i \mathcal{F}(a)_i = 1$. We will use a similar approach to deriving HLB but replacing the Fourier Transform with the Hadamard transform, making the HRR a key baseline. Last, the Multiply Add Permute (MAP) [11] is derived by taking only the diagonal of the tensor product from [38]'s TPR. This results in a surprisingly simple representation of using element-wise multiplication for both binding/unbinding, making it a key baseline. The MAP binding is also notable for its continuous (MAP-C) and binary (MAP-B) forms, which will help elucidate the importance of the difference in our unbinding step compared to the initialization avoiding values near zero. HLB differs in devising for the unbinding step, and we will later show an additional corrective term that HLB employs for ρ different items bound together, that dramatically improve performance.

Our motivation for using the Hadamard Transform comes from its parallels to the Fourier Transform (FT) used to derive the HRR and the HRR's relatively high performance. The Hadamard matrix has a simple recursive structure, making analysis tractable, and its transpose is its own inverse, which simplifies the design of the inverse function \mathcal{B}^* . Like the FT, WHT can be computed in log-linear time, though in our case, the derivation results in linear complexity as an added benefit. The WHT is already associative and distributive, making less work to obtain the desired properties. Finally, the WHT involves only $\{-1, 1\}$ values, avoiding numerical instability that can occur with the HRR/FT. This work shows that these motivations are well founded, as they result in a binding with comparable or improved performance in our testing.

Our interest in VSAs comes from their utility in both classical symbolic tasks and as useful priors in designing deep learning systems. In classic tasks VSAs are popular for designing power-efficient systems from a finite set of operations [15, 24, 18, 30]. HRRs, in particular, have shown biologically plausible models of human cognition [22, 6, 40, 7] and solving cognitive science tasks [9]. In deep learning the TPR has inspired many prior works in natural language processing [34, 17, 35]. To wit, The HRR operation has seen the most use in differentiable systems [43, 41, 42, 27, 29, 33, 1, 2, 28]. To study our method, we select two recent works that make heavy use of the neuro-symbolic capabilities

of HRRs. First, an Extreme Multi-Label (XML) task that uses HRRs to represent an output space of tens to hundreds of thousands of classes C in a smaller dimension d < C [10], and an information privacy task that uses the HRR binding as a kind of "encrypt/decrypt" mechanism for heuristic security [4]. We will explain these methods in more detail in the experimental section.

B Similarity Augmentation Proof

Proof of Theorem 2.2. We start with the definition of cosine similarity and insert the value of \hat{x}_i . The step-by-step breakdown is shown in Equation 8.

$$\phi = \frac{\sum_{i=1, j \neq i}^{d} x_{i} \cdot \hat{x}_{i}}{\|x_{i}\|_{2} \cdot \|\hat{x}_{i}\|_{2}} = \frac{\sum_{i=1, j \neq i}^{d} x_{i} \cdot \left(x_{i} + \sum_{j=1, j \neq i}^{\rho} \frac{x_{j}y_{j}}{y_{i}}\right)}{\|x_{i}\|_{2} \cdot \|x_{i} + \sum_{j=1, j \neq i}^{\rho} \frac{x_{j}y_{j}}{y_{i}}\|_{2}} = \frac{\sum_{i=1, j \neq i}^{d} x_{i} \cdot \left(\sum_{j=1, j \neq i}^{\rho} \frac{x_{j}y_{j}}{y_{i}}\right)}{\|x_{i}\|_{2} \cdot \|x_{i} + \sum_{j=1, j \neq i}^{\rho} \frac{x_{j}y_{j}}{y_{i}}\|_{2}}$$
(8)

Employing Properties 2.1 we can derive that $||x_i||_2 = \sqrt{\sum x_i \cdot x_i} = \sqrt{\mu^2 d}$ and $||\frac{x_j y_j}{x_i}|| = \sqrt{\mu^2 d}$. Thus, the square of the $||x_i| + \sum_{i=1}^{p} \frac{x_j y_j}{||x_i||_2}$ can be expressed as

