

GRÖBNER BASES OF NEURAL IDEALS

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ABSTRACT. The brain processes information about the environment via neural codes. The neural ideal was introduced recently as an algebraic object that can be used to better understand the combinatorial structure of neural codes. Every neural ideal has a particular generating set, called the canonical form, that directly encodes a minimal description of the receptive field structure intrinsic to the neural code. On the other hand, for a given monomial order, any polynomial ideal is also generated by its unique (reduced) Gröbner basis with respect to that monomial order. How are these two types of generating sets – canonical forms and Gröbner bases – related? Our main result states that if the canonical form of a neural ideal is a Gröbner basis, then it is the universal Gröbner basis (that is, the union of all reduced Gröbner bases). Furthermore, we prove that this situation – when the canonical form is a Gröbner basis – occurs precisely when the universal Gröbner basis contains only pseudo-monomials (certain generalizations of monomials). Our results motivate two questions: (1) When is the canonical form a Gröbner basis? (2) When the universal Gröbner basis of a neural ideal is *not* a canonical form, what can the non-pseudo-monomial elements in the basis tell us about the receptive fields of the code? We give partial answers to both questions. Along the way, we develop a representation of pseudo-monomials as hypercubes in a Boolean lattice.

Keywords: neural code, receptive field, canonical form, Gröbner basis, Boolean lattice

MSC classes: 92-04 (Primary), 13P25, 68W30 (Secondary)

1. INTRODUCTION

The brain is tasked with many important functions, but one of the least understood is how it builds an understanding of the world. Stimuli in one’s environment are not experienced in isolation, but in relation to other stimuli. How does the brain represent this organization? Or, to quote from Curto, Itskov, Veliz-Cuba, and Youngs, “What can be inferred about the underlying stimulus space from neural activity alone?” [7].

Curto *et al.* pursued this question for codes where each neuron has a region of stimulus space, called its *receptive field*, in which it fires at a high rate. They introduced algebraic objects that summarize neural-activity data, which are in the form of *neural codes* (0/1-vectors where 1 means the corresponding neuron is active, and 0 means silence) [7]. The *neural ideal* of a neural code is an ideal that contains the full combinatorial data of the code. The *canonical form* of a neural ideal is a generating set that is a minimal description of the receptive-field structure. Hence, the questions posed above have been investigated via the neural ideal or the canonical form [6, 7, 8, 10]. As a complement to algebraic approaches, combinatorial and topological arguments are employed in related works [5, 11, 12].

The aim of our work is to investigate, for the first time, how the canonical form is related to other generating sets of the neural ideal, namely, its Gröbner bases. This is a natural mathematical question, and additionally the answer could improve algorithms for computing the canonical form. Currently, there are two distinct methods to compute the canonical form of a neural ideal: the original method proposed in [7] and an iterative method introduced in [14]. The former method requires the computation of primary decomposition of pseudo-monomial ideals. As a result, this method is rather inefficient. Even in dimension 5, one can find codes for which this algorithm takes hundreds or even thousands of seconds to terminate or halts due to lack of memory. The

more recent iterative method relies entirely on basic polynomial arithmetic. This algorithm can efficiently compute canonical forms for codes in up to 10 dimensions; see [14]. On the other hand, Gröbner basis computations are generally computationally expensive. Nevertheless, we take full advantage of tailored methods for Gröbner basis over Boolean rings [3]. As we show in Table I, for small dimensions less or equal to 8, Gröbner basis computations are faster than canonical form ones. For larger dimensions, we have observed that in general Gröbner basis computations are faster but the standard deviation on computational time is much larger. In dimension 9, the average time to compute a Gröbner basis is around 3 seconds, but there are codes for which that computation takes close to 10 hours to finish.

Nevertheless, we believe that a thorough study of Gröbner basis of neural ideals is not only of theoretical interest, but it can lead to better procedures able to perform computations in larger dimensions. Indeed, among small codes, surprisingly many have canonical forms that are also Gröbner bases. Moreover, the iterative nature of the newer canonical form algorithm hints towards the ability to compute canonical forms and Gröbner bases of neural codes in large dimensions by ‘gluing’ those of codes on small dimensions. Such decomposition results are a common theme in other areas of applied algebraic geometry [1, 9].

The outline of this paper is as follows. Section 2 provides background on neural ideals, canonical forms, and Gröbner bases. In Section 3, we prove our main result: if the canonical form of a neural ideal is a Gröbner basis, then it is the universal Gröbner basis (Theorem 3.1). We also prove a partial converse: if the universal Gröbner basis of a neural ideal contains only so-called pseudo-monomials, then it is the canonical form (Theorem 3.12). Our results motivate other questions:

- (1) When is the canonical form a Gröbner basis?
- (2) If the universal Gröbner basis of a neural ideal is *not* a canonical form, what can the non-pseudo-monomial elements in the basis tell us about the receptive fields of the code?

Sections 4 and 5 provide some partial answers these questions. Finally, a discussion is in Section 6.

2. BACKGROUND

This section introduces neural ideals and related topics, which were first defined by Curto, Itskov, Veliz-Cuba, and Youngs [7], and recalls some basics about Gröbner bases. We use the notation $[n] := \{1, 2, \dots, n\}$.

2.1. Neural codes and receptive fields. A **neural code** (also known as a **combinatorial code**) on n neurons is a set of binary firing patterns $C \subset \{0, 1\}^n$, that is, a set of binary strings of neural activity. Note that neither timing nor rate of neural activity are recorded in a neural code.

An element $c \in C$ of a neural code is a **codeword**. Equivalently, a codeword is determined by the set of neurons that fire:

$$\text{supp}(c) := \{i \in [n] \mid c_i = 1\} \subseteq [n].$$

Thus, the entire code is identified with a set of subsets of co-firing neurons: $\text{supp}(C) = \{\text{supp}(c) \mid c \in C\} \subseteq 2^{[n]}$.

In many areas of the brain, neurons are associated with **receptive fields** in a *stimulus space*. Of particular interest are the receptive fields of *place cells*, which are neurons that fire in response to an animal’s location. More specifically, each place cell is associated with a **place field**, a convex region of the animal’s physical environment where the place cell has a high firing rate [13]. The discovery of place cells and related neurons (grid cells and head direction cells) won neuroscientists John O’Keefe, May Britt Moser, and Edvard Moser the 2014 Nobel Prize in Physiology and Medicine.

