Optimal Quadratic Binding for Relational Reasoning in Vector Symbolic Neural Architectures

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Binding operation is fundamental to many cognitive processes, such as cognitive map formation, relational reasoning, and language comprehension. In these processes, two different modalities, such as location and objects, events and their contextual cues, and words and their roles, need to be bound together, but little is known about the underlying neural mechanisms. Previous work has introduced a binding model based on quadratic functions of bound pairs, followed by vector summation of multiple pairs. Based on this framework, we address the following questions: Which classes of quadratic matrices are optimal for decoding relational structures? And what is the resultant accuracy? We introduce a new class of binding matrices based on a matrix representation of octonion algebra, an eight-dimensional extension of complex numbers. We show that these matrices enable a more accurate unbinding than previously known methods when a small number of pairs are present. Moreover, numerical optimization of a binding operator converges to this octonion binding. We also show that when there are a large number of bound pairs, however, a random quadratic binding performs, as well as the octonion and previously proposed binding methods. This study thus provides new insight into potential neural mechanisms of binding operations in the brain.

1 Introduction

In many cognitive tasks, the brain has to construct a compositional representation by binding various properties of things like objects, events, or words. However, little is known about how the brain solves this binding...
Figure 1: Schematics of the binding problem. (A) A scene with three objects: pink cube (left), green pyramid (middle), and red cylinder (right). (B) Representation of the scene in VSA (vector symbolic architecture). Vector representation of objects \((a)\) and their positions \((b)\) are combined into a compositional representation of the entire scene \((c)\).

Problem (Feldman, 2013). For example, the scene depicted in Figure 1A is decomposed into a set of object-location pairs as

\[
\text{[scene]} = \{(\text{pink-cube}, \text{left}), (\text{green-pyramid}, \text{middle}), (\text{red-cylinder}, \text{right})\}. \tag{1.1}
\]

This compositional representation of the object-location pairs is crucial for scene understanding. For instance, by having this representation in your working memory, you can answer questions like, “What is the left-most object?” (answer: pink cube), and “What is the position of the red cylinder?” (answer: right) from your memory. However, it remains elusive how the brain binds neural representations of objects and locations and creates a compositional representation. Similarly, in the context of natural language processing, a sentence is interpreted as a set of word-position pairs:

\[
\text{["Man bites dog"]} = \{(\text{"man,"}, 1), (\text{"bites,"}, 2), (\text{"dog,"}, 3)\}. \tag{1.2}
\]

Here, the syntactic position information paired with the words differentiate the sentence “man bites dog” from “dog bites man,” implying that the binding of words and their syntactic positions is essential for language processing (Jackendoff, 2002). Similar compositional representations are also suggested to be essential for relational inference, object-based navigation, and episodic memory formation (Eliasmith et al., 2012; Whittington et al., 2020). Moreover, the binding problem is also an important topic in machine learning literature (Greff, van Steenkiste, & Schmidhuber, 2020), particularly in knowledge graph construction (Socher, Chen, Manning, & Ng, 2013; Nickel, Rosasco, & Poggio, 2016; Ma, Hildebrandt, Tresp, & Baier, 2018) and relational reasoning (Johnson et al., 2017; Santoro et al., 2017).

Mathematically speaking, this is a problem of vector representation construction. Let us consider a vector representation of a set of pairs...
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$S = \{(a_\mu, b_\mu)\}_{\mu=1}^L$, where $L$ is the number of the pairs and $a$ and $b$ are $N$-dimensional vectors. For instance, in the case of the scene recognition depicted in Figure 1A, $a_1$ is a vector representation of “pink cube,” while $b_1$ is a representation of the position “left,” and so on (see Figure 1B). In the brain, the number of neurons recruited for a representation of an object or its position is expectedly large, whereas previous human studies indicate that the number of pairs, $L$, the brain can hold in short-term memory is fewer than 10 (Miller, 1956; Cowan, 2001). Therefore, we will mainly focus on the parameter regime where $1 \lesssim L \ll N$ is satisfied.

Previous work has proposed vector symbolic architecture (VSA) as a biological-plausible solution for the binding problem (Smolensky, 1990; Plate, 1995; Gayler, 2003; Kanerva, 2009). In particular, VSA is capable of instantaneous construction of compositional structures essential for linguistic processing (Gayler, 2003). In the VSA framework, a vector representation of a set $S = \{(a_\mu, b_\mu)\}_{\mu=1}^L$ is constructed by

$$c_\mu = \psi(a_\mu, b_\mu) : \text{binding},$$

$$c = \sum_{\mu=1}^L c_\mu : \text{bundling},$$

where $c$ is a $N_c$-dimensional vector and $\psi$ is a nonlinear mapping $\psi : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}^{N_c}$. This means that we first create a representation of a pair $(a_\mu, b_\mu)$ by a nonlinear mapping $\psi(a_\mu, b_\mu)$, then generate a representation of the set $S$ by summing up the representation of the pairs (see Figure 1B). By constructing a representation of a set by taking the sum over pairs, the length of vector $c$ stays constant regardless of the cardinality of the set $L$. This is a desirable property when we consider population coding by a fixed number of neurons. However, it also causes interference between different pairs, as we will see.

In this article we study how we should choose the binding operator $\psi$. The answer depends on the objective, but it is often desirable for $c$ to maximize the unbinding performance. In other words, we should be able to retrieve $a_\mu$ from $c$ using $b_\mu$ as a query, and vice versa. In our example (see Figure 1A), representation of the scene, $c$, should enable us to answer a question like, “What is the left-most object?” (answer: pink cube) or “What is the position of the red cylinder?” (answer: right).

Previous work introduced two popular binding mechanisms for VSA architecture, the tensor product representation (Smolensky, 1990) and the holographic reduced representation (HRR; Plate, 1995), among others (Kanerva, 1997; Rachkovskij & Kussul, 2001; Gallant & Okaywe, 2013; Gosmann & Eliasmith, 2019; Frady, Kleyko, & Sommer, 2021). The tensor product representation enables an accurate representation of bound vectors, but it requires $N_c = N^2$ neurons for representing a composition. On the other hand,
HRR compresses the tensor product representation via circular convolution; thus, the size of composition \( c \) remains the same with its elements \( a, b \) (i.e., \( N_c = N \); see appendixes C.2 and C.1 for the details of the two binding methods). However, HRR representation is noisy due to this compression. Though their properties have been studied previously (Plate, 1997; Schlegel, Neubert, & Protzel, 2021; Steinberg & Sompolinsky, 2022), it remains elusive if HRR and the tensor product representation are the optimal binding under \( N_c = N \) and \( N_c = N^2 \), respectively. Moreover, little is known on how we should construct a binding operator under various composition sizes \( N_c \) and how the minimum achievable error scales with the number of bound pairs \( L \). We address these questions under a quadratic parameterization of the binding operators. We found that at \( L \sim O(1) \), there is a novel binding algorithm based on a matrix representation of the octonion algebra that significantly outperforms HRR and its extension. We also show that when \( L \gg 1 \) and \( N_c \ll N^2 \), there is no quadratic binding method that significantly outperforms a random binding method.

2 Quadratic Binding

Here, we introduce a specific class of binding operators that has a quadratic form. More specifically, using an \( N \times N \times N_c \) tensor \( P \), we define the \( k \)th element of a representation of set \( S = \{ (a_\mu, b_\mu) \}_{\mu=1}^L \) as

\[
c_k = \sum_{\mu=1}^L \sum_{i=1}^N \sum_{j=1}^N P_{ijk} a_\mu^i b_\mu^j,
\]

for \( k = 1, \ldots, N_c \), where \( a_\mu^i \) is the \( i \)th element of vector \( a_\mu \). There are several motivations for why we consider this quadratic parameterization. First, assuming that the norm of the vectors is constant (\( ||a||^2 = ||b||^2 = N \)), many previously proposed binding operators, such as HRR and the tensor product representation, are written as examples of quadratic binding. For instance, if we set \( P_{ijk} = \delta_{[i+j]N,k} \) with \( [i+j]N \equiv i+j \) (mod. \( N \)), we recover HRR, \( c_k = \sum_{\mu} \sum_i a_\mu^i b_\mu^{[k+j]} \) (see Frady et al., 2021, and appendix C.1). Moreover, when \( a \) and \( b \) are random gaussian variables, the quadratic parameterization should be enough to capture the statistical relationship between \( a \) and \( b \). Third, this formulation is simple enough to be biologically plausible, though the biological substrates for the multiplication are not yet fully understood.

From this vector representation \( c \), we consider unbinding of a vector using its bound pair as a query. For example, to answer the question, “What is the left-most object?” from a vector representation of the scene depicted in Figure 1A, we need to unbind “pink cube” from representation \( c \) by using
the position “left” as a query. Here, we also restrict this unbinding operation onto a quadratic form. Unbinding of $a_1$ with a query $b_1$ is defined by

$$\hat{a}_1^i = \sum_{j=1}^{N} \sum_{k=1}^{N_c} Q_{ijk} b_1^j c_k,$$  \hspace{1cm} (2.2)

where $Q$ is an $N \times N \times N_c$ tensor. Similarly, using an $N \times N \times N_c$ tensor $R$, unbinding of $b_1$ with $a_1$ is defined by

$$\hat{b}_1^j = \sum_{i=1}^{N} \sum_{k=1}^{N_c} R_{ijk} a_1^i c_k.$$  \hspace{1cm} (2.3)

Our objective is to find a set of tensors $P, Q, R$ that achieves the best unbinding performance. Using the mean-squared error as the loss, we define the unbinding error of $a_1$ and $b_1$ as

$$\ell_a (P, Q) \equiv \frac{1}{N} \langle \| a_1 - \hat{a}_1 \|^2 \rangle_{p(S)}$$  \hspace{1cm} (2.4)

and

$$\ell_b (P, R) \equiv \frac{1}{N} \langle \| b_1 - \hat{b}_1 \|^2 \rangle_{p(S)}.$$  \hspace{1cm} (2.5)

We consider the case when $a$ and $b$ are sampled from an independent and identically distributed (i.i.d.) gaussian distribution $N(0, I_N)$. This assumption is introduced partially for analytical tractability, but we would also expect the input vectors $a$ and $b$ to be whitened in the preprocessing.

Inserting equations 2.1 and 2.2 into the loss $\ell_a$, equation 2.4, we get

$$\ell_a = \frac{1}{N} \left( \sum_{i=1}^{N} \left( a_1^i - \sum_{\mu=1}^{L} \sum_{j=1}^{N} \sum_{l=1}^{N} \sum_{m=1}^{N_c} \left[ \sum_{k=1}^{N_c} Q_{ijk} P_{lmk} \right] b_1^j b_1^{\mu} a_1^l \right)^2 \right)_{p(a,b)}.$$  \hspace{1cm} (2.6)

Because the error depends only on the tensor product of $P$ and $Q$ over index $k$, there is an invariance in the choice of $P$ and $Q$. If we define $\tilde{Q}_{ijk} = \sum_n Q_{ijn} A_{nk}$ and $\tilde{P}_{lmk} = \sum_n P_{lmn} [A^{-1}]_{kn}$ with an $N_c \times N_c$ invertible matrix $A$, we get $\sum_k Q_{ijk} P_{lmk} = \sum_k \tilde{Q}_{ijk} \tilde{P}_{lmk}$, indicating that the choice of the optimal $P$ and $Q$ is not unique. Taking the expectation over $a$ and $b$, the equation above is rewritten as (see appendix A.1)
\[ \ell_a = 1 - \frac{2}{N} \sum_i \text{tr} [P_i Q_i^T] + \frac{1}{N} \sum_i \sum_l \left( \text{tr} [P_i Q_i^T] \right)^2 
+ \text{tr} \left[ P_i Q_i^T \left( L \cdot Q_i P_i^T + P_i Q_i^T \right) \right], \] (2.7)

where all summations run from 1 to \( N \), and \( P_i \) and \( Q_i \) are \( N \times N \) matrices corresponding to the \( i \)th component of tensors \( P \) and \( Q \), respectively:

\[ [P_i]_{jk} = P_{ijk}, \quad [Q_i]_{jk} = Q_{ijk}. \] (2.8)

Similarly, by taking the expectation over \( a \) and \( b \), the decoding loss of \( b \) is given as

\[ \ell_b = 1 - \frac{2}{N} \sum_i \text{tr} [P_i R_i^T] + \frac{1}{N} \sum_i \sum_l \left( \text{tr} [P_i R_i^T R_i P_i^T] \right) 
+ \text{tr} \left[ P_i R_i^T \left( L \cdot R_i P_i^T + R_i P_i^T \right) \right], \] (2.9)

where \([R_i]_{jk} = R_{ijk}\).

### 3 The Binding Solutions under \( L = 1 \)

How should we choose binding operator \( P \) and unbinding operators \( Q, R \) to minimize the loss \( \ell_a \) and \( \ell_b \)? We start from a simple scenario where only one pair is bound (i.e., \( L = 1 \)), and the size of the composition \( c \) is the same with its elements \( a \) and \( b \) (i.e., \( N_c = N \)). In this scenario, there is actually a trivial nonquadratic lossless algorithm in which binding and unbinding are performed by \( c = a + b \) and \( \hat{a} = c - b \), which we call the sum binding. However, this strategy scales badly to \( L > 1 \). This is because, for instance, under \( L = 2 \), we have \( c = a^1 + b^1 + a^2 + b^2 \); hence, it is impossible to tell whether \( a^1 \) is bound to \( b^1 \) or \( b^2 \) just by observing \( c \) and \( a^1 \). This superposition catastrophe can be avoided by introducing nonlinearity into the binding as \( c = \psi (a^1, b^1) + \psi (a^2, b^2) \). We first investigate the solution numerically using a fixed-point algorithm; subsequently, we study a sufficient condition for a local minimum of \( \ell_a \) and \( \ell_b \) analytically.

#### 3.1 Numerical Optimization of the Binding Tensor

To investigate the solution space of the quadratic binding operators, we first optimize the binding operators \( P, Q, R \) numerically for both \( \ell_a \) and \( \ell_b \) using a fixed-point algorithm. Taking the gradient of \( \ell_a \) with respect to \( P_l \) and rewriting this equation in a tensor form, the fixed-point condition is given as (see appendix A.2 for the details)

\[ \frac{\partial \ell_a}{\partial P_l} = 0 \Leftrightarrow Q_{ljk} = \sum_{m,n} \Gamma_{[jN+k],[mN+n]}^q P_{lmn}, \] (3.1)
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for \( j, k = 1, \ldots, N \), where \( \Gamma^q_{ij} \) is an \( N^2 \times N^2 \) matrix defined as

\[
\Gamma^q_{[jN+k],[mN+n]} = \sum_i \left( \delta_{jm} \sum_\beta Q_{ijk} Q_{i\beta n} + Q_{ijk} Q_{mn} + Q_{ijn} Q_{ink} \right).
\] (3.2)

Therefore, for a given unbinding tensor \( Q \), the binding tensor \( P \) satisfying

\[
\frac{\partial \ell_a}{\partial P_l} = 0
\]

for \( j, k = 1, \ldots, N \), where \( \Gamma^q \) is an \( N^2 \times N^2 \) matrix defined as

\[
\text{Vec}[P_l] = (\Gamma^q)^{-1} \text{Vec}[Q_l],
\] (3.3)

where \( \text{Vec}[P_l] \) and \( \text{Vec}[Q_l] \) are the vector representation of \( N \times N \) matrices \( P_l \) and \( Q_l \), respectively. From a similar calculation, for a given binding tensor \( P \), the fixed point of \( \ell_a \) with respect to \( Q \) is given as

\[
\text{Vec}[Q_l] = (\Gamma^w)^{-1} \text{Vec}[P_l],
\] (3.4)

where \( \Gamma^w \) is an \( N^2 \times N^2 \) matrix that only depends on \( P \). Moreover, we can update \( P \) and \( R \) with respect to \( \ell_b \) by

\[
\text{Vec}[\hat{P}_m] = (\Gamma')^{-1} \text{Vec}[	ilde{R}_m], \quad \text{Vec}[\hat{R}_j] = (\Gamma^{pb})^{-1} \text{Vec}[	ilde{P}_j],
\] (3.5)

respectively, where \( \tilde{R}_m \) and \( \tilde{P}_m \) are defined as \( [\tilde{R}_m]_{i,j,k} = R_{imk} \) and \( [\tilde{P}_m]_{i,j,k} = P_{imk} \), and \( \Gamma' \) and \( \Gamma^{pb} \) are \( N^2 \times N^2 \) matrices (defined at equations A.19 and A.22 in appendix A.2). Therefore, we can perform an iterative optimization of tensors \( P, Q, R \) with respect to both \( \ell_a \) and \( \ell_b \) by the fixed-point algorithm described in algorithm 1.