Thus, the square of the $||x_i + \sum_{j=1, j \neq i}^{\rho} \frac{x_j y_j}{y_i}||_2$ can be expressed as

$$= \|x_i\|_2^2 + \sum_{j=1, \ j\neq i}^{\rho} \left\|\frac{x_j y_j}{y_i}\right\|_2^2 + 2 \cdot \underbrace{\sum_{j=1, \ j\neq i}^d \frac{x_j y_j}{y_i}}_{\alpha} + \underbrace{\sum_{j=1, \ l\neq i}^d \sum_{l=1}^{\rho-1} \sum_{l=1 \atop l\neq j}^{\rho-1} \frac{x_j y_j}{y_i} \cdot \frac{x_l y_l}{y_i}}_{\beta} = \mu^2 d + (\rho - 1) \cdot \mu^2 d + 2\alpha + 2\beta = \rho \cdot \mu^2 d + 2\alpha + 2\beta$$
(9)

Therefore, using Equation 8 and Equation 9 we can write that

$$\mathbf{E}[\phi] = \frac{\mu^2 d + \alpha}{\sqrt{\mu^2 d} \cdot \sqrt{\rho \cdot \mu^2 d + 2\alpha + 2\beta}} \approx \frac{\mu^2 d}{\sqrt{\mu^2 d} \cdot \sqrt{\rho \cdot \mu^2 d}} = \frac{\mu^2 d}{\sqrt{\rho} \cdot \mu^2 d} = \frac{1}{\sqrt{\rho}} \qquad \Box$$



Figure 1: Empirical comparison of the corrected cosine similarity scores between $\phi'_{(+)}$ (on top) and $\phi'_{(-)}$ (on bottom) for varying n and ρ shown in heatmap. The dimension, i.e., $d = 2^n$ is varied from 2 to 1024 ($n \in \{1, 2, \dots, 10\}$) and the number of vector pairs bundled is varied from 1 to 50. This shows that we can accurately identify when a vector \boldsymbol{x} has been bound to a VSA or not when we keep track of how many pairs of terms ρ are included.

Empirical results of ϕ' for varying n and ρ are visualized and verified by a heatmap. In a composite representation $\chi'_{\rho} = \sum_{i=1}^{\rho} (x_i \odot y_i)$, when unbinding is applied using the query y_i , i.e., $\mathcal{B}^{*'}(\chi'_{\rho}, y_i) =$

¹Here, α and β are the noise terms and in expectation $E[\alpha] \approx 0$ and $E[\beta] \approx 0$.

 \hat{x}_i , a positive case is a similarity between x_i and \hat{x}_i . On the contrary, similarity between \hat{x}_i and any x_j where $j \in \{1, 2, \dots, \rho\}$ and $j \neq i$, is a negative case. Mean cosine similarity scores of 100 trials for both positive and negative cases in presented in Figure 1 where the scores for the positive cases are in the red (≈ 1) shades and the scores for the negative cases are in the blue (≈ 0) shades.

C Noise Decomposition

When a single vector pair is combined, one of the vector pairs can be exactly retrieved with the help of the other component and the inverse function, recalling the retrieved output does not contain any noise component for a single pair of vectors, i.e., $\rho = 1$. However, when more than one vector pairs are bundled, noise starts to accumulate. In this section, we will uncover the noise components accumulated with and without the projection to the inputs and analyze their impact on expectation. We first start with the noise component without the projection step η_i° .

$$\eta_i^\circ = \frac{1}{d} \cdot H(\frac{1}{Hy_i} \odot \sum_{\substack{j=1\\j \neq i}}^{\rho} (Hx_j \odot Hy_j)$$
(10)

Let, set the value of n to be 1 thus, $d = 2^n = 2$ and the number of vector pairs $\rho = 2$, i.e., $\chi_{\rho=2} = \mathcal{B}(x_1, y_1) + \mathcal{B}(x_2, y_2)$. We want to retrieve x_1 using the query y_1 , thereby, the expression of η_i° is uncovered step by step for $\rho = 2$ shown in Equation 11.