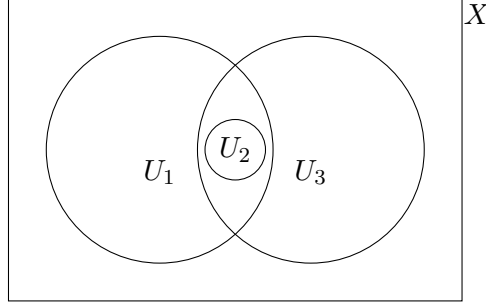


FIGURE 1. Receptive fields U_i for which the code is $C(\mathcal{U}) = \{\emptyset, 1, 123, 13, 3\}$.

Given a collection of sets $\mathcal{U} = \{U_1, \dots, U_n\}$ in a stimulus space X (here U_i is the receptive field of neuron i), the **receptive field code**, denoted by $C(\mathcal{U})$, is:

$$C(\mathcal{U}) := \left\{ c \in \{0, 1\}^n : \left(\bigcap_{i \in \text{supp}(c)} U_i \right) \setminus \left(\bigcup_{j \notin \text{supp}(c)} U_j \right) \neq \emptyset \right\}.$$

As mentioned earlier, we often identify this code with the corresponding set of subsets of $[n]$.

Example 2.1. Consider the sets U_i in a stimulus space X depicted in Figure 1. The corresponding receptive field code is $C(\mathcal{U}) = \{\emptyset, 1, 123, 13, 3\}$.

2.2. The neural ideal and its canonical form. A **pseudo-monomial** in $\mathbb{F}_2[x_1, \dots, x_n]$ is a polynomial of the form

$$f = \prod_{i \in \sigma} x_i \prod_{j \in \tau} (1 + x_j),$$

where $\sigma, \tau \subseteq [n]$ with $\sigma \cap \tau = \emptyset$. Every term in a pseudo-monomial $f = \prod_{i \in \sigma} x_i \prod_{j \in \tau} (1 + x_j)$ divides its highest-degree term, $\prod_{i \in \sigma \cup \tau} x_i$. We will use this fact several times in this work.

Each $v \in \{0, 1\}^n$ defines a pseudo-monomial ρ_v as follows:

$$\rho_v := \prod_{i=1}^n (1 - v_i - x_i) = \prod_{\{i|v_i=1\}} x_i \prod_{\{j|v_j=0\}} (1 + x_j) = \prod_{\{i \in \text{supp}(v)\}} x_i \prod_{\{j \notin \text{supp}(v)\}} (1 - x_j).$$

Notice that ρ_v is the **characteristic function** for v , that is, $\rho_v(x) = 1$ if and only if $x = v$.

Definition 2.2. Let $C \subseteq \{0, 1\}^n$ be a neural code. The **neural ideal** J_C is the ideal in $\mathbb{F}_2[x_1, \dots, x_n]$ generated by all ρ_v for $v \notin C$:

$$J_C := \langle \{\rho_v | v \notin C\} \rangle.$$

It follows that the variety of the neural ideal is the code itself: $V(J_C) = C$. The following lemma provides the algebraic version of the previous statement:

Lemma 2.3 (Curto, Itskov, Veliz-Cuba, and Youngs [7, Lemma 3.2]). *Let $C \subset \{0, 1\}^n$ be a neural code. Then*

$$I(C) = J_C + \langle x_i(1 + x_i) \mid i \in [n] \rangle,$$

where $I(C)$ is the ideal of the subset $C \subset \{0, 1\}^n$.

Note that the ideal generated by the Boolean relations $\langle x_i(1 + x_i) : i \in [n] \rangle$ is contained in $I(C)$, regardless of the structure of C .

A pseudo-monomial f in an ideal J in $\mathbb{F}_2[x_1, \dots, x_n]$ is **minimal** if there does not exist another pseudo-monomial $g \in J$, with $g \neq f$, such that $f = gh$ for some $h \in \mathbb{F}_2[x_1, \dots, x_n]$.

Definition 2.4. The **canonical form** of a neural ideal J_C , denoted by $\text{CF}(J_C)$, is the set of all minimal pseudo-monomials of J_C .

Algorithms for computing the canonical form were given in [7, 8, 14]. In particular, [14] describes an iterative method to compute the canonical form that is significantly more efficient than the original method presented in [7].

The canonical form $\text{CF}(J_C)$ is a particular generating set for the neural ideal J_C [7]. The main goal in this work is to compare $\text{CF}(J_C)$ to other generating sets of J_C , namely, its Gröbner bases.

Example 2.5. Returning to Example 2.1, the codewords v that are *not* in $C(\mathcal{U}) = \{\emptyset, 1, 123, 13, 3\}$ are 2, 12, and 23, so the neural ideal is $J_C = \langle \{x_2(1+x_1)(1+x_3), x_1x_2(1+x_3), x_2x_3(1+x_1)\} \rangle$. The canonical form is $\text{CF}(J_C(\mathcal{U})) = \{x_2(1+x_1), x_2(1+x_3)\}$. We will interpret these canonical-form polynomials in Example 2.7 below.

2.3. Receptive-field relationships. It turns out that we can interpret pseudo-monomials in J_C (and thus in the canonical form) in terms of relationships among receptive fields. First we need the following notation: for any $\sigma \subseteq [n]$, define:

$$x_\sigma := \prod_{i \in \sigma} x_i \quad \text{and} \quad U_\sigma := \bigcap_{i \in \sigma} U_i,$$

where, by convention, the empty intersection is the entire space X .

Lemma 2.6 (Curto, Itskov, Veliz-Cuba, and Youngs [7, Lemma 4.2]). *Let X be a stimulus space, let $\mathcal{U} = \{U_i\}_{i=1}^n$ be a collection of sets in X , and consider the receptive field code $C = C(\mathcal{U})$. Then for any pair of subsets $\sigma, \tau \subseteq [n]$,*

$$x_\sigma \prod_{i \in \tau} (1+x_i) \in J_C \iff U_\sigma \subseteq \bigcup_{i \in \tau} U_i.$$

Thus, three types of receptive-field relationships (RF relationships) can be read off from pseudo-monomials in a neural ideal (e.g., those in the canonical form) [7]:

Type 1: $x_\sigma \in J_C \iff U_\sigma = \emptyset$ (where $\sigma \neq \emptyset$).

Type 2: $x_\sigma \prod_{i \in \tau} (1+x_i) \in J_C \iff U_\sigma \subseteq \bigcup_{i \in \tau} U_i$ (where $\sigma, \tau \neq \emptyset$).

Type 3: $\prod_{i \in \tau} (1+x_i) \in J_C \iff X \subseteq \bigcup_{i \in \tau} U_i$ (where $\tau \neq \emptyset$), and thus $X = \bigcup_{i \in \tau} U_i$.