Figures 2A and 2B describe the learning curves of this algorithm from 10 random initializations. Both decoding errors \( \ell_a \) and \( \ell_b \) first plateau around \( \ell_a \approx 0.35 \), then converge to \( 1/5 \), robustly. To evaluate the performance of this optimized binding operator, we compare it with HRR (Plate, 1995), a
Figure 2: Iterative optimization of binding operators $P, Q, R$ under $N = 48$ and $L = 1$. (A) Learning dynamics of the fixed-point algorithm from random initializations. Here, we evaluated the loss $\ell_a$ directly from equation 2.7. Each line represents a learning curve of the decoding error $\ell_a$ from a random initialization. The black dashed line represents the error after convergence, and the gray dashed line is the error under HRR. (B) The same as panel A, but the $y$-axis is $\ell_b$, not $\ell_a$. (C) Change in distance measures during learning. We defined the distances using the Frobenius norm as $\|Q - \gamma P\|^2 \equiv \sum_{i,j,k} (Q_{ijk} - \gamma P_{ijk})^2$, where $\gamma = \frac{\max Q}{\max P}$, $\|Q - R\|^2 \equiv \sum_{i,j,k} (Q_{ijk} - R_{ijk})^2$, and $\sum_i \|P_i Q_i^T - Q_i P_i^T\|^2 \equiv \sum_{i,j,k} \left(\|P_i Q_i^T\|_{jk} - \|P_i Q_i^T\|_{kj}\right)^2$.

binding method using the circular convolution (see appendix C.1). Under HRR, the binding and the unbinding operators are given as

$$P_{ijk} = Q_{ijk} = R_{ijk} = \frac{1}{\sqrt{2(N+1)}} \delta_{[i+j]N, k},$$

where $[x]_N \equiv x \ (\text{mod. } N)$, and the decoding error is $\ell_a = \ell_b = 1/2$ under a large $N$ (gray dashed lines in Figures 2A and 2B). This means that the numerically optimized binding operator achieves a better decoding performance than HRR under $L = 1$.

To see if the numerically optimized binding operators $P, Q, R$ have some specific structures, we next investigate the values of $P, Q, R$ after learning. First, upon optimization, $Q$ and $R$ converge to the same values (i.e., $Q = R$; orange lines in Figure 2C), but $P \neq Q, R$ even under a rescaling (blue lines; here we plotted a normalized distance $\sum_{i,j,k} (Q_{ijk} - \gamma P_{ijk})^2$ with $\gamma = \frac{\max Q}{\max P}$). Moreover, the matrix products $P_1 Q_1^T, \ldots, P_N Q_N^T$ converge to symmetry matrices after the optimization (green lines).

Elements of matrix $P_1$ look random even after an optimization (see Figure 3A; here we plotted $P_1, \ldots, P_5$ out of $N = 48$ matrices $P_1, \ldots, P_{48}$) potentially due to an invariance in the solution space, and the same is true for the elements of $Q_1$ (see Figure 3B). To untangle the invariance and extract the hidden structure in $P, Q, R$, we process the tensors in the following way:
Figure 3: Binding matrices obtained after the convergence from one random initialization ($N = 48$, $L = 1$). (A) $P_1, \ldots, P_5$ (of $P_1, \ldots, P_{48}$) after 100 iterations of the numerical optimization. (B) $Q_1, \ldots, Q_5$ after the numerical optimization. (C, D) The same as the binding matrices depicted in panels A and B, respectively but transformed into a space where $\bar{P}_1$ is diagonal.

1. Because $P_1Q_1^T$ converges to a symmetric matrix, we can decompose it as $P_1Q_1^T = U_1 \Sigma_1 U_1^T$, where $U_1$ is an $N \times N$ orthogonal matrix and $\Sigma_1$ is an $N \times N$ diagonal matrix.

2. We introduce an $N \times N$ matrix $A_1$ by $A_1 = P_1^{-1}U_1 \Sigma_1^{1/2}$.

3. We transform the binding matrices $P_i$ by $\bar{P}_i = U_1^T P_i A_1$ for $i = 1, \ldots, N$.

This transformation cancels out the invariance in the choice of $P$ and $Q$ and maps $P_i$ onto the space where $\bar{P}_1$ is a diagonal matrix ($\bar{P}_1 = \Sigma_1^{1/2}$). After this preprocessing, we found an $8 \times 8$ block structure in all $\bar{P}_i$ (see Figure 3C; we plotted $\bar{P}_1, \ldots, \bar{P}_3$ out of $\bar{P}_1, \ldots, \bar{P}_{48}$ as before). Note that there is no constraint that enforces the $8 \times 8$ structure in the learning algorithm or the data processing, except that $N = 48$ is a multiple of eight. Similarly, by preprocessing $Q_i$, we have $\bar{Q}_i = U_1^T Q_i B_1$ with $B_1 = Q_1^{-1}U_1 \Sigma_1^{1/2}$, we recover the $8 \times 8$ block structure (see Figure 3D). Moreover, $\bar{P}_i = \bar{Q}_i$ is satisfied for all $i = 1, \ldots, N$ (compare Figures 3C and 3D). Notably, $P_iQ_i^T$ is rewritten as

$$P_iQ_i^T = U_1^T P_i P_1^{-1} U_1 \Sigma_1 U_1^T (Q_1^T)^{-1} Q_i U_1^T = U_1^T P_i Q_i^T U_1.$$ (3.7)
Therefore, under the transformation \( \{P_i, Q_i\} \rightarrow \{\bar{P}_i, \bar{Q}_i\} \), the loss \( \ell_a \) (see equation 2.7) is preserved. This means that up to a linear transformation with an orthogonal matrix, these numerically optimized operators are symmetric (\( Q = \bar{R} \) and \( P = \bar{Q} \)) and have a hidden \( 8 \times 8 \) block structure. In the rest of the section, we discuss why we see the \( 8 \times 8 \) structure in the optimized binding operators from an algebraic perspective.

### 3.2 Composition Algebra-Based Solution for the Quadratic Binding Problem

Our numerical optimization indicates that there is a nontrivial binding method with a \( 8 \times 8 \) block diagonal structure that outperforms a previously proposed method. To understand the origin of this structure, we next analytically study a sufficient condition for a local minimum of both \( \ell_a \) and \( \ell_b \). We introduce \( P = Q = R \) constraint for the binding and unbinding tensors. This is motivated by the symmetric structure we saw in the numerical optimization (see Figures 2C and 3CD). Note that two popular binding methods, HRR and the tensor product representation, also satisfy this \( P = Q = R \) constraint (see appendix C). Taking the gradient of \( \ell_a \) under the symmetric constraint \( P = Q \), the fixed-point condition is given as

\[
P_i = \sum_{l=1}^{N} \left( \text{tr} \left[ P_l P_i^T \right] I_N + P_l P_i^T + P_i P_l^T \right) P_l \tag{3.8}
\]

for \( i = 1, \ldots, N \), where \( I_N \) is the size \( N \) identity matrix. Similarly, introducing the \( P = R \) constraint, the fixed-point condition for \( \ell_b \) is written as

\[
P_i = \sum_{l=1}^{N} \left( P_l P_i^T P_l + P_i P_l^T P_l + P_l P_i^T P_l \right). \tag{3.9}
\]

What kind of \( P = \{P_1, P_2, \ldots, P_N\} \) satisfies equations 3.8 and 3.9? A sufficient condition for both is

\[
P_l P_i^T + P_i P_l^T = 2\lambda \delta_{il} I_N, \tag{3.10}
\]

for all \( i, l = 1, \ldots, N \), with the scaling factor \( \lambda = \frac{1}{N+2} \) (see appendix B.1). This set of equations is known as the Hurwitz matrix equations. It has been proved that there exists a family of \( N \) matrices of size \( N \times N \) that satisfies equation 3.10 only if \( N = 1, 2, 4, 8 \), and a solution is given by a real matrix representation of the composition algebra of dimension \( N \) (Shapiro, 2011). This means that when binding two vectors \( a, b \) having length \( N = 1, 2, 4, 8 \), you can locally minimize the decoding error by using a solution of the Hurwitz matrix equations as a binding operator \( P \).
For instance, when \( N = 2 \), by setting
\[
P_1 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P_2 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},
\]
(3.11)
equation 3.10 is satisfied. Then, from equation 2.1, the binding of two (real) vectors \( \mathbf{a} = (a_1, a_2) \) and \( \mathbf{b} = (b_1, b_2) \) becomes
\[
\mathbf{c} = \frac{1}{2} \begin{pmatrix} a_1 b_1 - a_2 b_2 \\ a_1 b_2 + a_2 b_1 \end{pmatrix},
\]
(3.12)
and the unbinding of \( \mathbf{a} \) is given as \( \hat{\mathbf{a}} = \frac{\sqrt{2}}{\sqrt{2}} (a_1, a_2) \). Notably, \( P_1 \) and \( P_2 \) consist of a basis of a matrix representation of the complex numbers up to a scaling factor. Let us define a projection \( \phi : \mathbb{C} \to \mathbb{R}^2 \times \mathbb{R}^2 \) by
\[
\phi (x + iy) = 2 (xP_1 + yP_2) = \begin{pmatrix} x & y \\ -y & x \end{pmatrix}.
\]
(3.13)
Then, for two complex numbers \( a = a_1 + ia_2 \) and \( b = b_1 + ib_2 \),
\[
\phi (a) \phi (b) = \begin{pmatrix} a_1 & a_2 \\ -a_2 & a_1 \end{pmatrix} \begin{pmatrix} b_1 & b_2 \\ -b_2 & b_1 \end{pmatrix}
= \begin{pmatrix} a_1 b_1 - a_2 b_2 & a_1 b_2 + a_2 b_1 \\ -(a_1 b_2 + a_2 b_1) & a_1 b_1 - a_2 b_2 \end{pmatrix} = \phi (ab).
\]
(3.14)
Thus, at \( N = 2 \), a matrix representation of the complex numbers provides a binding operator \( P = [P_1, P_2] \) that satisfies the fixed-point conditions, equations 3.8 and 3.9. Similarly, at \( N = 4 \), we can construct a binding operator \( P = [P_1, P_2, P_3, P_4] \) using a matrix representation of the quaternions:
\[
P_1 = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad P_2 = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},
\]
\[
P_3 = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad P_4 = \frac{1}{\sqrt{6}} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}.
\]
(3.15)
Under this binding operator, the composition \( c \) of the two vectors \( a \) and \( b \) is given as

\[
\begin{align*}
    c_1 &= \frac{1}{\sqrt{6}} (a_1 b_1 + a_2 b_2 + a_3 b_3 + a_4 b_4), \\
    c_2 &= \frac{1}{\sqrt{6}} (a_1 b_2 - a_2 b_1 - a_3 b_4 + a_4 b_3), \\
    c_3 &= \frac{1}{\sqrt{6}} (a_1 b_3 + a_2 b_4 - a_3 b_1 - a_4 b_2), \\
    c_4 &= \frac{1}{\sqrt{6}} (a_1 b_4 - a_2 b_3 + a_3 b_2 - a_4 b_1),
\end{align*}
\]

(3.16)

and using \( P \) as the unbinding tensor, from equation 2.2, we get

\[
\hat{a} = \frac{1}{6} (b_1^2 + b_2^2 + b_3^2 + b_4^2) a.
\]

(3.17)

Therefore, decoding of \( a \) is faithful up to a constant scaling factor under this quaternion-based binding. Similarly, we can construct a binding operator based on a matrix representation of the octonions, an extension of the quaternions to \( N = 8 \) dimensional space (see appendix B.2). However, this is not true for \( N > 8 \), because equation 3.10 does not admit a solution.

### 3.3 Sparse \( K \)-Compositional Bindings

Although solutions based on the composition algebra we have discussed are lossless, they cannot be directly extended to the case when \( N > 8 \) because the Hurwitz matrix equations do not have a solution. Nevertheless, we can apply this binding in a block-wise manner. Let us define a family of matrices that satisfies the Hurwitz matrix equations (equation 3.10) as \([A_1, A_2, \ldots, A_K]\), where \( K = 1, 2, 4, \) or 8 and each \( A_k \) is a \( K \times K \) matrix. Suppose \( N = \dim(a) \) satisfies \( N = qK \) for a positive integer \( q \). We define a sparse \( K \)-compositional binding by

\[
P_i = O_K \oplus \cdots \oplus O_K \oplus A_{\%K} \oplus O_K \oplus \cdots \oplus O_K,
\]

(3.18)

for \( i = 1, \ldots, N \), where \( O_K \) is the \( K \times K \) zero matrix, \( A \oplus B \) is the direct sum of matrices \( A \) and \( B \), \([x] \) represents the largest integer smaller or equal to \( x \), and \( x \% y \) is the remainder of \( x \) divided by \( y \) (for ease of notation, we define \( A_0 = A_K \)). We denote this binding mechanism as the sparse \( K \)-compositional binding because it is a sparse implementation of the composition algebra of dimension \( K \). For instance, if \( K = 2 \) and \( q = 3 \), we get
Figure 4: Performance of sparse $K$-compositional binding methods under $L = 1$. (A) Decoding error $\ell_a$ of sparse $K$-compositional binding methods with the core size $K = 1, 2, 4, 8$ and the holographic reduced representation (HRR) under various layer sizes $N$. Points are simulations, and lines are theory ($\ell_a = 2/(K + 2)$ for $K$-compositional and $\ell_a = \frac{N+2}{2(N+1)}$ for HRR). (B) Decoding error $\ell_a$ of the sparse $K$-compositional binding methods with various core sizes $K$ under $N = 128$. The solid line is $\frac{2}{K+2}$, while the dotted line is a linear interpolation. (C) The same as panel A, except that the binding operators were normalized so that the amplitude of the signal is maintained in the unbinding. Points are simulations and lines are theory ($\ell_a = 2/K$ for $K$-compositional, and $\ell_a = 1 + \frac{2}{N}$ for HRR).

\[ P_1 = \begin{pmatrix} A_1 & O & O \\ O & O & O \\ O & O & O \end{pmatrix}, \quad P_2 = \begin{pmatrix} A_2 & O & O \\ O & O & O \\ O & O & O \end{pmatrix}, \quad P_3 = \begin{pmatrix} O & O & O \\ O & A_1 & O \\ O & O & O \end{pmatrix}, \quad P_4 = \begin{pmatrix} O & O & O \\ O & A_2 & O \\ O & O & O \end{pmatrix}, \ldots \] (3.19)

When $q = 1$, they are matrix representations of the composition algebra we discussed in the previous section, whereas under $K = 1$, we get a binding by the Hadamard product, which was previously used in MAP (multiply, add, permute) coding (Gayler & Wales, 1998) and an HRR implementation in the Fourier space (Plate, 1994). Although $P = [P_1, P_2, \ldots, P_N]$ does not satisfy the Hurwitz matrix equations when $q > 1 (P_i P_i^T \neq \lambda I_N)$, it satisfies the fixed-point condition, equations 3.8 and 3.9 (see appendix B.3). This means that a sparse $K$-compositional tensor $P$ is a fixed-point solution of both $\ell_a$ and $\ell_b$. The decoding error under this binding is given as

\[ \ell_a = \ell_b = \frac{2}{K+2}. \] (3.20)

This error is significantly smaller than that of HRR under $K = 4$ and $K = 8$ (see Figure 4A, purple and orange lines versus blue line). In particular, under $K = 8$, we get $\ell_a = \ell_b = 1/5$, the same error we observed under a numerical optimization (compare Figures 2A and 2B with Figure 4A). It also
explains why we found $8 \times 8$ block structures (see Figures 3C and 3D). Among sparse $K$-compositional bindings, $K = 8$ yields the smallest error because it is the largest matrix family that satisfies the Hurwitz matrix equations. Note that if we normalize the loss by the norm of the unbound vector as $\tilde{\ell}_a = \ell_a / \frac{1}{N} \langle \| \hat{a} \| \rangle$, we have $\tilde{\ell}_a = \tilde{\ell}_b = \frac{2}{K}$, because $\frac{1}{N} \langle \| \hat{a} \| \rangle = \frac{K}{K+2}$.