$$\begin{split} \eta_{i}^{\circ} &= \frac{1}{d} \cdot H(\frac{1}{Hy_{1}} \odot (Hx_{2} \odot Hy_{2})) \\ &= \frac{1}{d} \cdot \sqrt{d} \cdot H\left(\frac{\frac{1}{y_{1}^{(0)} + y_{1}^{(1)}}}{y_{1}^{(0)} - y_{1}^{(1)}} \odot (x_{2}^{(0)} + x_{2}^{(1)}) \cdot (y_{2}^{(0)} + y_{2}^{(1)})}{(x_{2}^{(0)} - x_{2}^{(1)}) \cdot (y_{2}^{(0)} - y_{2}^{(1)})}\right) \\ &= \frac{1}{d} \cdot d \cdot \left(\frac{\frac{(x_{2}^{(0)} + x_{2}^{(1)})(y_{2}^{(0)} + y_{2}^{(1)})(y_{1}^{(0)} - y_{1}^{(1)}) + (x_{2}^{(0)} - x_{2}^{(1)})(y_{2}^{(0)} - y_{2}^{(1)})(y_{2}^{(0)} - y_{$$

Here, $\varphi_k \forall k \in \mathbb{N} : 1 \leq k \leq d$ are the polynomials comprises of (x_2, y_2) , and the query vector y_1 . \mathcal{P} is the vector of polynomials consisting of φ_k . From the noise expression, we can observe that the numerator is a polynomial and the denominator is the product of all the elements of the Hadamard transformation of the query vector. This is true for any value of n and ρ . Thus, in general, for any query y_i we can express η_i° as shown in Equation 12.

$$\eta_i^{\circ} = \frac{\stackrel{\rho}{\mathcal{P}}_{j=1, \ j \neq i}(x_j, y_j, y_i)}{\prod_{k=1}^d (Hy_i)_k}$$
(12)

The noise accumulated after applying the projection to the inputs is quite straightforward as given in Equation 13.

$$\eta_i^{\pi} = \frac{\sum_{j=1, \ j \neq i}^{\rho} (x_j \odot y_j)}{y_i}$$
(13)

Although the vectors $x_i, y_i \forall i \in \mathbb{N} : 1 \le i \le \rho$ are sampled from a MiND with an expected value of 0 given in Equation 6, the sample mean of x_i or y_i would be $\hat{\mu} \approx 0$ but $\hat{\mu} \neq 0$. Both the numerator of η_i° and η_i^{π} are the polynomials thus the expected value would be very close to 0. However, the expected value of the denominator of η_i° would be $\mathbb{E}[\prod_{k=1}^d (Hy_i)_k] = \prod_{k=1}^d \mathbb{E}[(Hy_i)_k] = \hat{\mu}^d$ whereas the expected value of the denominator of η_i^{π} is $\mathbb{E}[y_i] = \hat{\mu}$. Since, $\hat{\mu}^d < \hat{\mu}$, hence, in expectation $\eta_i^{\pi} < \eta_i^{\circ}$. This is also verified by an empirical study where n, i.e., the dimension $d = 2^n$ is varied along with the no. of bound vector pairs ρ and the amount of absolute mean noise in retrieval is estimated.

Figure 2 shows the heatmap visualization of the noise for both η_i° and η_i^π in natural log scale. The amount of noise accumulated without any projection to the inputs is much higher compared to the noise accumulation with the projection. For varying n and ρ , the maximum amount of noise accumulated when projection is applied is 7.18 and without any projection, the maximum amount of noise is 19.38. Also, most of the heatmap of η_i^π remains in the blue region whereas as n and ρ increase, the heatmap of η_i° moves towards the red region. Therefore, it is evident that the projection to the inputs diminishes the amount of accumulated noise with the retrieved output.