Example 2.7. The canonical form in Example 2.5, which is $\{x_2(1+x_1), x_2(1+x_3)\}$, encodes two Type 2 relationships: $U_2 \subseteq U_1$ and $U_2 \subseteq U_3$. Indeed, we can verify this in Figure 1.

In this work, we reveal more types of RF relationships, which arise from non-pseudo-monomials. They often appear in Gröbner bases of neural ideals (see Section 5).

2.4. Gröbner bases. Here we recall some basics about Gröbner bases [2, 4].

Fix a monomial ordering $<$ of a polynomial ring $R = k[x_1, \dots, x_n]$ over a field k , and let I be an ideal in R . Let $LT_{<}(I)$ denote the ideal generated by all leading terms, with respect to the monomial ordering $<$, of elements in I .

Definition 2.8. A **Gröbner basis** of I , with respect to $<$, is a finite subset of I whose leading terms generate $LT_{<}(I)$.

One useful property of a Gröbner basis is that given a polynomial f and a Gröbner basis G , the remainder of f when divided by the set of elements in G is uniquely determined.

A Gröbner basis is **reduced** if (1) every $f \in G$ has leading coefficient 1, and (2) no term of any $f \in G$ is divisible by the leading term of any $g \in G$ for which $g \neq f$. For a given monomial ordering, the reduced Gröbner basis of an ideal is unique.

Definition 2.9. A **universal Gröbner basis** of an ideal I is a Gröbner basis that is a Gröbner basis with respect to *every* monomial ordering. **The universal Gröbner basis** of an ideal I is the union of all the reduced Gröbner bases of I .

The set of all distinct reduced Gröbner bases of an ideal I is finite [2, pg. 515], so *the* universal Gröbner basis is an instance of *a* universal Gröbner basis.

3. MAIN RESULT

In this section, we give the main result of our paper: if the canonical form is a Gröbner basis, then it is the universal Gröbner basis (Theorem 3.1). Beyond being a natural expansion of some of Curto *et al.*'s results [7], our theorem is also of mathematical interest since there are few classes of ideals whose universal Gröbner bases are known. Indeed, such characterizations in general are known to be computationally difficult.

Theorem 3.1. *If the canonical form of a neural ideal J_C is a Gröbner basis of J_C with respect to some monomial ordering, then it is the universal Gröbner basis of J_C .*

The proof of Theorem 3.1, which appears in Section 3.3, requires the following related results:

Lemma 3.2. *For a pseudo-monomial $f = x_\sigma \prod_{j \in \tau} (1 + x_j)$ in $\mathbb{F}_2[x_1, \dots, x_n]$, the leading term of f with respect to any monomial ordering is its highest-degree term, $x_{\sigma \cup \tau}$.*

Proof. This follows from the fact that every term of f divides $x_{\sigma \cup \tau}$, and two properties of a monomial ordering [4]: it is a well-ordering (so, $1 < x_i$), and $x_\alpha < x_\beta$ implies $x_{\alpha \cup \gamma} < x_{\beta \cup \gamma}$. \square

Proposition 3.3. *If the canonical form of a neural ideal J_C is a Gröbner basis of J_C with respect to some monomial ordering, then it is a universal Gröbner basis of J_C .*

Proof. Let G denote the canonical form, and assume that G is a Gröbner basis with respect to some monomial ordering $<_1$. Let $<_2$ denote another monomial ordering. As always, we have the containment $\text{LT}_{<_2}(G) \subseteq \text{LT}_{<_2}(J_C)$, which we must prove is an equality. Accordingly, let $f \in J_C$. We must show that $\text{LT}_{<_2}(f) \in \text{LT}_{<_2}(G)$. With respect to $<_1$, the reduction of f by G is 0, so we can write f as a polynomial combination of some of the $g_i \in G$ in the following form:

$$(1) \quad f = \frac{\text{LT}_{<_1}(f)}{\text{LT}(g_1)} g_1 + \frac{\text{LT}_{<_1}(r_1)}{\text{LT}(g_2)} g_2 + \cdots + \frac{\text{LT}_{<_1}(r_{t-1})}{\text{LT}(g_t)} g_t = h_1 + \cdots + h_t,$$

where (for $i = 1, \dots, t$) we have $g_i \in G$, $h_i := \frac{\text{LT}_{<_1}(r_{i-1})}{\text{LT}(g_i)} g_i$, $r_0 := f$, and $r_i = f - h_1 - \cdots - h_i$ is the remainder after the i -th division of f by G . Note that in equation (1), the polynomial g_i may appear multiple times, but this does not affect our arguments. By Lemma 3.2, the leading term of g_i does not depend on the monomial ordering. Moreover, each h_i is the product of a monomial and a pseudo-monomial, g_i , so by a straightforward generalization of Lemma 3.2, the leading term of h_i with respect to *any* monomial ordering is $\text{LT}_{<_1}(h_i)$. Also note that when dividing by the Gröbner basis G , $\text{LT}_{<_1}(r_i) <_1 \text{LT}_{<_1}(r_{i-1})$ so the $\text{LT}_{<_1}(r_i)$ are distinct. This implies that the $\text{LT}_{<_1}(h_i)$ are distinct since $\text{LT}_{<_1}(h_i) = \text{LT}_{<_1}(r_{i-1})$.

Hence, among the list of monomials $\{\text{LT}(h_i)\}_{i=1}^t$, there is a unique largest monomial with respect to $<_2$, which we denote by $\text{LT}(h_{i^*})$. Next, by examining the sum in (1), and noting that every term of h_i divides the leading term of h_i , we see that $\text{LT}_{<_2}(f) = \text{LT}(h_{i^*})$. Thus, because g_{i^*} divides h_{i^*} , it follows that $\text{LT}(g_{i^*})$ divides $\text{LT}_{<_2}(f)$, and so, $\text{LT}_{<_2}(f) \in \text{LT}_{<_2}(G)$.

Thus, if the canonical form is a Gröbner basis with respect to *some* monomial ordering, then it is a Gröbner basis with respect to *every* monomial ordering. \square

3.1. Pseudo-monomials and hypercubes. To prove our main result (Theorem 3.1), we need to develop the connection between pseudo-monomials and hypercubes in the Boolean lattice. The **Boolean lattice** on $[n]$ is the power set $P([n]) := 2^{[n]}$, partially ordered by inclusion. The **support** of a monomial $\prod_{i=1}^n x_i^{a_i}$ is the set $\{i \in [n] \mid a_i > 0\}$.