Under this normalization, HRR binding loss becomes $\tilde{\ell}_{HRR}^a = 1 + \frac{2}{N}$; thus, sparse $K$-compositional bindings with $K = 4$ and $K = 8$ still outperform HRR.

Using Cayley-Dickson construction (Baez, 2002), we can in principle construct sparse $K$-compositional binding tensors for $K = 16$ (sedenions), 32 (trigintaduonions), and so on. However, it does not improve the unbinding performance (right side of Figure 4B), because they do not satisfy the Hurwitz matrix equations. Thus, the binding tensor with $K = 8$ provides the best unbinding performance among the sparse $K$-compositional bindings. Below, we denote this $K = 8$ solution of equation 3.18 as the octonion binding, because it employs a matrix representation of the octonions.

The octonion binding solution we constructed is not the same with the numerically optimized one, in a sense that only one of the block diagonal components is nonzero, while all block diagonal components are nonzero in the numerically optimized matrices (see Figures 3C and 3D). However, we found that the error of the sparse $K$-compositional binding is conserved under a transformation with any orthogonal matrix, which makes all block diagonal components nonzero (see appendix B.3). This result suggests that the numerically optimized solutions are consistent with the octonion binding. Note that unlike $K$-compositional bindings with $K \leq 8$, HRR does not satisfy equations 3.8 and 3.9 at a finite $N$ (see appendix C.1).

A binding operator $P$ derived by minimizing $\ell_a$ shrinks the amplitude of the signal in the reconstructed vector $\hat{a}_1$ as shown in equation 3.17 ($\langle \hat{a} \rangle_{P(b)} = \frac{2}{3} a$ under the quaternion binding), meaning that the decoding is biased. However, it might be desirable to use an unbiased binding operator, which keeps the signal amplitude in the decoded vector $\hat{a}_1$ the same with the original signal $a_1$ (i.e., $\langle \hat{a}_1 - a_1 \rangle = 0$). Taking the expectation over $b$, the reconstructed vector $\hat{a}_1^1$ (see equation 2.2) on average satisfies

$$\langle \hat{a}_1^1 \rangle_{P(b)} = \sum_{j=1}^{N} \sum_{l=1}^{N} \left( \sum_{k=1}^{N} Q_{ijk} P_{ljk} \right) a_1^l. \quad (3.21)$$

Thus, in order to keep the reconstructed signal amplitude the same with the original signal, under $P = Q$, $P$ should be normalized as

$$\sum_{j=1}^{N} \sum_{k=1}^{N} P_{ijk}^2 = 1, \quad (3.22)$$
Figure 5: Local stability of the quaternion and the octonion bindings at $N = 48$ and $L = 1$. (A) Learning curve from the quaternion binding ($K = 4$) plus perturbation. We constructed the initial $P, Q, R$ by adding random gaussian noise with the standard deviation $\sigma / N$ to the sparse-quaternions binding. (B) Learning curve from the octonion binding ($K = 8$) plus perturbation. In both panels A and B, we measure the unbinding error by $\ell_a$. for $i = 1, 2, \ldots, N$. Under this normalization, the unbinding error tends to be larger, but the relative performance of various binding methods is preserved (see Figure 4C versus 4A). In particular, the sparse $K$-compositional bindings with $K = 4$ and 8 still outperform HRR with the same unbiased normalization (see the orange and purple lines versus blue line in Figure 4C).

To gain further insights into the space of the quadratic binding mechanisms, we next study the stability of the quaternion and the octonion bindings (see equation 3.18 with $K = 4$ and 8, respectively) against a perturbation. If we initialize $P, Q, R$ as the quaternion binding plus a small random perturbation, then run the iterative optimization process (see algorithm 1), the error converges to one-third, the original error level under the quaternion binding (see the blue lines in Figure 5A). On the other hand, under a large perturbation, the error instead converges to one-fifth, the error level under the octonion binding (see the purple and pink lines). These results indicate that the quaternion binding is a local minimum in the space of binding operators. The octonion binding is, on the contrary, stable against perturbation (see Figure 5B), although $P, Q, R$ converge to different tensors when a large perturbation is added. This result suggests that the octonion binding has a large basin of attraction in the parameter space, though it only indicates a local optimality of the octonion binding, not a global one.

4 The Binding Solutions under $L > 1$

Our theoretical and numerical analyses in the previous section suggest that a binding method based on a matrix representation of octonions, the
Figure 6: Numerical optimization of $P, Q, R$ under $N = 48, L = 3$. (A) Learning dynamics from 10 random initializations (the same as Figure 2A but under $L = 3$). Black and gray horizontal dashed lines are the error under the octonion binding ($\ell = \frac{9}{13}$), and HRR ($\ell = \frac{3}{4}$), respectively. (B, C) Examples of the learned binding matrices after 300 iterations. The panels are the same with Figures 3C and 3D, but calculated under $L = 3$. Note that $\bar{P}_i = \bar{Q}_i$ holds for all $i$.

octonion binding, outperforms HRR binding under $L = 1$. How does this method scale to an unbinding from a composition $c$ that consists of multiple bound pairs ($L > 1$)?

The numerical optimization method (algorithm 1) can be straightforwardly applied to $L > 1$. For instance, an update of $P$ with respect to loss $\ell_a$ is done by $\text{Vec}[P] = (\Gamma^{q,L})^{-1} \text{Vec}[Q]$, where $N^2 \times N^2$ matrix $\Gamma^{q,L}$ is defined as (see appendix A.2),

$$\Gamma^{q,L}_{[N+k],[mN+n]} = \sum_i \left( \delta_{jm} I \sum_{\beta} Q_{ij\beta k \beta} Q_{ij\beta n} + Q_{ijk} Q_{imn} + Q_{ijn} Q_{imk} \right).$$

(4.1)

Applying this numerical optimization to the case when $L = 3$, we found $8 \times 8$ block diagonal structures in the converged binding matrices as before (see Figures 6B and 6C). The decoding performance of the obtained binding is better than HRR (black versus gray dashed lines in Figure 6A), though the relative advantage was smaller compared to the case when $L = 1$ (see Figure 6A versus Figure 2A). Moreover, the octonion binding satisfies the fixed-point condition for both $\ell_a$ and $\ell_b$ even when $L > 1$ (see appendix B.3). These results indicate that the octonion binding may have an edge even when $L > 1$. However, it is only suggestive because both the octonion and HRR bindings perform poorly when we directly apply them to $L > 1$ (see Figure 6A; the noise-to-signal ratio is above 0.7 for both).

Below, we first show that the performance of all unbiased quadratic binding operators is lower-bounded by $\ell_a \geq \frac{NL}{N_c} + O(1)$ under a mild condition; hence, equi-sized binding operators (i.e., $N_c = N$), such as HRR or the octonion binding, inevitably scale poorly under $L > 1$. To overcome this...
problem, we consider two extensions: decoding with a dictionary (Plate, 1995; Smolensky, Goldrick, & Mathis, 2014) and decoding from a composition \( c \) larger than the size of elements \( a \) and \( b \) \((N_c > N)\) (Smolensky, 1990; Frady et al., 2021). We show that under both extensions, the proposed octonion binding outperforms both HRR and a random binding under \( L \sim O(1) \), but its advantage disappears at the large \( L \) limit.

### 4.1 Lower Bound on the Unbinding Error.

Let us first focus on the case when \( L \gg 1 \) and consider minimization of the decoding error \( \ell_a \) under a general quadratic parameterization. As we discussed previously, in order to retain the signal amplitude in the unbinding process, and thus to make the estimation unbiased, from equation A.24, \( P \) and \( Q \) need to be normalized as

\[
\sum_{j=1}^{N} \sum_{k=1}^{N_c} P_{ijk} Q_{ijk} = 1. \tag{4.2}
\]

Taking the large \( L \) limit of the loss \( \ell_a \) under this constraint, as a function of \( L \), the loss \( \ell_a \) follows (see appendix A.3)

\[
\frac{\ell_a}{L} = \frac{1}{N} \sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} \left[ P_l Q_i^T Q_i P_l^T \right] + O \left( \frac{1}{L} \right). \tag{4.3}
\]

Thus, at \( L \gg 1 \), minimization of the loss \( \ell_a \) under the signal amplitude constraint is reformulated as the minimization of a Lagrangian:

\[
\mathcal{L}_a = \frac{1}{2} \sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} \left[ P_l Q_i^T Q_i P_l^T \right] - \sum_{i=1}^{N} \lambda_i \left( \text{tr} \left[ P_i Q_i^T \right] - 1 \right). \tag{4.4}
\]

Solving this Lagrangian under an assumption that \( \sum_i P_i P_i^T \) is invertible and applying Jensen’s inequality, the lower bound of \( \ell_a \) is given as

\[
\frac{\ell_a}{L} \geq \frac{N}{N_c} + O \left( \frac{1}{L} \right), \tag{4.5}
\]

where \( N \equiv \text{dim}(a) = \text{dim}(b) \), and \( N_c \equiv \text{dim}(c) \). This means that the error under any quadratic bindings satisfying the invertibility condition is lower-bounded by \( \ell_a \geq \frac{N}{N_c} + C \), where \( C \) is a term that does not depend on \( L \). In particular, under an equisized composition \((N_c = N)\), the error is bounded by \( \ell_a \geq L + C \).

Figure 7 describes the unbinding error \( \ell_a \) as a function of the number of bound pairs \( L \) under \( N_c = N \) for three different binding mechanisms. Under
Figure 7: Comparison of the loss $\ell_a$ under the octonion, HRR, and the sum bindings at $N_c = N = 128$ for various $L$. Points are simulations and lines are theory ($\ell_a = 2L - 1, L + \frac{2}{N}$, and $L - \frac{3}{4}$ for the sum binding, HRR, and the octonion, respectively).

the octonion binding, the error follows $\ell_a = L - \frac{3}{4}$ (see the orange line in Figure 7), whereas under HRR, $\ell_a = L + \frac{2}{N}$ (blue line). It means that both binding methods tightly follow the lower bound (see equation 4.5) though the octonion binding has a smaller intercept $C$ than HRR. On the contrary, the sum binding ($c = \sum_{\mu} (a_\mu + b_\mu)$ and $\hat{a}_1 = c - b_1$) yields $\ell_a = 2L - 1$ (see the green line in Figure 7). Thus, it performs progressively worse compared to the two other methods as $L$ becomes larger, though it has the smallest error under $L = 1$. Notably, all three methods yield errors larger than one for $L > 1$, meaning that the signal-to-noise ratio is smaller than one. Therefore, we need to modify these methods to perform decoding from a composition of multiple pairs. We first consider decoding with the help of a dictionary, then study binding with an expanded composition ($N_c > N$).

4.2 Decoding with a Dictionary. Previous studies have shown that if the system knows the dictionary from which vectors $\{a_\mu\}_{\mu=1}^L$ and $\{b_\mu\}_{\mu=1}^L$ are sampled, accurate decoding is possible even if multiple pairs are bound together (Plate, 1995; Smolensky et al., 2014). Hence, we introduce a dictionary containing $D$ words $D = \{a_d\}_{d=1}^D$, where each word $a_d$ is sampled from an i.i.d. gaussian distribution $N(0, I_N)$. With this dictionary, we conduct unbinding of $a_1$ from a composition $c$ with a query $b_1$ in the following steps:

1. Unbind $a_1$ by $\hat{a}_1 = \sum_j \sum_k Q_{ijk} b_j k$, as before.
2. Calculate $z_\mu = \hat{a} \cdot a_\mu$ for all the words in the dictionary ($\mu = 1, \ldots, D$).
3. Pick the word $a_{\mu_o}$ with $\mu_o \equiv \arg\max_\mu z_\mu$. 
Note that because all $a_\mu$ have roughly the same norm ($\|a_\mu\|^2 \approx N$), argmax$_\mu \hat{a} \cdot a_\mu$ is equivalent to argmin$_\mu \|\hat{a} - a_\mu\|^2$ at the large $N$ limit. Approximating $p(z_1, \ldots, z_D)$ with a gaussian distribution, we can derive the probability of misclassification similar to previous work (see appendix A.4 and Murdock, 1982; Plate, 1995; Frady, Kleyko, & Sommer, 2018; Steinberg & Sompolinsky, 2022),

$$P[\mu_o \neq 1] = 1 - \int \frac{dz}{\sqrt{2\pi}} \exp \left(-\frac{1}{2} \left(z - \frac{1}{\sigma_s}\right)^2\right) \left(\Phi \left[\frac{\sigma_s z}{\sigma_l}\right]\right)^{L-1} \left(\Phi \left[\frac{\sigma_s z}{\sigma_d}\right]\right)^{D-L},$$

(4.6)

where $\Phi[z]$ is the cumulative gaussian distribution, and $\sigma_s, \sigma_l, \sigma_d$ are the standard deviations of $z_\mu$ under $\mu = 1$ (the target), $2 \leq \mu \leq L$ (the bound words), and $L + 1 \leq \mu \leq D$ (the rest of words in the dictionary), respectively.

The standard deviations $\sigma_s, \sigma_l$ and $\sigma_d$ depend on the choice of the binding and unbinding methods. For instance, under the octonion binding, we get

$$\sigma_s^2 = \frac{1}{N} \left(L + \frac{3}{2}\right), \quad \sigma_l^2 = \frac{1}{N} \left(L + \frac{1}{2}\right), \quad \sigma_d^2 = \frac{1}{N} \left(L + \frac{1}{4}\right),$$

(4.7)

whereas under HRR, assuming $N \gg 1$,

$$\sigma_s^2 = \frac{1}{N} (L + 3), \quad \sigma_l^2 = \frac{1}{N} (L + 2), \quad \sigma_d^2 = \frac{1}{N} (L + 1).$$

(4.8)

Thus, the performance should converge to the same accuracy under $L \gg 1$. In fact, our theoretical result recovers equation 2.35 of Frady et al. (2018) in this limit. On the contrary, $L \sim O(1)$, we expect the classification error of two binding methods to be different. In particular, a small $\sigma_s$ effectively amplifies the signal, $1/\sigma_s$, while a small $\sigma_s/\sigma_d$ makes a misclassification with nonbound words in the dictionary less likely (note that $[\sigma_s/\sigma_d]_{\text{oct}} \leq [\sigma_s/\sigma_d]_{\text{HRR}}$ for $L \geq 1$).