Figure 2: Heatmap of the empirical comparison of the noise components η_i° and η_i^{π} for varying n and ρ shown in natural logarithm scale. The dimension, i.e., $d = 2^n$ is varied from 2 to 1024 $(n \in \{1, 2, \dots, 10\})$ and the number of vector pairs bundled is varied from 2 to 50.

D Norm Relation

Theorem D.1 ($\chi_{\rho} - \rho$ Relationship). Given $x_i, y_i \sim \Omega(\mu, 1/d) \in \mathbb{R}^d \ \forall \ i \in \mathbb{N} : 1 \leq i \leq \rho$, the norm of the composite representation χ_{ρ} is proportional to $\sqrt{\rho}$ and approximately equal to the $\mu^2 \sqrt{\rho \cdot d}$.

Proof of Theorem D.1. Given χ_{ρ} is the composite representation of the bound vectors, i.e., the summation of ρ no. of individual bound terms. First, let's compute the norm of the single bound term as shown in Equation 14.

$$\begin{aligned} \|\mathcal{B}(x_{i}, y_{i})\|_{2} &= \|x_{i} \cdot y_{i}\|_{2} \\ &= \sqrt{(x_{i}^{(1)}y_{i}^{(1)})^{2} + (x_{i}^{(2)}y_{i}^{(2)})^{2} + \dots + (x_{i}^{(d)}y_{i}^{(d)})^{2}} \\ &= \sqrt{(\pm\mu^{2})^{2} + (\pm\mu^{2})^{2} + \dots + (\pm\mu^{2})^{2}} \quad \left[E[x^{(1)}] \cdot E[y^{(1)}] = \pm\mu \cdot \pm\mu = \pm\mu^{2}\right] \\ &= \sqrt{\mu^{4}d} \end{aligned}$$

$$(14)$$

Now, let's expand and compute the square norm of the composite representation given in Equation 15.

$$\begin{aligned} \|\chi_{\rho}\|_{2}^{2} &= \|\mathcal{B}(x_{1}, y_{1}) + \mathcal{B}(x_{2}, y_{2}) + \dots + \mathcal{B}(x_{\rho}, y_{\rho})\|_{2}^{2} \\ &= \|\mathcal{B}(x_{1}, y_{1})\|_{2}^{2} + \|\mathcal{B}(x_{2}, y_{2})\|_{2}^{2} + \dots + \|\mathcal{B}(x_{\rho}, y_{\rho})\|_{2}^{2} + \xi \\ \text{where } \xi \text{ is the rest of the terms of square expansion.} \\ &= \mu^{4}d + \mu^{4}d + \dots + \mu^{4}d + \xi \\ &= \rho \cdot \mu^{4}d + \xi \\ &= \rho \cdot \mu^{4}d + \xi \\ \|\chi_{\rho}\|_{2} &= \sqrt{\rho \cdot \mu^{4}d} + \xi \\ &\approx \sqrt{\rho \cdot \mu^{4}d} \quad [\xi \text{ is the noise term and discarded to make an approximation }] \\ &= \mu^{2}\sqrt{\rho \cdot d} \quad \Box \end{aligned}$$
(15)

Thus, given the composite representation and the mean of the MiND distribution, we can estimate the no. of bound terms bundled together by $\rho \approx \|\chi_{\rho}\|_2^2 / \mu^4 d$.

Figure 3 shows the comparison between the theoretical relationship and actual experimental results where the norm of the composite representation is computed for $\mu = 0.5$ and $\rho = \{1, 2, \dots, 200\}$. The figure indicates that the theoretical relationship aligns with the experimental results. However, as the no. of bundled pair increases, the variation in the norm increases. This is because of making the approximation by discarding ξ in Equation 15.



Figure 3: Comparison between the theoretical and experimental relationship of Theorem D.1. The norm of the composite representation of the bound vectors is computed for no. of bundled vectors from 1 to 200 of dimension d = 1024. The figure shows how the experimental value of the norm closely follows the theoretical relation between $\|\chi_{\rho}\|_2$ and ρ .