Definition 3.4. Let $f = x_\sigma \prod_{j \in \tau} (1 + x_j)$ be a pseudo-monomial in $\mathbb{F}_2[x_1, \dots, x_n]$. The **hypercube of f** , denoted by $H(f)$, is the sublattice of the Boolean lattice on $[n]$ formed by the support of each term of f .

Remark 3.5. The hypercube of f is the *interval* of the Boolean lattice from σ to $\sigma \cup \tau$:

$$H(f) = \{\omega \mid \sigma \subseteq \omega \subseteq \sigma \cup \tau\} \subseteq P([n]),$$

and thus its Hasse diagram is a hypercube (this justifies its name). This is because:

$$f = x_\sigma \prod_{j \in \tau} (1 + x_j) = \sum_{\{\theta \mid \theta \subseteq \tau\}} x_{\sigma \cup \theta}.$$

Example 3.6. Let $f = x_1 x_2 (1 + x_3)(1 + x_4) = x_1 x_2 x_3 x_4 + x_1 x_2 x_3 + x_1 x_2 x_4 + x_1 x_2$. Figure 2 shows part of the Hasse diagram of $P([4])$, with the hypercube of f indicated by circles and solid lines.

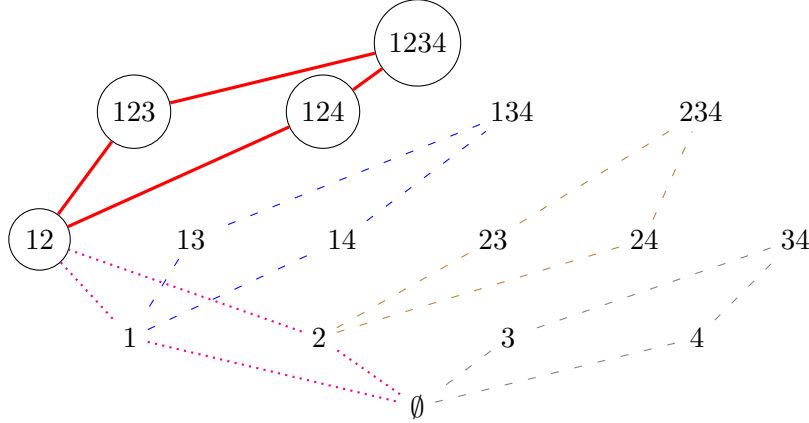


FIGURE 2. Displayed is part of the Hasse diagram of the Boolean lattice $P([4])$. The hypercube of $f = x_1 x_2 (1 + x_3)(1 + x_4)$ is indicated by circles and solid lines, and $P([2])$ is marked by dotted lines. If g is a pseudo-monomial that divides f , then its hypercube is contained in either the hypercube of f or one of the dashed-line squares “parallel” to the hypercube of f (see Example 3.8).

Via hypercubes, divisibility of pseudo-monomials has a nice geometric interpretation:

Lemma 3.7. For pseudo-monomials $f = x_\sigma \prod_{j \in \tau} (1 + x_j)$ and $g = x_\alpha \prod_{j \in \beta} (1 + x_j)$, the following are equivalent:

- (1) $g \mid f$,
- (2) $\alpha \subseteq \sigma$ and $\beta \subseteq \tau$,
- (3) $H(g) \subseteq P(\sigma \cup \tau)$ and $H(g) \cap P(\sigma) = \{\alpha\}$, and
- (4) $H(g) \subseteq P(\sigma \cup \tau)$ and $|H(g) \cap P(\sigma)| = 1$.

Proof. The implication (1) \Leftrightarrow (2) is clear, and (1) \Rightarrow (2) follows from the fact that $\mathbb{F}_2[x_1, \dots, x_n]$ is a unique factorization domain. For (2) \Rightarrow (3), assume that $\alpha \subseteq \sigma$ and $\beta \subseteq \tau$. Then $H(g) \subseteq P(\alpha \cup \beta) \subseteq P(\sigma \cup \tau)$. So, we need only show that $H(g) \cap P(\sigma) = \{\alpha\}$. To see this, we first recall:

$$(2) \quad H(g) = \{\alpha \cup \theta \mid \theta \subseteq \beta\}$$

from Remark 3.5. Thus,

$$H(g) \cap P(\sigma) = \{\alpha \cup \theta \mid \theta \subseteq \beta \text{ and } \theta \subseteq \sigma\} = \{\alpha\},$$

where the second equality follows from hypotheses: $\alpha \subseteq \sigma$ and $\sigma \cap \beta \subseteq \sigma \cap \tau = \emptyset$ (because $\beta \subseteq \tau$).

(3) \Rightarrow (4) is clear, so we need only show (2) \Leftarrow (4). Accordingly, suppose $H(g) \subseteq P(\sigma \cup \tau)$ and $I := H(g) \cap P(\sigma)$ consists of only one element. We claim that this element is α . Indeed, let $\omega \in I$ (i.e., $\omega \in H(g)$ and $\omega \subseteq \sigma$); then, α also is in I (because $\alpha \in H(g)$ and $\alpha \subseteq \omega \subseteq \sigma$). So, $\alpha = \omega \subseteq \sigma$.

To complete the proof, we must show that $\beta \subseteq \tau$. To this end, let $k \in \beta$. Then $\alpha \cup \{k\}$ is in $H(g)$, by equation (2), so it is *not* in $P(\sigma)$ (because $H(g) \cap P(\sigma) = \{\alpha\}$). So, $k \in (\beta \setminus \sigma)$. Finally, $(\beta \setminus \sigma) \subseteq \tau$, because $\alpha \cup \beta \subseteq \sigma \cup \tau$ follows from the hypothesis $H(g) \subseteq P(\sigma \cup \tau)$. So, $k \in \tau$. \square

Example 3.8. We return to the pseudo-monomial $f = x_1x_2(1+x_3)(1+x_4)$, which we rewrite as $f = x_\sigma \prod_{j \in \tau} (1+x_j)$, where $\sigma = \{1, 2\}$ and $\tau = \{3, 4\}$. In Figure 2, $P(\sigma) = P(\{2\})$ is marked by the dotted line. According to Lemma 3.7, a pseudo-monomial h divides f if and only if the hypercube of h satisfies two conditions: it includes a vertex from $P(\sigma)$, and it is contained within either the hypercube of f or one of the dashed-line squares “parallel” to the hypercube of f in Figure 2.

3.2. Multivariate division by pseudo-monomials. The following result concerns reducing a given pseudo-monomial by a set of pseudo-monomials.