Figure 8A describes the probability of incorrect classification ($P[\mu_o \neq 1]$) under the octonion binding and HRR, and also under a random binding introduced as a control. The random binding was constructed by sampling the elements of $P$ from a gaussian distribution $\mathcal{N}(0, 1/N^2)$ and setting $Q = R = P$. As in the case of unbinding without a dictionary, the performance becomes worse as the number of bound pairs goes up (compare Figure 8A with Figure 7). However, even when a dozen pairs are bound to the composition, the misclassification rate is far below the chance level ($P(\mu_o \neq 1) = 1 - \frac{1}{D}$) in all three binding methods. Moreover, we found that the error under the octonion binding is smaller than a random binding under a small $L$ (orange versus red in Figure 8A), while that of HRR is roughly
Figure 8: Decoding performance in the presence of a dictionary. (A) Error rates (probability of incorrect classification) of the octonion, HRR, and the random bindings under various various number of bound pairs $L$. We set the number of the items in the dictionary to $D = 5000$ and the vector size as $N_c = N = 96$. Points are simulations, and lines are theory (see appendix A.4 for details). Analytical lines for the random binding are omitted because that is exactly the same as the line for HRR. (B) Error rates of the octonion, HRR, and the random bindings under various dictionary sizes $D$. Three panels represent the errors under different $L$ and $N$ under a fixed ratio $N/L$. Points are simulations, and lines are theory. The lines deviate from the points under $L = 5$ because the gaussianity assumption made for the theoretical lines is violated in this regime.

the same with the random binding (blue versus red; some blue points are hidden under the red points).

In the comparison above, all three methods perform worse when a large number of pairs are bound to the composition, making the comparison difficult in this regime. To clarify the issue, using the fact that the signal-to-noise ratio roughly scales with $N/L$ (see equations 4.7 and 4.8), we plotted the misclassification probability for different $L$ while scaling the vector size as $N \propto L$ (see Figure 8B). In this parameterization, the octonion binding exhibits similar error curves as a function of the dictionary size $D$ regardless of $L$ (orange lines). On the contrary, HRR and the random binding show higher errors under $L = 5$ and $L = 10$ (orange versus blue and red points in Figure 8B, left and middle panels), though their performance converges to that of the octonion binding under $L = 20$ (right panel). This result suggests that the performance of HRR and the random binding are suboptimal under $L \sim O(1)$, while all three methods perform similarly under a large $L$.

Because the number of things humans can keep in the working memory is suggested to be fewer than 10 (Miller, 1956; Cowan, 2001), in a cognitive process that requires binding in the working memory such as scene understanding, we expect $L \leq 10$ to be the biologically relevant parameter regime. Our result indicates that the octonion binding outperforms HRR and the random binding in this regime, though its advantage goes away under a large $L$. 
Figure 9: Comparison of the random, tensor-HRR, and the extended octonion bindings under various expansion ratios $N_c/N$ at $L = 3$ (A) and $L = 10$ (B). We set $N = 128$. Points are simulation results, and lines are theoretical results from equations B.24 (extended octonions), C.22 (tensor-HRR), and A.59 (random).

4.3 Extension of the Octonion Binding and HRR to $N_c > N$. Even if the brain does not know the dictionary from which words are sampled, it can achieve a good decoding performance with an expansion of the composition layer. Indeed, equation 4.5 indicates that if the size of composition $N_c$ scales with the (maximum) number of bound pairs $L$, the system can reliably perform an unbinding from a composition of multiple pairs. Thus, we next consider an extension of the octonion, HRR, and random binding mechanisms to $N_c > N$.

When $N_c$ is a multiple of $N$ but smaller than $N^2/8$, the octonion binding is straightforwardly extended to $N_c > N$ by adding shifted block-diagonal components (see appendix B.4). Under this extended octonion binding mechanism, the decoding error becomes $\ell_a = \frac{N}{N_c} \left( L - 1 + \frac{2}{N} \right)$ (see the orange lines in Figures 9A and 9B). Notably, the leading term of $\ell_a$ with respect to $L$ is still the same with the lower bound (see equation 4.5).

HRR can also be extended to $N_c > N$ by considering an interpolation of HRR and the tensor product representation (Smolensky, 1990). Because the binding tensor $P$ is given as $P_{ijk} = \frac{1}{\sqrt{N}} \delta_{i+j} \delta_{N+k}$ for HRR and $P_{ijk} = \frac{1}{\sqrt{N}} \delta_{(i+j)N+k}$ for the tensor product representation, we can interpolate these two bindings by setting $P_{ijk} = \frac{1}{\sqrt{N}} \delta_{[i+j]N+k}$ for $N_c = dN$ (see appendix C.3). The decoding error approximately follows $\ell_a \approx \frac{NL}{N_c} + \frac{1}{N}$ under this tensor-HRR binding (see the blue lines in Figures 9A and 9B, partially occluded by the red lines).

Finally, an extension of the random binding is done straightforwardly by sampling the elements of $P$ from a gaussian distribution with the mean zero and the variance $1/(NN_c)$, while setting $Q = R = P$. Under this method, assuming $N, N_c \gg 1$, the decoding error becomes (see appendix A.6)

$$\ell_a = \frac{LN}{N_c} \left( 1 + \frac{N_c}{N^2} \right). \quad (4.9)$$
Thus, at $N_c \ll N^2$, the leading-order term of the error follows the lower bound $LN/N_c$ (see the red lines in Figures 9A and 9B) while at the $N_c \to N^2$ limit, the error of this random binding becomes the double of the lower bound.

Because it has a small intercept, the extended octonion binding outperforms both tensor-HRR interpolation and the random binding under $L \sim O(1)$ (see Figure 9A; here $L = 3$). This result again indicates that the octonion-based binding method is preferable in the parameter regime relevant to working memory-based cognitive processes. However, at $L \gg 1$, the random binding is as good as the extended octonion bindings (see Figure 9B; $L = 10$). In fact, comparing the lower bound (see equation 4.5) with equation 4.9, we can conclude that there is no quadratic binding method with invertible $\sum_i P_i P_i^T$ that significantly outperforms the random binding when $L \gg 1$ and $N_c \ll N^2$.

5 Discussion

In this work, we investigated optimal methods for pair-wise binding based on the VSA framework (Smolensky, 1990; Plate, 1995; Gayler, 2003). We first numerically optimized the binding and unbinding operators for the best unbinding performance assuming only one pair is bound to the composition vector. We found that the numerically optimized binding operators outperform HRR, a popular method for binding (see Figure 2). Moreover, we revealed that there is a hidden $8 \times 8$ block structure in the optimized binding and unbinding matrices (see Figure 3). By analytically deriving a sufficient condition for a fixed point of the loss function, we show that the $8 \times 8$ block structure originates from a matrix representation of the octonion algebra, an eight-dimensional extension of the complex numbers (see Figure 4). Furthermore, we showed that even when several pairs are bound into a composition, the proposed binding method based on the octonion outperforms previously proposed methods under both the dictionary decoding (see Figure 8) and unbinding from an expanded composition (see Figure 9). When there are many bound pairs in a composition, however, the advantage of the proposed method vanishes, and even a random binding shows approximately the optimal unbinding performance under a mild condition (see Figures 8 and 9).

We introduced two key assumptions for deriving these conclusions: Both binding and unbinding operators have quadratic forms, and input vectors are i.i.d. random gaussian vectors. The former assumption is reasonable under the latter assumption because a quadratic binding should be enough to capture the statistical relationship between the inputs when the inputs are gaussian. We leave an investigation of the optimal binding under general input statistics for future work.

Our work contains several novel aspects relative to previous VSA work. First, we optimized the binding operator using a fixed-point algorithm...
instead of handcrafting a binding operator. By analyzing the structure of
the numerically optimized binding matrices, we discovered a new family
of binding operators based on solutions of the Hurwitz matrix equations.
We also extended previous analyses on the dictionary decoding to arbitrary
quadratic binding matrices. Our analysis revealed that binding with ran-
dom matrices is asymptotically optimal among quadratic binding methods
when many pairs are bound together.

Many binding mechanisms have been proposed previously in the frame-
work of VSA (Smolensky, 1990; Plate, 1995; Kanerva, 1997; Rachkovskij &
Kussul, 2001; Gallant & Okaywe, 2013; Gosmann & Eliasmith, 2019; Frady
et al., 2021; see Kleyko, Rachkovskij, Osipov, & Rahimi, 2022, for a review).
In particular, Frady and colleagues (2021) proposed a block-wise circular
convolution method to conserve the sparsity of the composition. At the
limit where each block is a $2 \times 2$ matrix, their binding method corresponds
to our sparse $K$-compositional binding with $K = 2$ in which a matrix repre-
sentation of the complex numbers is used for binding. However, their analy-
sis is limited to the case when the input is a block-wise, one-hot vector,
and they did not investigate other block-wise binding mechanisms. In ad-
dition, the relationship between the Clifford algebra, a generalization of the
quaternion algebra, and HRR was previously investigated by Aerts and col-
leagues (2009), though they did not study the space of binding mechanisms
or the optimization of binding methods. Recently, Ganesan and colleagues
(2021) proposed a modification of HRR by introducing a projection step and
demonstrating that it improves HRR by over $100 \times$. However, this claim was
supported by a comparison with a naive HRR, which is known to be unstab-
le (see appendix C.1 and section 3.6.4 of Plate, 1994).

Recent experimental results found a mixed representation of sensory
stimuli and context cues in the prefrontal cortex (Rigotti et al., 2013) and hip-
locampus (Nieh et al., 2021). However, it remains unclear whether mixed
representation in the brain is random or structured (Hirokawa, Vaughan,
Masset, Ott, & Kepecs, 2019). Our results suggest that depending on the
task configuration, random binding might be enough for an accurate un-
binding, though it is unclear if unbinding is crucial in the tasks employed in
these experiments. Wiring should be minimized in the brain; hence, sparse
connectivity of the proposed octonion binding is potentially beneficial from
this additional biological constraint. The sparse connectivity should be also
beneficial for an implementation in neuromorphic hardwares (Kleyko et al.,
2021).

The binding problem is also an important topic in machine learning
(Greff et al., 2020). In knowledge graph embedding tasks (Nickel, Mur-
phy, Tresp, & Gabrilovich, 2015), Nickel and colleagues (2016) showed that
HRR yields a better generalization performance than methods based on
nonlinear projection of a concatenated vector. Moreover, in visual ques-
tion answering tasks, binding of an image representation and a query rep-
resentation is crucial for solving the task. The Hadamard product is often
employed for this binding (Antol et al., 2015; Santoro et al., 2017), but more elaborate binding mechanisms, such as self-attention on concatenated vectors, are suggested to improve learning performance (Teney, Anderson, He, & Van Den Hengel, 2018). Another related task is a vector factorization problem, in which both $a_\mu$ and $b_\mu$ are estimated simultaneously given composition $c$ (Frady, Kent, Olshausen, & Sommer, 2020; Kent, Frady, Sommer, & Olshausen, 2020).

Finally, unlike the quaternions, the octonions are rarely applied to the domain of science (Baez, 2002). Our work provides a rare practical application of octonion algebra. More generally, our work indicates a potential link between the mathematics of quadratic forms and the binding problem in cognitive science and machine learning.

**Appendix A: Quadratic Binding**

**A.1 Fixed-Point Condition of the Mean-Squared Error.** From equations 2.1, 2.2, and 2.4, the loss function $\ell_a$ is written as

$$\ell_a = \frac{1}{N} \left\langle \sum_{i=1}^{N} (a_i^1 - \hat{a}_i^1)^2 \right\rangle_{p(S)}$$

$$= \frac{1}{N} \left\langle \sum_{i=1}^{N} \left( a_i^1 - \sum_{\mu=1}^{L} \sum_{j=1}^{N} \sum_{l=1}^{N} \sum_{m=1}^{N} \left[ \sum_{k=1}^{N_c} Q_{ijk} P_{lmk} b_{ij}^\mu m \right] b_{1j}^\mu b_{1i}^\mu \right)^2 \right\rangle_{p(S)}, \quad (A.1)$$

where $\langle \cdot \rangle_{p(S)}$ is the expectation over random vectors $a_\mu$ and $b_\mu$ sampled i.i.d. from a gaussian distribution $N(0, I_N)$. For simplicity, we introduce a fourth-order tensor $M$ as

$$M_{li}^{mj} = \sum_{k=1}^{N_c} Q_{ijk} P_{lmk}. \quad (A.2)$$

Then the loss is rewritten as

$$\ell_a = \frac{1}{N} \left\langle \sum_{i=1}^{N} \left( a_i^1 \right)^2 - 2 \sum_{\mu=1}^{L} \sum_{j=1}^{N} \sum_{l=1}^{N} \sum_{m=1}^{N} M_{mj}^{li} b_{ij}^\mu b_{lj}^\mu b_{1j}^\mu \right) \right\rangle_{p(S)}, \quad (A.3)$$
The expectation over the last quadratic term becomes

\[
\langle \sum_{i=1}^{N} \left( \sum_{\mu=1}^{L} \sum_{j=1}^{N} \sum_{l=1}^{N} \sum_{m=1}^{N} M_{mj}^{li} a_{i}^{\mu} b_{j}^{1\mu} b_{m}^{1\mu} \right)^{2} \rangle
\]

\[
= \sum_{\mu=2}^{L} \sum_{i} \sum_{l} \sum_{j} \sum_{m} \left( M_{mj}^{li} \right)^{2}
\]

\[
+ \sum_{i} \sum_{l} \left( \sum_{j} \sum_{m} M_{mj}^{li} M_{mj}^{li} + \sum_{j} \sum_{m} M_{mj}^{li} M_{jm}^{li} + \sum_{j} \sum_{m} M_{ij}^{li} M_{jm}^{li} \right)
\]

\[
= \sum_{i} \sum_{l} \left( \left( \sum_{j} M_{jj}^{li} \right)^{2} + \sum_{j} \sum_{m} M_{mj}^{li} \left[ L \cdot M_{mj}^{li} + M_{jm}^{li} \right] \right). \tag{A.4}
\]

where summation runs from 1 to \(N\) unless otherwise stated. In the second line, we used

\[
\langle b_{i}^{1\mu} b_{j}^{1\mu} b_{k}^{1\mu} \rangle = \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}. \tag{A.5}
\]

Thus, the loss \(\ell_{a}\) is written as

\[
\ell_{a} = 1 - \frac{2}{N} \sum_{i} \sum_{j} M_{jj}^{li}
\]

\[
+ \frac{1}{N} \sum_{i} \sum_{l} \left( \left( \sum_{j} M_{jj}^{li} \right)^{2} + \sum_{j} \sum_{m} M_{mj}^{li} \left[ L \cdot M_{mj}^{li} + M_{jm}^{li} \right] \right). \tag{A.6}
\]

Using \(P\) and \(Q\) instead of \(M\) via equation A.2, this equation is also written as

\[
\ell_{a} = 1 - \frac{2}{N} \sum_{i} \text{tr} [P_{i} Q_{i}^{T}]
\]

\[
+ \frac{1}{N} \sum_{i} \sum_{l} \left( (\text{tr} [P_{i} Q_{i}^{T}])^{2} + \text{tr} [P_{i} Q_{i}^{T} \left( L \cdot Q_{i} P_{i}^{T} + P_{i} Q_{i}^{T} \right)] \right). \tag{A.7}
\]

Here we defined \(N \times N\) matrices \(\{P_{i}\}_{i=1}^{N}\) and \(\{Q_{i}\}_{i=1}^{N}\) by \([P_{i}]_{jk} = P_{ijk}\) and \([Q_{i}]_{jk} = Q_{ijk}\) as in the main text. By taking the gradient with respect to \(P_{i}\)
and $Q_i$, we get

$$\frac{\partial \ell_a}{\partial P_l} = 0 \Leftrightarrow Q_l = \sum_i (\text{tr} [P_l Q_i^T] I_N + L \cdot P_l Q_i^T + Q_i P_l^T) Q_i,$$

$$\frac{\partial \ell_a}{\partial Q_i} = 0 \Leftrightarrow P_i = \sum_l (\text{tr} [P_l Q_i^T] I_N + L \cdot Q_i P_l^T + P_l Q_i^T) P_l,$$ \hspace{1cm} (A.8)

where $I_N$ is the size $N$ identity matrix. Under $P = Q$ constraint, the above equations are rewritten as

$$P_l = \sum_i (\text{tr} [P_i P_l^T] I_N + L \cdot P_l P_i^T + P_i P_l^T) P_l.$$ \hspace{1cm} (A.9)

On the other hand, as a function of $\{P_i\}$ and $\{R_i\}$, the decoding error for $b$ is given as

$$\ell_b = 1 - \frac{2}{N} \sum_i \text{tr} [P_i R_i^T]$$

$$+ \frac{1}{N} \sum_i \sum_l (\text{tr} [P_i R_i^T R_l P_l^T] + \text{tr} [P_l R_i^T (L \cdot R_i P_l^T + R_l P_i^T)]) .$$ \hspace{1cm} (A.10)

Taking the gradient with respect to $P$ and $R$, we get

$$\frac{\partial \ell_b}{\partial P_l} = 0 \Leftrightarrow R_l = \sum_i (L \cdot P_l R_i^T R_l + P_l [R_l^T R_l + R_l^T R_l]) ,$$

$$\frac{\partial \ell_b}{\partial R_i} = 0 \Leftrightarrow P_i = \sum_l (L \cdot R_i P_l^T P_l + R_l [P_l^T P_l + P_l^T P_i]) .$$ \hspace{1cm} (A.11)

In particular, under $P = R$ constraint, the fixed-point condition on $\{P_i\}$ with respect to $\ell_b$ is given as

$$P_l = \sum_i (L \cdot P_i P_l^T P_l + P_l P_i^T P_l + P_i P_l^T P_i)$$ \hspace{1cm} (A.12)

for $i = 1, \ldots, N$.