E Cosine Relation

Theorem 2.2 shows how the cosine similarity ϕ between the original x_i and retrieved vector \hat{x}_i is approximately equal to the inverse square root of the number of vector pairs in a composite representation ρ . In this section, we will perform an empirical analysis of the theorem and compare it with the theoretical results. For $\rho = \{1, 2, \dots, 50\}$, similarity score ϕ is calculated for vector dimension d = 512. Additionally, the theoretical cosine similarity score is also calculated using the value of ϕ following the theorem. Figure 4 shows the comparison between the two results where the experimental result closely follows the theoretical result. The figure also shows the standard deviation for 100 trials indicating a minute change from the actual value.



Figure 4: Comparison between the theoretical and experimental $\phi - \rho$ relationship. Vectors of dimension d = 512 are combined and retrieved with a varied number of vectors from 1 to 50. The zoom portion shows how closely experimental results match with the theoretical conclusion.

F Classical VSA Results



Figure 5: The area under the accuracy curve due to the change of no. of bundled pairs ρ for dimensions d. All the dimensions are chosen to be perfect squares due to the constraint of VTB.



Figure 6: When repeatedly binding different random (left) or a single vector (right), HLB consistently returns the ideal similarity score of 1 for a present item (top row) and has a constant magnitude (bottom row), avoiding exploding/vanishing values.

G CSPS Details and Results

Deploying deep learning networks on a remote third-party compute environment is quite common for training and inference purposes due to the need of large computing demand. However, if the remote third party is not trusted, a user may want to obfuscate the data and the model to prevent theft. Since provable Homomorphic Encryption is too expensive [12], Connectionist Symbolic Pseudo Secrets (CSPS) [3] was proposed a fast, heuristic, pseudo-encryption. It mimics a "one-time-pad" by taking a random VSA vector s as the *secret* and binding it to the input x. The value $\mathcal{B}(s, x)$ obscures the original x, and the third-party runs the bulk of the network on their platform. A result \tilde{y} is returned, and a small local network computes the final answer after unbinding with the secret $\mathcal{B}^*(\tilde{y}, s)$. Other than changing the VSA used, we follow the same training, testing, architecture size, and validation procedure of [3].

Table 4: Clustering results of the main network inputs (top rows) and outputs (bottom rows) in terms of Adjusted Rand Index (ARI). Because CSPS is trying to hide information, scores near zero are better. Cell color corresponds to the cell absolute value, with blue indicating lower ARI and red indicating higher ARI. All numbers in percentages, and show HLB is better at information hiding.

0 0				1	0						C
CLUSTERING		VTB					-				
METHODS	MNIST	SVHN	CR10	CR100	MIN	MNIST	SVHN	CR10	CR100	MIN	-
K-MEANS	-0.02	-0.01	0.18	0.54	0.42	-0.00	-0.01	-0.01	0.02	0.00	
GMM	0.01	0.00	0.09	0.61	0.44	4.67	1.37	-0.01	0.02	0.01	
BIRCH	0.20	0.00	0.14	0.45	0.35	0.02	0.03	0.04	0.08	0.03	
HDBSCAN	0.00	-0.24	1.23	0.01	0.02	0.00	0.00	0.00	0.00	0.00	
K-MEANS	1.28	0.06	0.21	0.03	0.08	8.52	0.13	1.11	0.05	0.12	
GMM	1.28	0.06	0.17	0.04	0.09	8.63	0.14	1.63	0.05	0.00	
BIRCH	1.51	0.03	0.13	0.05	0.07	3.24	0.00	0.64	0.06	0.17	
HDBSCAN	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00	
CLUSTERING				HLB							
METHODS	MNIST	SVHN	CR10	CR100	MIN	MNIST	SVHN	CR10	CR100	MIN	-
K-MEANS	0.17	0.01	0.01	0.00	0.00	0.09	0.00	0.00	0.00	0.00	
GMM	3.39	-0.01	0.01	0.00	0.00	2.53	0.00	0.00	0.00	0.00	
BIRCH	0.84	-0.00	0.00	0.01	0.00	0.83	0.00	0.00	0.01	0.00	
HDBSCAN	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
K-MEANS	15.91	0.09	0.00	0.03	0.01	13.67	-0.04	0.01	0.02	-0.00	
GMM	42.43	0.11	0.00	0.03	0.00	14.96	-0.04	0.01	0.02	0.00	
Birch	7.09	-0.07	-0.02	0.01	-0.00	18.44	-0.07	0.00	0.01	0.02	
HDBSCAN	0.48	0.00	0.00	0.00	0.00	7.60	0.01	0.00	0.00	0.00	