Theorem 3.9. *Consider a pseudo-monomial $f = x_\sigma \prod_{i \in \tau} (1+x_i) \in \mathbb{F}_2[x_1, \dots, x_n]$, and let G be a finite set of pseudo-monomials in $\mathbb{F}_2[x_1, \dots, x_n]$. If some remainder upon division of f by G is 0 for some monomial ordering, then there exists $g \in G$ such that g divides f .*

Proof. Suppose that some remainder on division of f by G is 0:

$$(3) \quad f = \frac{\text{LT}(f)}{\text{LT}(g_1)}g_1 + \frac{\text{LT}(r_1)}{\text{LT}(g_2)}g_2 + \dots + \frac{\text{LT}(r_{t-1})}{\text{LT}(g_t)}g_t = h_1 + \dots + h_t,$$

where, as in the proof of Proposition 3.3, for $i = 1, \dots, t$, we have $g_i \in G$, $h_i := \frac{\text{LT}(r_{i-1})}{\text{LT}(g_i)}g_i$, and $r_i = f - h_1 - \dots - h_i$ is the remainder after the i -th division (and $r_0 := f$). Also, each term of h_i divides the leading term of h_i .

By construction, $g_i | h_i$. So, it suffices to show that there exists i such that $h_i | f$.

We now claim that $\text{LT}(h_i) | \text{LT}(f)$ holds for all i . We prove this claim by induction on i . For the $i = 1$ case, $\text{LT}(h_1) = \text{LT}(f)$. If $i \geq 2$, then $\text{LT}(h_i)$ is the leading term of:

$$(4) \quad r_{i-1} = f - h_1 - \dots - h_{i-1}.$$

We now examine the summands in (4). As f is a pseudo-monomial, each term in f divides $\text{LT}(f)$, and the same holds for each remaining summand h_i : as noted above, its terms divide $\text{LT}(h_i)$, and thus (by induction hypothesis) divide $\text{LT}(f)$. So, $\text{LT}(h_i) = \text{LT}(r_{i-1}) | \text{LT}(f)$, proving our claim.

We now assert that h_i is a pseudo-monomial. To see this, recall that h_i is the product of a monomial and a pseudo-monomial (namely, g_i), so we just need to show that its leading term is square-free. Indeed, this follows from two facts: $\text{LT}(h_i) | \text{LT}(f)$ and f is a pseudo-monomial.

Hence, $H(h_i) \subseteq P(\sigma \cup \tau)$ for every i , because every term in h_i divides $\text{LT}(h_i)$ which in turn divides $x_{\sigma \cup \tau} = \text{LT}(f)$. Thus, by Lemma 3.7, it is enough to show that $|H(h_i) \cap P(\sigma)| = 1$ for some i (because this would imply that $h_i | f$).

The sum in (3) is over \mathbb{F}_2 , so the polynomials f, h_1, \dots, h_t together must contain an even number of each term. We focus now on only those terms with support in $P(\sigma)$. The pseudo-monomial f has only one such term (namely, x_σ). Thus, some h_i has an odd number of terms in $P(\sigma)$, i.e., $|H(h_i) \cap P(\sigma)|$ is odd. On the other hand, both $H(h_i)$ and $P(\sigma)$ are hypercubes in the Boolean lattice, so their intersection, if nonempty, also is a hypercube and thus has size 2^q for some $q \geq 0$. Hence, $q = 0$, so $|H(h_i) \cap P(\sigma)| = 1$. This completes our proof. \square

3.3. Proof of Theorem 3.1. Theorem 3.9 allows us to prove that when a canonical form is a Gröbner basis, it is reduced:

Proposition 3.10. *If the canonical form of a neural ideal J_C is a Gröbner basis of J_C , then it is a reduced Gröbner basis of J_C .*

Proof. Suppose for contradiction that $\text{CF}(J_C)$ is a Gröbner basis, but not a reduced Gröbner basis. Then there exist $f, g \in \text{CF}(J_C)$, with $f \neq g$, such that $\text{LT}(g)$ divides some term of f . Thus, $\text{LT}(g)$ divides $\text{LT}(f)$ (because every term in a pseudo-monomial divides the leading term). Thus, $\text{CF}(J_C)$ and $\text{CF}(J_C) \setminus \{f\}$ both generate the same ideal of leading terms, and hence $\text{CF}(J_C) \setminus \{f\}$ is also a Gröbner basis of J_C . It follows that the remainder on division of f by $\text{CF}(J_C) \setminus \{f\}$ is 0, so by Theorem 3.9, there exists $h \in \text{CF}(J_C) \setminus \{f\}$ such that $h|f$. Hence, f is a non-minimal element of the canonical form, which is a contradiction. \square

Now we can prove Theorem 3.1, which states that a canonical form that is a Gröbner basis is the universal Gröbner basis:

Proof of Theorem 3.1. Follows from Propositions 3.3 and 3.10. \square

3.4. Every pseudo-monomial in a reduced Gröbner basis is in the canonical form. In this subsection, we prove the following partial converse of Theorem 3.1: if the universal Gröbner basis of a neural ideal consists of only pseudo-monomials, then it equals the canonical form (Theorem 3.12).

We first show that every pseudo-monomial in a reduced Gröbner basis is in the canonical form.

Proposition 3.11. *Let J_C be a neural ideal.*

- (1) *Let G be a reduced Gröbner basis of J_C . Then every pseudo-monomial in G is in the canonical form of J_C .*
- (2) *Let \widehat{G} be the universal Gröbner basis of J_C . Then every pseudo-monomial in \widehat{G} is in the canonical form of J_C .*

Proof. Let f be a pseudo-monomial in G . Suppose that f is *not* a minimal pseudo-monomial in J_C : for some pseudo-monomial $h \in J_C$ such that $\deg(h) < \deg(f)$, $h|f$. Then for some $g \in G$, $\text{LT}(g)|\text{LT}(h)$. Hence, $\text{LT}(g)|\text{LT}(f)$ (because $\text{LT}(h)|\text{LT}(f)$) and also $g \neq f$ (because $\deg(g) \leq \deg(h) < \deg(f)$). This is a contradiction: f and g cannot both be in a reduced Gröbner basis.