**A.2 Details of the Numerical Optimization Algorithm.** Rewriting the fixed-point condition of $P_l$ with respect to the loss $\ell_a$ (see equation A.8), we get
\[ Q_{ijk} = \sum_m \sum_n \sum_i \left( \delta_{jm} L \sum_{\beta} Q_{ij\beta n} + Q_{ijk} Q_{imn} + Q_{ijn} Q_{imk} \right) P_{lmn}, \]  
(A.13)

for \( j, k = 1, \ldots, N \). Thus, introducing an \( N^2 \times N^2 \) matrix \( \Gamma^q \) by

\[ \Gamma^q_{[jN+k],[mN+n]} \equiv \sum_i \left( \delta_{jm} L \sum_{\beta} Q_{ij\beta n} + Q_{ijk} Q_{imn} + Q_{ijn} Q_{imk} \right), \]  
(A.14)

we get \( Q_{ijk} = \sum_{m,n} \Gamma^q_{[jN+k],[mN+n]} P_{lmn} \). Therefore, we can derive the binding tensor \( P \) that minimizes the loss \( \ell_a \) under a fixed \( Q \) by solving this linear equation as

\[ \text{Vec}[P] = (\Gamma^q)^{-1} \text{Vec}[Q], \]  
(A.15)

where \( \text{Vec}[P] \) and \( \text{Vec}[Q] \) are the vector representations of \( N \times N \) matrices \( P \) and \( Q \), respectively. From a similar calculation, the unbinding tensor \( Q \) that minimizes the loss \( \ell_a \) under a fixed \( P \) is given by

\[ \text{Vec}[Q] = (\Gamma^{pa})^{-1} \text{Vec}[P], \]  
(A.16)

where \( \Gamma^{pa} \) is an \( N^2 \times N^2 \) matrix:

\[ \Gamma^{pa}_{[jN+k],[mN+n]} \equiv \sum_i \left( \delta_{il} L \sum_{\alpha} R_{\alpha jn} R_{\alpha jk} + \sum_j R_{ijk} R_{ijn} + \sum_j R_{ijn} R_{ijk} \right). \]  
(A.17)

To consider minimization of \( \ell_b \), we rewrite the fixed-point condition of \( P_i \) with respect to \( \ell_b \) (see equation A.11) as

\[ R_{lmk} = \sum_i \sum_n \Gamma_{kin} P_{mn}, \]  
(A.18)

where

\[ \Gamma_{[lN+k],[iN+n]} \equiv \delta_{ik} L \sum_j R_{\alpha jn} R_{\alpha jk} + \sum_j R_{ijk} R_{ijn} + \sum_j R_{ijn} R_{ijk} \]  
(A.19)

is an \( N^2 \times N^2 \) matrix. Let us construct \( N \times N \) matrices \( \check{R}_m \) and \( \check{P}_m \) by \( [\check{R}_m]_{l,k} = R_{lmk} \) and \( [\check{P}_m]_{l,k} = P_{lmn} \), respectively (for \( m = 1, \ldots, N \)). Then, for a given \( R \), the tensor \( P \) that satisfies the fixed-point condition of \( \ell_b \) is derived as

\[ \text{Vec}[\check{P}_m] = (\Gamma^r)^{-1} \text{Vec}[\check{R}_m] \]  
(A.20)
for \( m = 1, \ldots, N \). Similarly, the fixed-point condition for \( R \) is written as

\[
P_{ijk} = \sum_l \sum_n \Gamma^{ib}_{jlk} R_{ljn}, \tag{A.21}
\]

where

\[
\Gamma^{ib}_{j[N+k],[N+n]} \equiv \delta_{il} L \sum_{\alpha} \sum_m P_{\alpha mk} P_{\alpha mn} + \sum_m P_{imk} P_{imn} + \sum_m P_{imn} P_{lmk}. \tag{A.22}
\]

Therefore, for a given \( P, R \) should satisfy

\[
\text{Vec} [\tilde{R}_j] = (\Gamma^{ib})^{-1} \text{Vec} [\tilde{P}_j] \tag{A.23}
\]

for \( j = 1, \ldots, N \).

Combining the fixed-point algorithms for \( P, Q \) in the main text, and for \( P, R \) described above, we obtain an iterative optimization algorithm of \( P, Q, R \). In pseudocode, this algorithm is written as algorithm 1. In Figures 2 and 3, we initialized \( P, Q, R \) randomly by setting their elements from i.i.d gaussian with variance \( \frac{1}{NN_c} \), then performed algorithm 1 for \( T = 100 \) iterations under \( L = 1 \). In Figure 5, we instead initialized \( P, Q, R \) as a sparse \( K \)-compositional binding tensor plus an element-wise gaussian perturbation with variance \( \sigma^2 / N^2 \). Noise was added to \( P, Q, R \) independently (hence, \( P \neq Q \neq R \) after the perturbation). Figure 6 describes the optimization process under \( L = 3 \). The optimization process becomes slower and the advantage over HRR gets smaller (compare Figure 6A with Figure 2A). However, the obtained binding matrices exhibit \( 8 \times 8 \) block diagonal structures when projected to the space where \( \tilde{P}_1 \) is diagonal (see Figures 6B and 6C).

**A.3 Lower Bound on the Cardinality Dependence.** Taking the expectation over \( b \), the readout (see equation 2.2) becomes

\[
\{a^1_i\}_{p(b)} = \left( \sum_{\mu} \sum_j \sum_l \sum_m \left( \sum_k Q_{ijk} P_{lmk} \right) b^1_m a^\mu_j \right)_{p(b)}
\]

\[
= \sum_j \sum_l \left( \sum_k Q_{ijk} P_{ljk} \right) a^1_j. \tag{A.24}
\]

Thus, in order to retain the amplitude of the signal in the readout, \( P \) and \( Q \) need to satisfy

\[
\sum_{j=1}^N \sum_{k=1}^{N_c} P_{ijk} Q_{ijk} = 1. \tag{A.25}
\]
Note that $P$ and $Q$ that minimize $\ell_a$ do not necessarily satisfy this condition. However, the readout becomes unbiased against the original signal under this condition (i.e., $\langle \hat{a}_1^l - a_1^l \rangle = 0$). Under this constraint, equation A.7 is rewritten as

$$\ell_a = \frac{1}{N} \sum_i \sum_{l \neq i} (\text{tr} [P_i Q_i^T])^2 + \frac{1}{N} \sum_i \sum_l \text{tr} [P_i Q_i^T (P_i Q_i^T + L Q_l P_l^T)] \tag{A.26}$$

Therefore, at the large $L$ limit, the last term, $\text{tr} [P_i Q_i^T Q_i P_i^T]$, becomes the dominant factor of the loss function. Hence, we consider minimization of this dominant term under the constraint equation A.25. The Lagrangian for this constrained minimization is given by

$$\mathcal{L}_a = \frac{1}{2} \sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} [P_i Q_i^T Q_i P_i^T] - \sum_{i=1}^{N} \lambda_i (\text{tr} [P_i Q_i^T] - 1) \tag{A.27}$$

where $\lambda_i \geq 0$ is a Lagrange multiplier. The minimizer $Q_i$ needs to satisfy

$$\frac{\partial \mathcal{L}_a}{\partial Q_i} = 0 \iff \lambda_i P_i = Q_i \sum_{l=1}^{N} P_l^T P_l \tag{A.28}$$

for $i = 1, \ldots, N$. Let us assume that $\sum_{i=1}^{N} P_i^T P_i$ is invertible. Note that $\sum_{i=1}^{N} P_i^T P_i$ might not be invertible especially under $N \ll N_c$, because $P_i$ is a $N \times N_c$ matrix. However, because $\sum_{i=1}^{N} P_i^T P_i$ is an positive semidefinite matrix, if it is not invertible, the composition $c$ spans a subspace of $N_c$-dimensional space, which should not provide any advantage over smaller $N_c$. Under the invertibility assumption, $Q_i$ should satisfy

$$Q_i = \lambda_i P_i \left( \sum_{l=1}^{N} P_l^T P_l \right)^{-1} \tag{A.29}$$

Substituting $Q_i$ in equation A.25 with the equation above, we get

$$1 = \text{tr} [P_i Q_i^T] = \lambda_i \text{tr} \left[ P_i^T P_i \left( \sum_{l=1}^{N} P_l^T P_l \right)^{-1} \right] \tag{A.30}$$

Because $P_i \left( \sum_{l} P_l^T P_l \right)^{-1} P_i^T$ is a positive semidefinite matrix, $\text{tr} [P_i^T P_i \left( \sum_{l} P_l^T P_l \right)^{-1}] > 0$ (if all the eigenvalues are zero, the equation above does not hold). Thus,
\[ \lambda_i = \left( \text{tr} \left[ p_i^T P_i \left( \sum_{l=1}^{N} p_l^T P_l \right)^{-1} \right] \right)^{-1}. \tag{A.31} \]

Multiplying equation A.28 with \( Q_i^T \) from the right, taking the trace, and summing over \( i \),

\[ \sum_{i=1}^{N} \lambda_i \text{tr} \left[ P_i Q_i^T \right] = \sum_{i=1}^{N} \text{tr} \left[ Q_i^T Q_i \sum_{l=1}^{N} P_l^T P_l \right]. \tag{A.32} \]

Therefore,

\[ \sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} \left[ P_i Q_i^T Q_l P_l^T \right] = \sum_{i=1}^{N} \lambda_i \]

\[ = \sum_{i=1}^{N} \left( \text{tr} \left[ p_i^T P_i \left( \sum_{l=1}^{N} p_l^T P_l \right)^{-1} \right] \right)^{-1} \]

\[ \geq \frac{N^2}{\sum_{i=1}^{N} \text{tr} \left[ P_i^T P_i \left( \sum_{l=1}^{N} p_l^T P_l \right)^{-1} \right] } = \frac{N^2}{N_c}. \tag{A.33} \]

In the last line, we used Jensen’s inequality with \( 1/x \) (i.e., \( \left( \frac{1}{N} \sum_i x_i \right)^{-1} \leq \frac{1}{N} \sum_i \frac{1}{x_i} \)). Therefore, as long as \( \sum_{i=1}^{N} p_i^T P_l \) is invertible, the dominant error term of \( \ell_a \) is lower-bounded by \( LN/N_c \).

**A.4 Decoding with a Dictionary.** Although decoding in vector-symbolic architecture is typically noisy, especially when \( L > N_c/N \), if we know the dictionary of vectors from which \( a \) is sampled, it is possible to recover \( a \) accurately by matching the decoded vector \( \hat{a} \) with vectors \( \{a_\mu\}_{\mu=1}^{D} \) in the dictionary. Below, we set \( \mu = 1 \) as the target vector (as before), \( \mu = 2, \ldots, L \) as the other vectors bound to the composition \( c \), and \( \mu = L + 1, \ldots, D \) as the rest of the vectors in the dictionary. We denote the inner product between the retrieved vector \( \hat{a}_1 \) and \( \mu \)th vector in the dictionary \( a_\mu \) as

\[ z_\mu \equiv \hat{a}_1^T a_\mu, \tag{A.34} \]

then pick \( a_\mu \) with the largest \( z_\mu \) as the decoded vector. Because all \( a_\mu \) has nearly the same norm (\( \|a_\mu\|^2 \approx N \)), this is approximately equivalent to choosing \( a_\mu \) closest to \( \hat{a}_1 \) in terms of L2-norm (i.e., \( \text{argmin}_\mu \|\hat{a}_1 - a_\mu\|^2 \)). The probability of a correct classification under this decoding method is
\[ P_{\text{correct}} = \int dz_1 \ldots dz_DP [z_1, \ldots, z_D] \hat{\theta} [z_1 > z_2, \ldots, z_1 > z_D]. \]  

(A.35)

where \( \hat{\theta} [x] \) is the indicator function. Because \( \{z_\mu\} \) are not independent of each other, \( P_{\text{correct}} \) is generally not analytically tractable. However, we can approximately estimate \( P_{\text{correct}} \) under \( N \gg 1 \) for any quadratic binding methods satisfying equation A.25 in a similar manner to previous work (Murdock, 1982; Plate, 1995; Frady et al., 2018; Steinberg & Sompolinsky, 2022). We first normalize variables \( \{z_\mu\}_{D=1}^{D} \) as

\[ \hat{z}_\mu = \frac{a_\mu^T a_\mu}{a_1^T a_1}. \]  

(A.36)

This normalization improves the accuracy of the gaussian approximation we introduce below. Because the normalization does not change the relative order among \( \{z_\mu\}_{D=1}^{D} = 1 \), the probability of a correct classification is written as

\[ P_{\text{correct}} = \int d\hat{z}_1 \ldots d\hat{z}_D P [\hat{z}_1, \ldots, \hat{z}_D] \hat{\theta} [\hat{z}_1 > \hat{z}_2, \ldots, \hat{z}_1 > \hat{z}_D]. \]  

(A.37)

To evaluate this integral, we approximate the probability distribution \( P [\hat{z}_1, \ldots, \hat{z}_D] \) with a gaussian distribution,

\[ P [\hat{z}_1, \ldots, \hat{z}_D] \approx q [\hat{z}_1, \ldots, \hat{z}_D] \equiv N (z; \bar{z}, \Sigma), \]  

(A.38)

where \( z = [\hat{z}_1, \ldots, \hat{z}_D]^T \). By definition, \( \hat{z}_\mu \) follows

\[ \hat{z}_\mu = \frac{1}{\sum_{k=1}^{N} (a_1^k)^2} \sum_{i=1}^{L} \sum_{\nu=1}^{N} \sum_{l=1}^{M} \sum_{m=1}^{N} M_{i, j, l, m}^\mu (a_i^l)(a_\nu^m)(b_j^l b_\sigma^m), \]  