H XML Details

Extreme Multi Label (XML) classification is possible when only a small subset of classes exist for a given input \boldsymbol{x} . The VSA trick used by [10] was to define an additional "present" class \boldsymbol{p} and a "missing" class \boldsymbol{m} . Then the target output of the network $f(\cdot)$ is itself a vector composed of two parts added together. First $\mathcal{B}(\boldsymbol{p}, \sum_k \boldsymbol{c}_k)$ represents all *present* classes, and so the sum is over a finite smaller set. Then the absent classes compute the *missing* representing $\mathcal{B}(\boldsymbol{m}, \boldsymbol{a} - \sum_k \boldsymbol{c}_k)$, which again only needs to compute over the finite set of present classes, yet represents the set of all non-present classes by exploiting the symbolic properties of the VSA.

For XML classification, we have a set of K classes that will be present for a given input, where $K \approx 10$ is the norm. Yet, there will be L total possible classes where $L \ge 100,000$ is quite common. Forming a normal linear layer to produce L outputs is the majority of computational work and memory use in standard XML models, and thus the target for reduction. A VSA can be used to side-step this cost, as shown by [10], by leveraging the symbolic manipulation of the outputs. First, consider the target label as a vector $s \in \mathbb{R}^d$ such that $d \ll L$. By defining a VSA vector to represent "present" and "missing" classes as \mathbf{p} and \mathbf{m} , where each class is given its own vector $c_{1,...,L}$, we can shift the computational complexity form $\mathcal{O}(L)$ to $\mathcal{O}(K)$ by manipulating the "missing" classes as the compliment of the present classes as shown in Equation 16.

$$\boldsymbol{s} = \underbrace{\sum_{i \in y_i = 1}^{\text{Labels Present}\mathcal{O}(dK)}}_{i \in y_i = 1} + \underbrace{\sum_{j \in y_j = -1}^{\text{Labels Absent}\mathcal{O}(dL)}}_{j \in y_j = -1} = \underbrace{\mathcal{B}\left(\boldsymbol{p}, \left(\boldsymbol{a} = \sum_{i \in y_i = 1}^{\text{Labels Present}\mathcal{O}(dK)}\right) + \underbrace{\mathcal{B}\left(\boldsymbol{m}, \left(\boldsymbol{a} - \sum_{i \in y_i = 1}^{\text{Labels Absent}\mathcal{O}(dK)}\right)\right)}_{(16)}$$

Similarly, the loss to calculate the gradient can be computed based on the network's prediction \hat{s} by taking the cosine similarity between each expected class and one cosine similarity for the representation of all missing classes. The excepted response of 1 or 0 for an item being present/absent from the VSA is used to determine if we want the similarity to be 0 (1-cos) or 1 (just cos), as shown in Equation 17.

$$loss = \underbrace{\sum_{i \in y_i = 1}^{\text{Present Classes } \mathcal{O}(d \ K)}}_{i \in y_i = 1} (1 - \cos\left(\mathcal{B}^*(\boldsymbol{p}, \hat{\boldsymbol{s}}), \boldsymbol{c}_i\right))} + \underbrace{\cos\left(\mathcal{B}^*(\boldsymbol{m}, \hat{\boldsymbol{s}}), \sum_{i \in y_i = 1} \boldsymbol{c}_i\right)}^{\text{Absent classes } \mathcal{O}(d \ K)}$$
(17)