Finally, (2) follows directly from (1). \square

Theorem 3.12. *Let J_C be a neural ideal. The following are equivalent:*

- (1) *the canonical form of J_C is a Gröbner basis of J_C ,*
- (2) *the canonical form of J_C is the universal Gröbner basis of J_C , and*
- (3) *the universal Gröbner basis of J_C consists of pseudo-monomials.*

Proof. The implication (1) \Rightarrow (2) is Theorem 3.1, and both (1) \Leftarrow (2) and (2) \Rightarrow (3) are clear. For (3) \Rightarrow (1), assume that the universal Gröbner basis \widehat{G} consists of pseudo-monomials. Then, by Proposition 3.11(2), \widehat{G} is contained in the canonical form of J_C . Thus, the canonical form contains a Gröbner basis of J_C (namely, \widehat{G}) and hence is itself a Gröbner basis. \square

Remark 3.13. Suppose we want to know whether a code's canonical form is a Gröbner basis. Theorem 3.12 tells us how to do so *without* computing the canonical form: compute the universal Gröbner basis, and then check whether it contains only pseudo-monomials. See Example 3.14.

Under certain conditions, e.g. small number of neurons, computing the Gröbner basis is more efficient than computing the canonical form, but is there some way to avoid computations entirely and yet still decide whether the canonical form is a Gröbner basis? In the next section, we give conditions under which we can resolve this decision problem quickly.

Example 3.14. Consider the neural code $C = \{0100, 0101, 0111\}$. The universal Gröbner basis of J_C is $\widehat{G} = \{x_3(x_4 + 1), x_2 + 1, x_1\}$, so it contains only pseudo-monomials. Thus, by Theorem 3.12, \widehat{G} is the canonical form.

Example 3.15. Consider the neural code $C = \{0101, 1100, 1110\}$. The universal Gröbner basis of J_C is $\widehat{G} = \{x_4x_3, x_3(x_1 + 1), x_1 + x_4 + 1, x_2 + 1\}$, which contains the non-pseudo-monomial $x_1 + x_4 + 1$. Thus, by Theorem 3.12, the canonical form is not a universal Gröbner basis of J_C . Indeed, the canonical form is $\text{CF}(J_C) = \{x_3(x_1 + 1), x_2 + 1, (x_4 + 1)(x_1 + 1), x_4x_1, x_4x_3\}$, and, for a monomial ordering where $x_4 > x_1$, the leading term of the non-pseudo-monomial $x_1 + x_4 + 1$ is x_4 , which is *not* divisible by any of the leading terms from the canonical form.

4. WHEN IS THE CANONICAL FORM A GRÖBNER BASIS?

In this section we present some results that partially solve the question of when is the canonical form a Gröbner basis for the neural ideal. A complete answer to this question is not only of theoretical interest but perhaps also of practical relevance. Extensive computations suggest that, under certain conditions, Gröbner bases of neural ideals can be computed more efficiently than canonical forms. This is true for small neural codes. Moreover, the iterative nature of the newer canonical form algorithm hints towards the ability to compute canonical forms and Gröbner bases of neural codes in large dimensions by ‘gluing’ those of codes on small dimensions. Such decomposition results are a common theme in other areas of applied algebraic geometry such as algebraic statistics and phylogenetic algebraic geometry [1, 9].

Table I displays a runtime comparison between the iterative canonical form algorithm described in [14] and a specialized Gröbner basis algorithm for Boolean rings implemented in SageMath based on the work in [3]. We report the mean time (in seconds) of 100 randomly generated codes on n neurons for $n = 4, \dots, 8$. More precisely, for each code, a number m was chosen uniformly at random from $\{1, \dots, 2^n - 1\}$ and then m codewords were chosen at random. These computations were performed on SageMath 7.2 running on a Macbook Pro with a 2.8 GHz Intel Core i7 processor and 16 GB of memory.

Dimension	4	5	6	7	8
Canonical form	0.0016	0.0076	0.108	0.621	1.964
Gröbner basis	0.00147	0.00202	0.00496	0.01604	0.16638

TABLE I. Runtime comparison of canonical form versus Gröbner basis computations.

For codes on a larger number of neurons, our computations indicate that in general Gröbner bases computations are still more efficient than canonical form computations. However, even in the case of $n = 9$ neurons we found codes whose Gröbner bases took over 6 hours to be computed.

Proposition 4.1. *Let C be a neural code on n neurons. If $|C| = 1$ or $|C| = 2^n - 1$, then the canonical form of J_C is the universal Gröbner basis of J_C .*

Proof. If $C = \{c\}$, then Lemma 2.3 implies that $J_C = \langle x_1 - c_1, x_2 - c_2, \dots, x_n - c_n \rangle$. When $|C| = 2^n - 1$, then by definition $J_C = \langle \rho_v \rangle$ for the unique $v \notin C$. In either case, the indicated generating set is both the canonical form and the universal Gröbner basis of J_C . \square

A set of subsets $\Delta \subseteq 2^{[n]}$ is an (abstract) **simplicial complex** if $\sigma \in \Delta$ and $\tau \subseteq \sigma$ implies $\tau \in \Delta$. A neural code C is a simplicial complex if its support $\text{supp}(C)$ is a simplicial complex.

Proposition 4.2. *If C is a simplicial complex, then the canonical form of J_C is the universal Gröbner basis of J_C .*

Proof. If C is a simplicial complex, then J_C is a monomial ideal generated by the minimal Type 1 relationships (indeed, it is the Stanley-Reisner ideal of the simplicial complex $\text{supp}(C)$) [7, Lemma 4.4]. These minimal Type-1 relationships comprise the canonical form of J_C , and also form the universal Gröbner basis of J_C . \square

The next result gives conditions that guarantee that the canonical form is not a Gröbner basis.

Proposition 4.3. *Let $\mathcal{U} = \{U_i\}_{i=1}^n$ be a collection of sets in a stimulus space X , and let $C = C(\mathcal{U})$ denote the corresponding receptive field code. If one of the following conditions hold, then the canonical form of J_C is not a Gröbner basis of J_C :*

- (1) *Two proper, nonempty receptive fields coincide: $\emptyset \neq U_i = U_j \subsetneq X$ for some $i \neq j \in [n]$.*
- (2) *Two nonempty receptive fields are complementary: $U_i = X \setminus U_j$ for some $i \neq j \in [n]$ with $U_i \neq \emptyset$ and $U_j \neq \emptyset$.*

Proof. (1) Suppose $U_i, U_j \in \mathcal{U}$ are two sets with $\emptyset \neq U_i = U_j \subsetneq X$. By Lemma 2.6, both $f = x_i(x_j + 1)$ and $g = x_j(x_i + 1)$ are in J_C . In fact, f and g are minimal pseudo-monomials in J_C (because $\emptyset \neq U_i = U_j \neq X$), so $f, g \in \text{CF}(J_C)$. Under any monomial ordering, $\text{LT}(f) = \text{LT}(g) = x_i x_j$ (by Lemma 3.2), so the set $\text{CF}(J_C)$ is not reduced and thus cannot be a reduced Gröbner basis. Hence, by Proposition 3.10, $\text{CF}(J_C)$ cannot be a Gröbner basis.