(A.39)

where \( M_{i, j, l, m}^\mu = \sum_k P_{lmk} Q_{ijk} \) (see equation A.2). Taking the expectation over randomly sampled \( \{a_\mu\}_{D=1}^{D} \) and \( \{b_\mu\}_{L=1}^{L} \), the mean is estimated as

\[ \langle \hat{z}_\mu \rangle = \left( \frac{1}{\sum_{k=1}^{N} (a_1^k)^2} \sum_{i=1}^{L} \sum_{j=1}^{M} M_{i, j}^\mu (a_i^1)^2 \right) = \delta_{1, \mu}. \]  

Here, we used equation A.25. On the other hand, the covariance becomes

\[ \Sigma_{\mu \nu} = \left( \langle \hat{z}_\mu - \delta_{1, \mu} \rangle (\hat{z}_\nu - \delta_{1, \nu}) \right) \]

\[ = \sum_{\rho, \sigma} \sum_{i, j} \sum_{l, m} \sum_{j', l', m'} M_{i, j, l, m}^\mu M_{i', j', l', m'}^\nu \left( \langle b_i^l b_\sigma^m b_j^l b_\sigma^m \rangle \right) \frac{1}{\sum_{k} (a_1^k)^2} \left( \delta_{1, \mu} \delta_{1, \nu} - \delta_{1, \mu} \delta_{1, \nu} \right). \]  

(A.40)
The expectation over $b$ is nonzero only when $\rho = \sigma$, but given $\rho = \sigma$, the expectation over $a$ is nonzero only when $\mu = \nu$. Therefore, $\Sigma_{\mu\nu} = 0$ for $\mu \neq \nu$, meaning that the joint distribution $q[\hat{z}_1, \ldots, \hat{z}_D]$ is factorized under the gaussian approximation. The second moment is evaluated as

$$
\langle (\hat{z}_\mu)^2 \rangle = \sum_{\rho=1}^L \sum_{i,j,f} \sum_{l,m,w} M_{m,j}^{li} M_{m,j}^{lf} \langle b_1^j b_1^f b_\rho^w b_\rho^m \rangle \left( \frac{1}{(\sum_k a_k^i a_k^j)} \right)^2 a_i^\mu a_i^\nu a_i^\rho a_i^\sigma.
$$

The expectation over $b$ is given as

$$
\langle b_1^j b_1^f b_\rho^w b_\rho^m \rangle = \delta_{jj} \delta_{mm'} + \delta_{1\rho} \left[ \delta_{jm} \delta_{jm'} + \delta_{jm'} \delta_{jm} \right],
$$

while the expectation over $a$ is estimated as (see appendix A.5)

$$
\langle \left( \frac{1}{(\sum_k a_k^i a_k^j)} \right)^2 a_i^\mu a_i^\nu a_i^\rho a_i^\sigma \rangle = \begin{cases} 
\delta_{\rho,\delta_{\mu,+\delta_{\nu,m'}+(\delta_{\mu,m'}\delta_{\nu,m'})}} & \mu \geq 2 \\
\frac{\delta_{\mu,\delta_{\nu,m'}+(\delta_{\mu,m'}\delta_{\nu,m'})}}{N(N-2)} + \frac{\delta_{\mu,\delta_{\nu,m'}+(\delta_{\mu,m'}\delta_{\nu,m'})}}{N(N+2)} & \mu = 1.
\end{cases}
$$

Thus, for $\mu > 2$, the variance $\langle (\hat{z}_\mu)^2 \rangle$ follows

$$
\langle (\hat{z}_\mu)^2 \rangle = \sigma_0^2 + \sigma_1^2 + [\mu \leq L] \sigma_2^2,
$$

where

$$
\sigma_0^2 = \frac{1}{(N-2)(N-4)} \sum_{i,j} \sum_{l,m,w} M_{m,j}^{li} M_{m,j}^{lf} \delta_{jj'} \delta_{mm'} \delta_{ii'} \delta_{ii'},
$$

$$
\sigma_1^2 = \frac{1}{(N-2)(N-4)} \sum_{i,j} \sum_{l,m,w} M_{m,j}^{li} M_{m,j}^{lf} \left[ \delta_{jm} \delta_{jm'} + \delta_{jm'} \delta_{jm} \right] \delta_{ii'} \delta_{ii'},
$$

$$
\sigma_2^2 = \frac{1}{(N-2)(N-4)} \sum_{i,j} \sum_{l,m,w} M_{m,j}^{li} M_{m,j}^{lf} \delta_{jj'} \delta_{mm'} \left[ \delta_{ii} \delta_{ii'} + \delta_{ii'} \delta_{ii} \right].
$$

Note that $\sigma_2^2$ term appears only when the vector $a_\rho$ is bound to the composition $c$ (i.e., $\mu \leq L$). Summing over the delta functions and using $N \gg 1$, the components $\sigma_0^2, \sigma_1^2, \sigma_2^2$ are rewritten as

$$
\sigma_0^2 = \frac{L}{N^2} \sum_{i,l} \sum_{j,m} \left( M_{m,j}^{li} \right)^2,
$$
\[
\sigma_1^2 = \frac{1}{N^2} \sum_{i,l} \left( \left[ \sum_j M_{ij}^l \right]^2 + \sum_{j,m} M_{mj}^l M_{jm}^l \right),
\]
\[
\sigma_2^2 = \frac{1}{N^2} \sum_{j,m} \left( \left[ \sum_i M_{mj}^l \right]^2 + \sum_{i,l} M_{il}^l M_{mj}^l \right). \tag{A.46}
\]

On the other hand, at \( \mu = 1 \), the variance follows
\[
\left( z_{1\mu} - \delta_{1\mu} \right)^2 \approx \sigma_0^2 + \sigma_1^2 + \sigma_2^2 + \sigma_3^2, \tag{A.47}
\]
where the extra term \( \sigma_3^2 \) is given as
\[
\sigma_3^2 = \frac{1}{N(N+2)} \sum_{i,i'} \sum_{j,j'} \sum_{l,l'} \sum_{m,m'} \sum_{i,j} M_{ij}^l M_{ij}^{l'} \left( \delta_{ii'} \delta_{jj'} + \delta_{ii'} \delta_{jj'} \right) \left( \delta_{jm} \delta_{jm'} - 1 \right)
+ \frac{1}{N(N+2)} \sum_{i,i'} \sum_{j,j'} \sum_{l,l'} \sum_{m,m'} \sum_{i,j} M_{ij}^l M_{ij}^{l'} \left( \delta_{ii'} \delta_{jj'} \delta_{jm} \delta_{jm'} \right)
+ \frac{1}{N(N+2)} \sum_{i,i'} \sum_{j,j'} \sum_{l,l'} \sum_{m,m'} \sum_{i,j} M_{ij}^l M_{ij}^{l'} \left( \delta_{ii'} \delta_{jj'} \delta_{jm} \delta_{jm'} \right)
+ \frac{2}{N} + \frac{1}{N^2} \left( \sum_{m,m'} \left[ \sum_{i,j} M_{ij}^l \right] \left[ \sum_{i,j} M_{ij}^{l'} \right] + \sum_{i,l} \left[ \sum_{j,m} M_{ij}^l \right] \left[ \sum_{m} M_{mj}^{Il} \right] + \sum_{i,l} \left[ \sum_{j,m} M_{ij}^l \right] \left[ \sum_{m} M_{mj}^{Il} \right] \right)
+ \sum_{i,l} \sum_{j,m} M_{mj}^{Il} M_{jm}^{Il} \tag{A.48}
\]
Notably, of the four terms, \( \sigma_0^2, \ldots, \sigma_3^2 \) consist of the variance, and only \( \sigma_0^2 \) scales with the number of bound pairs \( L \). Thus, at the large \( L \) limit, the variance of all \( \mu \) follows
\[
\left( z_{\mu} - \delta_{1\mu} \right)^2 = L \left( \sum_{i,l} \sum_{j,m} \left( M_{mj}^l \right)^2 + O \left( \frac{1}{L} \right) \right) \geq L \left( \frac{N^2}{N_c} + O \left( \frac{1}{L} \right) \right). \tag{A.49}
\]
The last inequality follows from equation A.33. On the other hand, under \( L \sim O(1) \), \( \sigma_s^2 \), \( \sigma_l^2 \), and \( \sigma_d^2 \) may play an important role. For convenience, let us denote

\[
\sigma_s^2 \equiv \sigma_0^2 + \sigma_1^2 + \sigma_2^2 + \sigma_3^2, \quad \sigma_l^2 \equiv \sigma_0^2 + \sigma_1^2 + \sigma_2^2, \quad \sigma_d^2 \equiv \sigma_0^2 + \sigma_1^2. \tag{A.50}
\]

The first term, \( \sigma_s^2 \), corresponds to the variance of the target readout \( \hat{z}_1 \), while \( \sigma_l^2 \) is the variance of readout \( \hat{z}_\mu \) for \( \mu = 2, \ldots, L \), and \( \sigma_d^2 \) is the variance of \( \hat{z}_\mu \) for \( \mu = L + 1, \ldots, D \). Because \( q[\hat{z}_1, \ldots, \hat{z}_D] \) is factorized, using \( \sigma_s^2 \), \( \sigma_l^2 \), \( \sigma_d^2 \), we get

\[
P_{\text{correct}} \approx \int d\hat{z}_1 q[\hat{z}_1] \prod_{\mu=2}^D \int d\hat{z}_\mu q[\hat{z}_\mu] \Theta[\hat{z}_1 > \hat{z}_\mu] = \int \frac{d\hat{z}_1}{\sqrt{2\pi \sigma_s^2}} e^{-(\hat{z}_1 - 1)^2/2\sigma_s^2} \left( \int_{-\infty}^{\hat{z}_1} \frac{dz_l}{\sqrt{2\pi \sigma_l^2}} e^{-z_l^2/2\sigma_l^2} \right)^{L-1} \times \left( \int_{-\infty}^{\hat{z}_1} \frac{dz_d}{\sqrt{2\pi \sigma_d^2}} e^{-z_d^2/2\sigma_d^2} \right)^{D-L} = \int \frac{dz}{\sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( z - \frac{1}{\sigma_s} \right)^2 \right] \left( \Phi \left[ \frac{\sigma_s z}{\sigma_l} \right] \right)^{L-1} \left( \Phi \left[ \frac{\sigma_s z}{\sigma_d} \right] \right)^{D-L},
\]

where \( \Phi[z] \equiv \int_{-\infty}^{z} \frac{dy}{\sqrt{2\pi}} e^{-y^2/2} \) is the cumulative distribution function of a gaussian distribution \( \mathcal{N}(0, 1) \). Here, \( \left( \Phi \left[ \frac{\sigma_s z}{\sigma_l} \right] \right)^{L-1} \) evaluates the probability of correct classification against vectors in the composition \( c \), while \( \left( \Phi \left[ \frac{\sigma_s z}{\sigma_d} \right] \right)^{D-L} \) captures the classification accuracy against the rest of words in the dictionary.

Because \( \sigma_s^2, \sigma_l^2, \sigma_d^2 \) depend on the choice of the binding and unbinding operators \( P \) and \( Q \), \( P_{\text{correct}} \) also depends on the binding methods. For instance, under the octonion binding, from equations A.46 and 3.18, we get

\[
\sigma_s^2 = \frac{1}{N} \left( L + \frac{3}{2} \right), \quad \sigma_l^2 = \frac{1}{N} \left( L + \frac{1}{2} \right), \quad \sigma_d^2 = \frac{1}{N} \left( L + \frac{1}{4} \right), \tag{A.51}
\]

whereas under HRR and also under the random binding, assuming \( N \gg 1 \),

\[
\sigma_s^2 = \frac{1}{N} (L + 3), \quad \sigma_l^2 = \frac{1}{N} (L + 2), \quad \sigma_d^2 = \frac{1}{N} (L + 1). \tag{A.52}
\]
Note that at the large $L$ limit, the probability of correct classification under all three binding methods converges to

$$P_{\text{correct}} \approx \int \frac{dz}{\sqrt{2\pi}} \exp \left[ -\left( z - \sqrt{\frac{N}{L}} \right)^2 \right] \left( \Phi \left[ z \right] \right)^{D-1}.$$  

(A.53)

This result matches with equation 2.35 of Frady et al. (2018). However, the theory from Frady et al. (2018) also indicates that all binding methods written as $c_k = \sum_i P_{ki}^b a_i$ with $P_{ki}^b = \left( \sum_j P_{ijk} b_j \right)$ should yield the same performance as long as $P^b$ is a unitary matrix even under a small $L$. Because both HRR and the octonion binding satisfy this unitary condition on average, their theory predicts $P_{\text{correct}} \approx \int \frac{dz}{\sqrt{2\pi}} e^{-h^2/2} \left[ \Phi \left( \sqrt{\frac{L}{L+1}} h + \sqrt{\frac{N}{L+1}} \right) \right]^{D-1}$ for both binding methods. Thus, it does not capture the performance difference between the two binding methods, though this estimate captures HRR decoding performance well.

Our analysis described in this section is based on previous analyses (Murdock, 1982; Plate, 1995; Frady et al., 2018; Steinberg & Sompolsky, 2022), but it is different in several ways. First, we derived the dictionary decoding performance for arbitrary quadratic binding methods, which enables us to capture the performance difference between HRR and the octonion binding methods (see Figure 8B). Second, we approximated the joint distribution with a multivariate Gaussian distribution as shown in equation A.38 instead of approximating it with a factorized distribution as $P[z_1, \ldots, z_D] \approx \prod_{i=1}^D \mathcal{N} \left( z_i; \mu_i, \sigma_i^2 \right)$. Although it does not change the resulting expression, it relies on fewer assumptions. We also normalized the inner product as shown in equation A.36. We found that this normalization suppresses the overestimation of variance in the Gaussian approximation.

**A.5 Estimation of $a$-Dependent Terms in the Variance.** Here, we estimate the expectation of $a_i^\mu a_i^\rho / \left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2$ over random Gaussian vectors $a$ under $N \gg 1$. First, for $\mu \geq 2$, we get

$$\left\langle \frac{1}{\left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2} a_i^\mu a_i^\rho a_i^\sigma / \left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2 \right\rangle = \left( \delta_{i\mu} \delta_{i\rho} + \delta_{\mu\rho} \left[ \delta_{i\mu} \delta_{i\rho} + \delta_{i\mu} \delta_{i\rho} \right] \right) \left\langle \frac{1}{\left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2} \right\rangle$$

$$+ \delta_{i\mu} \delta_{i\rho} \left( \left\langle \frac{a_i^1 a_i^1}{\left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2} \right\rangle - \left\langle \frac{1}{\left( \sum_{k=1}^N a_k^1 a_k^1 \right)^2} \right\rangle \right)$$
\[
\frac{1}{(N-2)(N-4)} \left( \delta_{ii} \delta_{ll'} + \delta_{ii} \delta_{ll'} + \delta_{ii} \delta_{ll'} \right) \\
- \frac{4 \delta_{ii} \delta_{ll'} \delta_{ll'}}{N(N-2)(N-4)}. \tag{A.54}
\]

In the last line, we used
\[
\left\langle \frac{1}{(\sum_k a_k^1 a_k^1)^2} \right\rangle_a = \left\langle \frac{1}{x^2} \right\rangle_{x \sim \chi_k^2} = \frac{1}{(N-2)(N-4)},
\]
\[
\left\langle \frac{a_i^1 a_i^1}{(\sum_k a_k^1 a_k^1)^2} \right\rangle_a = \left\langle \frac{x}{(x+y)^2} \right\rangle_{x \sim \chi_i^2; y \sim \chi_j^2} = \frac{1}{N(N-2)}, \tag{A.55}
\]

where \(\chi_k^2\) is the chi-squared distribution with degree \(k\). Similarly, under \(\mu = 1\),
\[
\left\langle \frac{1}{(\sum_k a_k^1 a_k^1)^2} \right\rangle = \left\langle \frac{1}{x^2} \right\rangle_{x \sim \chi_k^2} = \frac{1}{(N-2)(N-4)}.
\]
\[
\left\langle \frac{a_i^1 a_i^1}{(\sum_k a_k^1 a_k^1)^2} \right\rangle = \left\langle \frac{x}{(x+y+z)^2} \right\rangle_{x,y \sim \chi_i^2; z \sim \chi_j^2} = \frac{1}{N(N+2)}. \tag{A.57}
\]

Therefore, up to the leading-order terms,
\[
\left\langle \frac{1}{(\sum_k a_k^1 a_k^1)^2} \right\rangle = \begin{cases} \\
\frac{\delta_{ii} \delta_{ll'} + \delta_{ii} \delta_{ll'} + \delta_{ii} \delta_{ll'}}{(N-2)(N-4)} & \mu \geq 2 \\
\frac{\delta_{ii} \delta_{ll'}}{N(N-2)} + \frac{\delta_{ii} \delta_{ll'} + \delta_{ii} \delta_{ll'}}{N(N+2)} & \mu = 1.
\end{cases} \tag{A.58}
\]

**A.6 Performance of the Random Binding.** We construct a random binding tensor by setting \(P = Q = R\), and choosing their elements from i.i.d. gaussian with the mean zero and the variance \(\frac{1}{NN_c}\). Under this normalization, \(P\) satisfies equation A.25 under \(N, N_c \gg 1\). From equation A.6, the average error over randomly chosen \(P\) is given as
\[ \ell_a = \frac{LN}{N_c} \left( 1 + \frac{1}{N_c} + \frac{1}{N^2} \right) + \left( \frac{1}{N} + \frac{3}{N_c} + \frac{1}{NN_c} \right). \]  
(A.59)

If \( N_c \ll N^2 \), the leading order term is \( \ell_a \approx \frac{LN}{N_c} \), which is the same with the lower bound. On the other hand, at \( N_c = N^2 \) limit, the leading order term becomes \( \ell_a \approx \frac{2LN}{N_c} \), which is twice larger than that of the tensor product representation (see equation C.22).

### Appendix B: K-Compositional Binding and Its Extensions

#### B.1 Sufficiency of the Hurwitz Matrix Equations for the Fixed-Point Condition.

Here we show that Hurwitz matrix equations \( P_jP_i^T + P_iP_j^T = 2\lambda \delta_{ij}I_N \) with \( \lambda = \frac{1}{N^2+2} \) are sufficient for the fixed-point conditions with respect to both \( \ell_a \) (see equation A.9) and \( \ell_b \) (see equation A.12) under \( P = Q = R \) constraint. Recall that \( L \) is the number of bound pairs in the composition. Although we mainly focused on \( L = 1 \) in the main text, we prove the results for arbitrary \( L \). First, taking the trace of the Hurwitz matrix equations, we get \( tr[P_iP_j^T] = \lambda N \delta_{ij} \). Moreover, because \( P_i \) is a square matrix, \( P_iP_i^T = \lambda I_N \) implies \( P_i^T P_i = \lambda I_N \). Thus,

\[ \sum_{j=1}^{N} \left( tr[P_jP_i^T]I_N + LP_jP_i^T + P_jP_i^T \right) P_j \]

\[ = \sum_{j=1}^{N} (\lambda N \delta_{ij}I_N + 2\lambda \delta_{ij}I_N) P_j + (L - 1) P_i \sum_{j=1}^{N} P_j^T P_j \]

\[ = \lambda (LN + 2) P_i = P_i. \]  
(B.1)

Second, using \( \sum_j \left( P_jP_i^T + P_iP_j^T \right) P_j = 2\lambda P_i \), we get

\[ \sum_j \left( LP_jP_i^T P_j + P_jP_i^T P_j + P_jP_i^T P_i \right) \]

\[ = (L - 1) P_i \sum_{j=1}^{N} P_j^T P_j + \sum_{j=1}^{N} \left[ P_jP_i^T + P_iP_j^T \right] P_j + \sum_{j=1}^{N} P_jP_i^T P_i \]

\[ = \lambda (LN + 2) P_i = P_i. \]  
(B.2)

Hence, a family of matrices \( \{P_i\}_{i=1}^{N} \) satisfying equation 3.10 also satisfies equations A.9 and A.12. In particular, under \( L = 1 \), it satisfies equations 3.8 and 3.9.
B.2 Octonion Binding. Using the Cayley-Dickson construction, a matrix representation of an element \( a = (a_1, a_2, \ldots, a_8) \) of the octonion algebra is given as (Tian, 2000)

\[
\phi(a) = \begin{pmatrix}
a_1 & -a_2 & -a_3 & -a_4 & -a_5 & -a_6 & -a_7 & -a_8 \\
a_2 & a_1 & a_4 & -a_3 & a_6 & -a_5 & -a_8 & a_7 \\
a_3 & -a_4 & a_1 & a_2 & a_7 & a_8 & -a_5 & -a_6 \\
a_4 & a_3 & -a_2 & a_1 & a_8 & -a_7 & a_6 & -a_5 \\
a_5 & -a_6 & -a_7 & -a_8 & a_1 & a_2 & a_3 & a_4 \\
a_6 & a_5 & -a_8 & a_7 & -a_2 & a_1 & -a_4 & a_3 \\
a_7 & a_8 & a_5 & -a_6 & -a_3 & a_4 & a_1 & -a_2 \\
a_8 & -a_7 & a_6 & a_5 & -a_4 & -a_3 & a_2 & a_1
\end{pmatrix}. \tag{B.3}
\]

Because octonions are not associative under multiplication (i.e., there are octonions \( a, b, c \), such that \( a \cdot (b \cdot c) \neq (a \cdot b) \cdot c \), a matrix representation of an octonion is not faithful, unlike matrix representations of the quaternions and the complex numbers. However, from \( \phi(a) \), we can still construct a family of matrices \( P = [P_1, \ldots, P_8] \) that satisfies the Hurwitz matrix equations, which we can use as the basis of binding matrices. Under this binding, up to a constant factor, the composition \( c \) of two elements is calculated as

\[
\begin{align*}
c_1 &= a_1 b_1 + a_2 b_2 + a_3 b_3 + a_4 b_4 + a_5 b_5 + a_6 b_6 + a_7 b_7 + a_8 b_8, \\
c_2 &= a_1 b_2 - a_2 b_1 + a_3 b_4 - a_4 b_3 + a_5 b_6 - a_6 b_5 - a_7 b_8 + a_8 b_7, \\
c_3 &= a_1 b_3 - a_2 b_4 - a_3 b_1 + a_4 b_2 + a_5 b_7 + a_6 b_8 - a_7 b_5 - a_8 b_6, \\
c_4 &= a_1 b_4 + a_2 b_3 - a_3 b_2 - a_4 b_1 + a_5 b_8 - a_6 b_7 + a_7 b_6 - a_8 b_5, \\
c_5 &= a_1 b_5 - a_2 b_6 - a_3 b_7 - a_4 b_8 - a_5 b_1 + a_6 b_2 + a_7 b_3 + a_8 b_4, \\
c_6 &= a_1 b_6 + a_2 b_5 - a_3 b_8 + a_4 b_7 - a_5 b_2 - a_6 b_1 - a_7 b_4 + a_8 b_3, \\
c_7 &= a_1 b_7 + a_2 b_8 + a_3 b_5 - a_4 b_6 - a_5 b_3 + a_6 b_4 - a_7 b_1 - a_8 b_2, \\
c_8 &= a_1 b_8 - a_2 b_7 + a_3 b_6 + a_4 b_5 - a_5 b_4 - a_6 b_3 + a_7 b_2 - a_8 b_1.
\end{align*}
\]

Note that because matrix representation of octonions is not unique, there are various ways to construct binding matrices that have octonion structure.

B.3 Properties of the Sparse K-Compositional Bindings. In equation 3.18, we generated sparse \( K \)-compositional binding operators by a blockwise binding. However, there are many equivalent binding operators due to invariance. In particular, we can generate a family of binding operators using an \( N \times N \) orthogonal matrix \( W (WW^T = W^T W = I_N) \). Let us denote
\( A = \{A_1, \ldots, A_K\} \) as a family of \( K \times K \) matrices that satisfies the Hurwitz matrix equations,

\[
A_iA_j^T + A_jA_i^T = 2\lambda \delta_{ij}I_K,
\]

for \( i, j = 1, \ldots, K \), with the normalization factor:

\[
\lambda = \frac{1}{LK + 2}.
\]

Setting \( N = qK \) with a natural number \( q \), we construct a binding operator \( P_n \) by

\[
P_n = \left( \sum_{k=1}^{K} W_{n,k}A_k \right) \oplus \left( \sum_{k=1}^{K} W_{n,K+k}A_k \right) \oplus \cdots \oplus \left( \sum_{k=1}^{K} W_{n,(q-1)K+k}A_k \right).
\]

In other words, we set the \( r \)th block diagonal component of \( P_n \) to \( \sum_{k=1}^{K} W_{n,(r-1)K+k}A_k \). If we choose \( W = I_N \), we recover equation 3.18. We show that under this binding, for arbitrary positive integer \( L \), the decoding error becomes \( \ell_a = \ell_b = \frac{(L-1)K+2}{LK} \) and \( \{P_n\}_{n=1}^{N} \) satisfies the fixed-point conditions for both \( \ell_a \) and \( \ell_b \). In particular, we recover \( \ell_a = \ell_b = \frac{2}{K} \) under \( L = 1 \).

**B.3.1 Decoding Error of \( a \).** Here we show that, under this binding, the error \( \ell_a \), equation A.7, satisfies \( \ell_a = \lambda K \delta_{kn} \), \( \text{tr}[P_iP_l^T] \) becomes

\[
\text{tr}[P_iP_l^T] = \sum_{r=0}^{q-1} \text{tr} \left[ \left( \sum_{k=1}^{K} W_{l,rK+k}A_k \right) \left( \sum_{n=1}^{K} W_{l,rK+n}A_n^T \right) \right]
\]

\[
= \lambda K \sum_{r=0}^{q-1} \sum_{k=1}^{K} W_{l,rK+k}W_{l,rK+n}
\]

\[
= \lambda K [WW^T]_{il} = \lambda K \delta_{il}.
\]

In the last line, we used the fact that \( W \) is an orthogonal matrix. Similarly, using \( A_iA_j^T + A_jA_i^T = 2\lambda \delta_{ij}I_K \),

\[
\sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} \left[ P_i^TP_l^T (P_lP_i^T + P_lP_i^T) \right] = \sum_{i=1}^{N} \sum_{l=1}^{N} \sum_{r=0}^{q-1} \text{tr} \left[ \sum_{k=1}^{K} \sum_{k'=1}^{K} W_{l,rK+k}W_{l,rK+k'}A_kA_{k'}^T \right.
\]

\[
\left. \sum_{n=1}^{N} \sum_{n'=1}^{N} W_{l,rK+n}W_{l,rK+n'} (A_nA_n^T + A_{n'}A_{n'}^T) \right]
\]
\[= 2\lambda^2 K \sum_{r=0}^{q-1} \sum_{k=1}^{K} \sum_{n=1}^{K} \left( [W^T W]_{rK+k, rK+n} \right)^2 \]
\[= 2\lambda^2 N K. \tag{B.8} \]

Finally, 
\[
\sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} [P_i P_i^T P_l P_l^T] \\
= \sum_{r=0}^{q-1} \sum_{k=1}^{K} \sum_{m=1}^{K} \sum_{m'=1}^{K} [W^T W]_{rK+k, rK+k'} \left[ W^T W \right]_{rK+m, rK+m'} \text{tr} \left[ A_k A_m^T A_{m'} A_k^T \right] \\
= \sum_{r=0}^{q-1} \sum_{k=1}^{K} \sum_{m=1}^{K} \text{tr} \left[ A_k A_m^T A_m A_k^T \right] \\
= N\lambda^2 K^2. \tag{B.9} \]

Therefore, from equation A.7, the loss \( \ell_a \) becomes 
\[
\ell_a = 1 - 2\lambda K + (\lambda K)^2 + 2\lambda^2 K + (L - 1) \lambda^2 K^2 \]
\[= \frac{(L - 1)K + 2}{LK + 2}. \tag{B.10} \]

Moreover, the binding operator defined by equation B.6 satisfies the fixed-point condition, equation A.9. First, from equation B.7, 
\[
\sum_{l=1}^{N} \text{tr} \left[ P_i P_i^T \right] I_N P_l = \lambda K P_i. \tag{B.11} \]

The \((r + 1)\)th diagonal block component of \( \sum_l [P_i P_i^T + P_l P_l^T] P_i \) is written as 
\[
\left[ \sum_{l=1}^{N} (P_i P_i^T + P_l P_l^T) P_i \right]_{(r+1)} = \sum_{l=1}^{N} \left( \sum_{k=1}^{K} \sum_{m=1}^{K} W_{l,rK+k} W_{l,rK+m} [A_k A_m^T + A_m A_k^T] \right) \left( \sum_{n=1}^{N} W_{l,rK+n} A_n \right) \\
= 2\lambda \sum_{k=1}^{K} \sum_{n=1}^{K} W_{l,rK+k} \left( \sum_{l=1}^{N} W_{l,rK+k} W_{l,rK+n} \right) A_n \\
= 2\lambda \left[ P_i \right]_{(r+1)} \text{th block}. \tag{B.12} \]
In addition, we have

\[
\sum_{i=1}^{N} [P_i P_i^T]_{(r+1)-th\ block} = \sum_{i=1}^{N} \left( \sum_{k=1}^{K} W_{i,rK+k} A_k \right) \left( \sum_{n=1}^{N} W_{i,rK+n} A_n^T \right) = \sum_{k=1}^{K} \sum_{n=1}^{N} [W^T W]_{rK+k,rK+n} A_k A_n^T = K \lambda I_K. \tag{B.13}
\]

By combining the equations above, we get

\[
\sum_{i=1}^{N} \left( \text{tr} [P_i P_i^T] I_N + L \cdot P_i P_i^T + P_i P_i^T \right) P_i = (\lambda K + 2 \lambda + [L - 1] \lambda K) P_i = P_i. \tag{B.14}
\]

Thus, equation B.6 indeed satisfies the fixed-point condition, equation A.9.

### B.3.2 Decoding Error of \( b \)

We next consider the decoding error of \( b, \ell_b \). Under \( P = R \), the error \( \ell_b \) is written as

\[
\ell_b = 1 - \frac{2}{N} \sum_i \text{tr} [P_i P_i^T] + \frac{1}{N} \sum_i \sum_l \left( \text{tr} [P_i P_i^T P_l P_l^T] + \text{tr} [P_l P_l^T L \cdot P_i P_i^T + P_l P_i^T] \right). \tag{B.15}
\]

From equation B.13, we get

\[
\sum_{i=1}^{N} \sum_{l=1}^{N} \text{tr} [P_i P_i^T P_l P_l^T] = \text{tr} \left[ (K \lambda)^2 I_N \right] = NK^2 \lambda^2. \tag{B.16}
\]

Because the rest of terms are the same with \( \ell_a \), the error \( \ell_b \) also follows

\[
\ell_b = 1 - 2K \lambda_K + K^2 \lambda_K^2 + 2K \lambda_K^2 + (L - 1) \lambda^2 K^2 = \frac{(L - 1) K + 2}{LK + 2}. \tag{B.17}
\]

Moreover, \( \{P_i\}_{i=1}^{N} \) constructed by equation B.6 satisfies the fixed-point condition, equation A.12. From equations B.12 and B.13, it follows that

\[
\sum_{i=1}^{N} \left( L \cdot P_l P_l^T P_i + P_l P_l^T P_i + P_l P_i^T P_i \right) = (L - 1) P_l \sum_i P_i^T P_l + \sum_l (P_i P_i^T + P_l P_l^T) P_i + \sum_l P_l P_l^T P_i = (L - 1) \lambda K P_l + 2 \lambda P_l + \lambda L P_i = P_i. \tag{B.18}
\]
### B.4 Extended Octonion Binding

The sparse octonion binding can be naturally extended to $N_c > N$ when $N_c$ satisfies $N_c = dN$ for a positive integer $d$. As before, we set $N$ to be $N = qK$ for a positive integer $q$.