(2) Now assume that $U_i = X \setminus U_j$ for some $i \neq j \in [n]$, with $U_i \neq \emptyset$ and $U_j \neq \emptyset$. Thus, $U_i \cap U_j = \emptyset$ and $U_i \cup U_j = X$, so Lemma 2.6 implies that $f = x_i x_j$ and $g = (x_i + 1)(x_j + 1)$ are in J_C . Now we proceed as in the previous paragraph: f and g are minimal pseudo-monomials in $\text{CF}(J_C)$, and $\text{LT}(f) = \text{LT}(g) = x_i x_j$, so, by Proposition 3.10, $\text{CF}(J_C)$ cannot be a Gröbner basis. \square

The last result in this section concerns a class of codes that we call **complement-complete**.

Definition 4.4. The **complement** of $c \in \{0, 1\}^n$ is the codeword $\bar{c} \in \{0, 1\}^n$ defined by $\bar{c}_i = 1$ if and only if $c_i = 0$. A neural code C is **complement-complete** if for all $c \in C$, then \bar{c} is also in C .

Example 4.5. The complement of the codeword $c_1 = 1000$ is $\bar{c}_1 = 0111$, and the complement of $c_2 = 1010$ is $\bar{c}_2 = 0101$. Thus, the code $C = \{1000, 0111, 1010, 0101\}$ is complement-complete.

Definition 4.6. The **complement** of a pseudo-monomial $f = x_\sigma \prod_{i \in \tau} (1 + x_i)$ is the pseudo-monomial $\bar{f} = x_\tau \prod_{j \in \sigma} (1 + x_j)$.

Lemma 4.7. *Consider pseudo-monomials $f = x_\sigma \prod_{i \in \tau} (1 + x_i)$ and $g = x_{\sigma'} \prod_{i \in \tau'} (1 + x_i)$. If f divides g , then \bar{f} divides \bar{g} .*

Proof. This follows from the fact that $f \mid g$ if and only if $\sigma' \subseteq \sigma$ and $\tau' \subseteq \tau$ (Lemma 3.7). \square

Proposition 4.8. *Let C be a code on n neurons, with $C \subsetneq \{0, 1\}^n$. If C is complement-complete, then the canonical form of J_C is not a Gröbner basis of J_C .*

Proof. Note that since $C \neq \{0, 1\}^n$, J_C is not trivial. We make the following claim:

CLAIM: If h is a pseudo-monomial in J_C , then \bar{h} is also in J_C .

To see this, let S be the set of all degree- n pseudo-monomials in $\mathbb{F}_2[x_1, \dots, x_n]$ that are multiples of h (so, $S \subseteq J_C$). Degree- n pseudo-monomials in $\mathbb{F}_2[x_1, \dots, x_n]$ are characteristic functions ρ_v , so, every element of S is some ρ_v , where $v \notin C$. Thus, every element of $\bar{S} := \{\bar{f} \mid f \in S\}$ has the form $\bar{\rho}_v = \rho_{\bar{v}}$, where $v \notin C$, which is equivalent to $\bar{v} \notin C$, as C is complement-complete. So, $\bar{S} \subseteq J_C$.

Next, let $s \in S$, that is, $s = hq$ for some pseudo-monomial q . Then $h\bar{q}$ is also in S . Since $\text{gcd}(q, \bar{q}) = 1$, it follows that $h = \text{gcd}(hq, h\bar{q})$, so $h = \text{gcd}\{S\}$. Thus, $\bar{h} = \text{gcd}\{\bar{S}\}$, so $\bar{h} \in J_C$ (because $\bar{S} \subseteq J_C$), which proves the claim.

Now let $f \in \text{CF}(J_C)$. By the claim, \bar{f} is in J_C , and now we assert that, like f , the pseudo-monomial \bar{f} is in $\text{CF}(J_C)$. Indeed, if a pseudo-monomial d in J_C divides \bar{f} , then by Lemma 4.7, the pseudo-monomial \bar{d} divides f . Also, $\bar{d} \in J_C$ (by the claim), so $\bar{d} = f$ (because f is minimal),

and thus $d = \bar{f}$. Hence, \bar{f} is minimal, and so \bar{f} is also in $CF(J_C)$. Thus, $CF(J_C)$ contains two polynomials (f and \bar{f}) with the same leading term, and so is not a reduced Gröbner basis, and thus (by Proposition 3.10) is not a Gröbner basis of J_C . \square

Example 4.9. Consider again the complement-complete code $C = \{1000, 0111, 1010, 0101\}$ from Example 4.5. The canonical form is $CF(J_C) = \{(x_1 + 1)(x_2 + 1), (x_1 + 1)(x_4 + 1), x_1x_2, x_2(x_4 + 1), x_1x_4, x_4(x_2 + 1)\}$. Note that $CF(J_C)$ is itself complement-complete; for example, $f = x_2(x_4 + 1)$ and $\bar{f} = x_4(x_2 + 1)$ are both in $CF(J_C)$. Also, we can show directly that $CF(J_C)$ is not a Gröbner basis, which is consistent with Proposition 4.8: with respect to any monomial ordering, the leading term of $f + \bar{f} = x_2 + x_4$ is not divisible by any of the leading terms in $CF(J_C)$.

5. NEW RECEPTIVE-FIELD RELATIONSHIPS

We saw earlier that if the universal Gröbner basis of a neural ideal consists of only pseudo-monomials, then it equals the canonical form (Theorem 3.12). When this is not the case, there are non-pseudo-monomial elements in the universal Gröbner basis, so it is natural to ask what they tell us about the receptive fields of the code. In other words, what types of RF relationships, besides those of Types 1–3 (Lemma 2.6), appear in Gröbner bases? Here we give a partial answer:

Theorem 5.1. *Let $\mathcal{U} = \{U_i\}_{i=1}^n$ be a collection of sets in a stimulus space X . Let $C = C(\mathcal{U})$ denote the corresponding receptive field code, and let J_C denote the neural ideal. Then for any subsets $\sigma_1, \sigma_2, \tau_1, \tau_2 \subseteq [n]$, and m indices $1 \leq i_1 < i_2 < \dots < i_m \leq n$, with $m \geq 2$, we have RF relationships as follows:*

Type 4: $x_{\sigma_1} \prod_{i \in \tau_1} (1 + x_i) + x_{\sigma_2} \prod_{j \in \tau_2} (1 + x_j) \in J_C \Rightarrow U_{\sigma_1} \cap \left(\bigcap_{i \in \tau_1} U_i^c \right) = U_{\sigma_2} \cap \left(\bigcap_{j \in \tau_2} U_j^c \right)$.