Let us focus on the case when $N_c < N^2 / K$ for simplicity. Using a solution for equation B.4, $\{A_i\}_{i=1}^K$, we introduce a family of $N \times N$ matrix $\{B^{\mu \nu}\}$ as

$$B^{\mu \nu} \equiv O_K \oplus \cdots \oplus O_K \oplus A_\mu \oplus O_K \oplus \cdots \oplus O_K$$

for $\mu = 1, \ldots, K$ and $\nu = 0, \ldots, q - 1$. We then construct a family of $N \times N_c$ matrices $\{P_i\}_{i=1}^N$ from $B$ as

$$P_i = \left[ B^\left\lceil i/q \right\rceil, p, B^\left\lceil (i+1)/q \right\rceil, \ldots, B^\left\lceil (i+d-1)/q \right\rceil \right].$$

For instance, if $q = 3$ and $d = 2$, then

$$P_1 = \begin{pmatrix} A_1 & O & O & O & O & O \\ O & O & O & O & A_1 & O \\ O & O & O & O & O & O \end{pmatrix}, \quad P_2 = \begin{pmatrix} O & O & O & O & O & O \\ O & A_1 & O & O & O & O \\ O & O & O & O & A_1 & O \end{pmatrix},$$

$$P_3 = \begin{pmatrix} O & O & O & A_1 & O & O \\ O & O & O & O & O & O \\ O & O & A_1 & O & O & O \end{pmatrix}, \quad P_4 = \begin{pmatrix} A_2 & O & O & O & O & O \\ O & O & O & O & A_2 & O \\ O & O & O & O & O & O \end{pmatrix}, \ldots$$

Let us estimate the error under this binding method. From the definition, $P_i P_i^T$ is written as

$$P_i P_i^T = \sum_{r=0}^{d-1} [(i + r) \% q = (l + r) \% q] \oplus O_K \oplus \cdots \oplus O_K \oplus A^\left\lceil i/q \right\rceil A_i^T$$

$$\oplus O_K \oplus \cdots \oplus O_K,$$

where $[x]_+$ is an indicator function that returns 1 if $x$ is true and returns 0 if false. Thus, $tr[P_i P_i^T] = d \lambda K$. This means that in order to satisfy equation A.25, the scaling factor $\lambda K$ of $A_k$ in equation B.4 needs to be $\lambda K = 1/(dK)$.

The dominant term of the error becomes

$$\frac{L}{N} \sum_{i=1}^N \sum_{l=1}^N \left[ (i + r) \% q = (l + r) \% q \right]_+ tr \left[ A^\left\lceil i/q \right\rceil A_i^T A^\left\lceil l/q \right\rceil A_l^T \right]$$
Therefore, the dominant term is the same with the lower bound obtained in appendix A.3. Calculating the rest of terms in a similar manner, we get

\[ \ell_a = \frac{N}{N_c} \left( L - 1 + \frac{2}{K} \right). \]  

(B.24)

**B.5 Construction of Higher-Order Sparse K-Compositional Bindings.**

In the simulations depicted in Figures 4, 5, and 7 to 9, we constructed sparse K-compositional bindings by using a Python library for the Cayley-Dickson construction, developed by Travis Hoppe (https://github.com/thoppe/Cayley-Dickson). Source codes for the simulations are available at https://github.com/nhiratani/quadratic_binding.

**Appendix C: Tensor-HRR Bindings**

We review two commonly used binding mechanisms: holographic reduced representation (HRR; Plate, 1995, 1997; Nickel et al., 2016) and tensor product representation (Smolensky, 1990; Smolensky et al., 2014). Subsequently, we introduce a binding that morphs from HRR to the tensor product representation as you change the vector length of the representation.

**C.1 Holographic Reduced Representation (HRR).**

**C.1.1 Definition of HRR.** Under HRR, the length of the composition vector \( c \) is the same with that of \( a \) and \( b (N_c = N) \), and the \( k \)th element of binding \( \psi \) is constructed by

\[ \psi_k(a_\mu, b_\mu) = \sum_{i=1}^{N} a_\mu^i b_\mu^{[k-i]_N} \text{ for } k = 1, \ldots, N \]  

(C.1)

where \([k - i]_N \equiv k - i \pmod{N}\), and \( a_\mu^i \) is the \( i \)th element of vector \( a_\mu \). Because the indices run from 1 to \( N \), not 0 to \( N - 1 \), we set \( b_\mu^0 = b_\mu^N \) and \( c_0 = c_N \).
for the ease of notation. Given \( c = \sum_{\mu=1}^{L} \psi(a_{\mu}, b_{\mu}) \), we can unbind \( a_1 \) from \( c \) using a query \( b_1 \) as

\[
\hat{a}_1 = \frac{1}{\|b_1\|^2} \sum_{j=1}^{N} c_{[j+i]N} b_j^1.
\]

(C.2)

Because \( c \) is rewritten as

\[
c_k = \sum_{\mu=1}^{L} \sum_{i=1}^{N} a_i^\mu b_{[k-i]N}^\mu = \sum_{\mu=1}^{L} \sum_{i=1}^{N} \sum_{j=1}^{N} a_i^\mu b_j^\mu \delta_{[i+j]N,k},
\]

(C.3)

this is a quadratic binding with

\[
P_{ijk} = \delta_{[i+j]N,k}.
\]

(C.4)

Similarly, if the amplitude of \( a_\mu \) and \( b_\mu \) is normalized as \( \|a_\mu\|^2 = \|b_\mu\|^2 = N \), unbinding of \( a \) and \( b \) are given as

\[
Q_{ijk} = R_{ijk} = \frac{1}{\sqrt{N}} \delta_{[i+j]N,k}.
\]

(C.5)

Alternatively, by moving the half of the normalization factor to the binding operator, we can rewrite \( P, Q, R \) as

\[
P_{ijk} = Q_{ijk} = R_{ijk} = \frac{1}{\sqrt{N}} \delta_{[i+j]N,k}.
\]

(C.6)

C.1.2 Normalization of HRR for L2 Error Minimization. Under both normalizations specified above, the amplitude of the recovered signal becomes the same with the original signal amplitude (see equation A.24). However, this normalization does not necessarily minimize the mean-squared error \( \ell_a \) and \( \ell_b \). To see this, we define \( P_{ijk} = Q_{ijk} = R_{ijk} = \sqrt{2} \delta_{[i+j]N,k} \) where \( \lambda \) is a scaling factor. Then, from equation 2.7, assuming that \( N \) is an even number, the loss \( \ell_a \) becomes

\[
\ell_a = 1 - 2N\lambda + ((L + 1)N + 2)N\lambda^2.
\]

(C.7)

Thus, the loss is minimized at \( \lambda = \frac{1}{(L+1)N+2} \), under which the loss follows \( \ell_a = \frac{LN+2}{(L+1)N+2} \).

In particular, when only one pair is bound to the composition \( L = 1 \), the unbinding error \( \ell_a \) defined by equation 2.4 follows
\[
\ell_a \equiv \frac{1}{N} (\| a - \hat{a} \|^2)_{p(a,b)} = \frac{N + 2}{2N + 2} \overset{N \to \infty}{\rightarrow} \frac{1}{2}. \quad (C.8)
\]

The blue line in Figure 4A plots \( \ell_a = \frac{N + 2}{2N + 2} \), where as gray dashed lines in Figures 2A and 2B represent the loss at the large \( N \) limit, \( \ell_a = \frac{1}{2} \). Notably, decoded vector \( \hat{a} \) is biased under the optimized \( \lambda \), as the amplitude of the decoded vector shrinks to the half of the original under \( L = 1 \):

\[
\langle \hat{a} \rangle_{p(b)} = \frac{N}{2N+2}a.
\]

Because of it, if we normalize the loss by the norm of the decoded vector

\[
\frac{1}{\langle \| \hat{a} \|^2 \rangle_{p(a,b)}} \langle \| a - \hat{a} \|^2 \rangle_{p(a,b)} = \frac{N + 2}{N} \overset{N \to \infty}{\rightarrow} 1.
\]

If we instead set \( \lambda = \frac{1}{N} \) to make the decoding unbiased, the loss, defined in equation 2.4, also follows \( \ell_a = 1 + \frac{2}{N} \) under \( L = 1 \) (see the blue line in Figure 4C). The loss \( \ell_b \) becomes the same with \( \ell_a \) due to the symmetry between \( a \) and \( b \) under HRR (see equation C.6 is invariant against \( i \leftrightarrow j \)).

A recent work showed that the decoding performance of HRR improves significantly by introducing normalization to the encoding vectors, so that \( |F_j(b)| = 1 \) for all \( j \) under a discrete Fourier transform \( F \) (Ganesan et al., 2021). However, their claim is supported by a comparison with a naive implementation of HRR unbinding, in which unbinding is performed with \( \hat{a} = F^{-1} (F(c) \odot F(b^{-1})) \) where \( b^{-1} \) satisfies \( F(b) \odot F(b^{-1}) = 1 \). Thus, it remains questionable if it provides an advantage over the standard HRR with circular correlation unbinding (see equation C.2), considering that a naive HRR unbinding is known to be much more unstable than the standard HRR unbinding (section 3.6.4 of Plate (1994)).

C.1.3 Properties of HRR. It should be noted that HRR does not satisfy the fixed-point conditions (see equations A.9 and A.12) under a finite \( N \) regardless of the choice of the scaling factor. This is because the right-hand side of equation 3.8 becomes

\[
\sum_{i=1}^{N} (\text{tr} \left[ P_i P_i^T \right]) I_N + L \cdot P_i P_i^T + P_i P_i^T P_i = \lambda (L + 1) NP_i + \lambda P_i^{\text{res}}, \quad (C.10)
\]

where \( [P_i^{\text{res}}]_{jk} = \sqrt{\lambda} \sum_l \delta_{[2l],[i-j+k]N} \). Nonetheless, the fact that \( P = Q \) is satisfied under HRR is consistent with the condition on the optimal \( Q \) at \( L \gg 1 \) limit (see equation A.29). Under HRR,
\[
\left[ \sum_{l=1}^{N} P_l P_l^T \right]_{jm} = \sum_{l=1}^{N} \sum_{k=1}^{N} P_{ljk} P_{lmk} = \frac{1}{N} \sum_{l=1}^{N} \delta_{[l+j]N,[l+m]N} = \delta_{jm}. \tag{C.11}
\]

Thus, for a given \( P \), to minimize the Lagrangian, \( Q \) needs to satisfy \( Q_i = \lambda_i P_i \) for \( i = 1, \ldots, N \). This result supports the optimality of unbinding by circular correlation given a binding by circular convolution at \( L \gg 1 \). From the symmetry between \( a \) and \( b \) (\( P_{ijk} = P_{jik} \)), we expect \( R_i = \lambda_i P_i \) to be the optimal too at \( L \gg 1 \).

**C.2 Tensor Product Representation.** In the tensor product representation, \( S = \{ (a_\mu, b_\mu) \}_{\mu=1}^{L} \) is represented by a \( N \times N \) matrix \( C \):

\[
C = \sum_{\mu=1}^{L} a_\mu b_\mu^T. \tag{C.12}
\]

Alternatively, we can consider \( C \) as a length \( N_c = N^2 \) vector \( c = \text{Vec}[C] \). Given \( C \) and a query \( b_1 \), unbinding of \( a_1 \) is done by

\[
\hat{a}_1 = \frac{1}{\|b_1\|^2} C b_1. \tag{C.13}
\]

This unbinding is lossless if \( L = 1 \) because \( \frac{1}{\|b_1\|^2} a_1 b_1^T b_1 = a_1 \). The tensor product representation is also an example of the quadratic binding family in which, assuming \( \|a_\mu\|^2 = \|b_\mu\|^2 = N \), the tensors \( P, Q, R \) are set to

\[
P_{ijk} = Q_{ijk} = R_{ijk} = \frac{1}{\sqrt{N}} \delta_{k,(i+j)}. \tag{C.14}
\]

Notably, \( P = Q = R \) is satisfied in the tensor product representation too.

**C.3 Tensor-HRR Morphing.** For \( N_c = dN \) with \( d = 1, 2, \ldots, N \), we define tensor-HRR binding as

\[
P_{ijk} = Q_{ijk} = R_{ijk} = \frac{1}{\sqrt{N}} \delta_{[i+j]d,[i+m]d}. \tag{C.15}
\]

At \( N_c = N \) (\( d = 1 \)), this is the same with HRR (see equation C.6), whereas at \( N_c = N^2 \), \( \delta_{[i+j]N,[i+m]N} = \delta_{(i+j),k} \); thus, it becomes the tensor-product binding (see equation C.14). Noticing that \( M \) (see equation A.2) is written as
Optimal Quadratic Binding

\[ M_{m_j}^{l_i} = \frac{1}{N} \delta_{[id+j]_{LN},[ld+m]_{LN}}, \]  

(C.16)

unbinding of \( a_1 \) indeed yields

\[ \langle a_1^1 \rangle_{p(b)} = \left( \sum_j \sum_k P_{ijk} b_1^i \sum_m \sum_l P_{mka_1^\mu} b_m^\mu \right)_{p(b)} \]

\[ = \left( \sum_j \sum_l M_{l_j}^{i_j} (b_j^l)^2 a_1^1 \right)_{p(b)} \]

\[ = \frac{1}{N} \sum_j \sum_l \delta_{[id+j]_{LN},[ld+m]_{LN}} a_1^1 \]

\[ = a_1^i. \]  

(C.17)

In the last line, we used

\[ id + j \equiv ld + j \pmod{dN} \Leftrightarrow (i - l)d \equiv 0 \pmod{dN} \Leftrightarrow i = l, \]  

(C.18)

for \( i, l = 1, \ldots, N \). The decoding error, equation A.6, under this binding is estimated as below. First, from equation C.16,

\[ 1 - \frac{2}{N} \sum_i \sum_j M_{l_j}^{i_j} + \frac{1}{N} \sum_i \sum_l \left( \sum_j M_{l_j}^{i_j} \right)^2 = 1 - 2 + 1 = 0. \]  

(C.19)

On the other hand, under \( N \gg 1 \), the noise term is given as

\[ \frac{1}{N} \sum_i \sum_l \sum_j \sum_m M_{m_j}^{l_i} (LM_{m_j}^{l_i} + M_{m_j}^d) \]

\[ = \frac{1}{N^3} \sum_i \sum_l \sum_j \sum_m \left( L \delta_{[id+j]_{LN},[ld+m]_{LN}} + \delta_{[id+j]_{LN},[ld+m]_{LN}} \delta_{[id+j]_{LN},[ld+m]_{LN}} \right) \]

\[ \approx \frac{L}{d} + \frac{1}{N}. \]  

(C.20)

The last line follows under a large \( N \), because for randomly sampled integers \( 1 \leq i, l, j, m \leq N \),

\[ \Pr \left[ \delta_{[id+j]_{LN},[ld+m]_{LN}} = 1 \right] = \frac{1}{dN}. \]  

(C.21)
Combining the terms above, we get

\[ \ell_a \approx \frac{LN}{N_c} + \frac{1}{N}. \]  

(C.22)

Data Availability

The source code is available at https://github.com/nhiratani/quadratic_binding.

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