Type 5: $x_{i_1} + \dots + x_{i_m} \in J_C \Rightarrow U_{i_k} \subseteq \bigcup_{j \in [m] \setminus \{k\}} U_{i_j}$ for all $k = 1, \dots, m$, and if, additionally, m is odd, then $\bigcap_{k=1}^m U_{i_k} = \emptyset$.

Type 6: $x_{i_1} + \dots + x_{i_m} + 1 \in J_C \Rightarrow \bigcup_{k=1}^m U_{i_k} = X$.

Proof. Throughout the proof, for $p \in X$, we let $c(p)$ denote the corresponding codeword in C .

TYPE 4. Let $f_1 := x_{\sigma_1} \prod_{i \in \tau_1} (1 + x_i)$, and let $f_2 := x_{\sigma_2} \prod_{j \in \tau_2} (1 + x_j)$. Also, let $W_1 := U_{\sigma_1} \cap \left(\bigcap_{i \in \tau_1} U_i^c \right)$, and let $W_2 := U_{\sigma_2} \cap \left(\bigcap_{j \in \tau_2} U_j^c \right)$. By symmetry, we need only show that $W_1 \subseteq W_2$. To this end, let $p \in W_1$ (so, $c(p) \in C$). First, because $f_1 + f_2 \in J_C$ and $V(J_C) = C$, it follows that $f_1(c(p)) = f_2(c(p))$. Next, for $i = 1, 2$, we have $p \in W_i$ if and only if $f_i(c(p)) = 1$. Thus, $p \in W_2$.

TYPE 5. Let $g := x_{i_1} + \dots + x_{i_m}$. By symmetry, we need only show that $U_{i_1} \subseteq \bigcup_{l=2}^m U_{i_l}$. To this end, let $p \in U_{i_1}$ (so, $c(p)_{i_1} = 1$). Then $g \in J_C$ implies the following equality in \mathbb{F}_2 :

$$(5) \quad 0 = g(c(p)) = c(p)_{i_1} + c(p)_{i_2} + \dots + c(p)_{i_m} = 1 + c(p)_{i_2} + \dots + c(p)_{i_m}.$$

Thus, for some $k \geq 2$, we have $c(p)_{i_k} = 1$, i.e., $p \in U_{i_k}$. Hence, $p \in \bigcup_{l=2}^m U_{i_l}$.

Now assume, additionally, that m is odd. Suppose, for contradiction, that there exists $q \in \bigcap_{k=1}^m U_{i_k}$. Then, like the sum (5) above, we have $0 = g(c(q)) = 1 + \dots + 1 = m$, which contradicts the hypothesis that m is odd. So, $\bigcap_{k=1}^m U_{i_k} = \emptyset$.

TYPE 6. Let $h := x_{i_1} + \dots + x_{i_m} + 1$. Let $p \in X$ (so, $c(p) \in C$). We must show that $p \in \bigcup_{k=1}^m U_{i_k}$. Because $h \in J_C$, we have $0 = h(c(p)) = c(p)_{i_1} + \dots + c(p)_{i_m} + 1$. Thus, for some $k \in [m]$, we have $c(p)_{i_k} = 1$, i.e., $p \in U_{i_k}$. Hence, $p \in \bigcup_{k=1}^m U_{i_k}$. \square

Remark 5.2. Like the earlier RF relationships (those of Types 1–3 from Lemma 2.6), some of our new ones (Types 4–6) are containments and some are equalities.

Example 5.3. Recall the code $C = \{0101, 1100, 1110\}$, from Example 3.15, for which the universal Gröbner basis of J_C is $\widehat{G} = \{x_4x_3, x_3(x_1 + 1), x_1 + x_4 + 1, x_2 + 1\}$. The polynomial $x_1 + x_4 + 1$ encodes a Type 6 relationship: $U_1 \cup U_4 = X$. Also, the polynomial $x_2 + 1$ encodes a Type 3

relationship: $U_2 = X$, which together gives us $U_1 \cup U_4 = U_2$. The canonical form also contains the polynomial x_1x_4 , which encodes a Type 1 relationship: $U_1 \cap U_4 = \emptyset$. We conclude that $U_1 \dot{\cup} U_4 = U_2$.

Example 5.4. Consider the code $C = \{00, 11\}$. The universal Gröbner basis of C is $\widehat{G} = \{x_1(1 + x_1), x_1 + x_2, x_2(1 + x_2)\}$. The polynomial $x_1 + x_2$ encodes a Type 4 relationship: $U_1 = U_2$. (The polynomial $x_1 + x_2$ also encodes Type 5 relationships.) This points to one of the advantages of our new RF relationships: we can read off some set equalities more quickly than from the canonical form. Indeed, the canonical form is $\text{CF}(J_C) = \{x_1(1 + x_2), x_2(1 + x_1)\}$, in which the Type 2 relationships are $U_1 \subseteq U_2$ and $U_2 \subseteq U_1$ – and only from there do we infer the equality $U_1 = U_2$.

6. DISCUSSION

In this work, we proved that if a code’s canonical form is a Gröbner basis of the neural ideal, then it is the universal Gröbner basis. Additionally, we gave conditions that guarantee or preclude this situation, and found three new types of receptive-field relationships that arise in neural ideals. Going forward, there are natural extensions to pursue:

- (1) Give a complete characterization of codes for which the canonical form is a Gröbner basis.
- (2) Beyond those of Types 1–6, what other receptive-field relationships can be read off from a Gröbner basis, and what do they tell us about a code?

Solutions to these problems would help us extract information about the receptive-field structure directly from the neural code.

Finally, we expect that our results can be used to improve canonical-form algorithms. Indeed, our experiments indicate that under certain conditions, Gröbner bases can be computed more efficiently than canonical forms. Moreover, every pseudo-monomial in the universal Gröbner basis of a neural ideal is in the canonical form – so, that subset of the canonical form can be obtained directly from the universal Gröbner basis. And, in the case when the universal Gröbner basis contains only pseudo-monomials, then we can conclude immediately that the basis is in fact the canonical form. Moreover, we hope to develop decomposition results to build canonical forms and Gröbner basis of codes in large dimensions by ‘gluing’ those of codes in smaller dimensions.

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