GRÖBNER BASES OF NEURAL IDEALS

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ABSTRACT. A major area in neuroscience is the study of how the brain processes spatial information. Neurons in the brain represent external stimuli via neural codes. These codes often arise from regions of space called receptive fields: each neuron fires at a high rate precisely when the animal is in the corresponding receptive field. Much research in this area has focused on understanding what features of receptive fields can be extracted directly from a neural code. In particular, Curto, Itskov, Veliz-Cuba, and Youngs recently introduced the concept of neural ideal, which is an algebraic object that encodes the full combinatorial data of a neural code. 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

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?” [6].

To pursue this question, Curto et al. 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) [9]. 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 stimulus space structure. Hence, the questions posed above have been investigated via the neural ideal or the canonical form [5, 6, 7, 8]. As a complement to algebraic approaches, combinatorial and topological arguments are employed in related works [4, 9, 10].

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. Indeed, among small codes, surprisingly many have canonical forms that are also Gröbner bases. 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 3.11). We also prove
a partial converse: if the universal Gröbner basis of a neural ideal contains only so-called pseudo-
ideal is a Gröbner basis, then it is the universal Gröbner basis (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 underlying stimulus space?

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 [6], and recalls some basics about Gröbner bases. We use the notation
[n] := {1, 2, . . . , 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 ⊆ {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 ∈ 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 co-firing neurons: supp(C) = \{supp(c) \mid c ∈ C\} ⊆ 2^[n].

In many areas of the brain, neurons are associated with receptive fields in a stimulus space.
We are particularly interested in 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 [11]. 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.

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

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

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 \( C(U) = \{\emptyset, 1, 123, 13, 3\} \).

2.2. The neural ideal and its canonical form. A pseudo-monomial in \( \mathbb{F}_2[x_1, \ldots, x_n] \) 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 \( \sigma \cap \tau = \emptyset \). Note that 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, \( \prod_{i \in \sigma, j \in \tau} x_i \). We will use this fact several times in this work.

Each \( v \in \{0, 1\}^n \) defines a pseudo-monomial \( \rho_v \) as follows:

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

Notice that \( \rho_v \) 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 \textbf{neural ideal} \( J_C \) is the ideal in \( \mathbb{F}_2[x_1, \ldots, x_n] \) generated by all \( \rho_v \) for \( v \not\in C \):
\[
J_C := \langle \{\rho_v | v \not\in C\} \rangle.
\]

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 [6, Lemma 3.2]). Let \( C \subseteq \{0, 1\}^n \) be a neural code. Then
\[
I(C) = J_C + \langle x_i(1 + x_i) | i \in [n] \rangle,
\]

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

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

Definition 2.4. The \textbf{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 [6, 7, 12]. In particular, [12] describes an iterative method to compute the canonical form that is significantly more efficient than the original method presented in [6].

The canonical form \( \text{CF}(J_C) \) is a particular generating set for the neural ideal \( J_C \) [6]. 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 \( C(U) = \{\emptyset, 1, 123, 13, 3\} \) 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 \( \text{CF}(J_{C(U)}) = \{x_2(1 + x_1), x_2(1 + x_3)\} \). 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 [6, 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) [6]:

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 [1, 3].

Fix a monomial ordering \( < \) of a polynomial ring \( R = k[x_1, \ldots, x_n] \) 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 [1, 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 a universal Gröbner basis (Theorem 3.1). Beyond being a natural expansion of some of Curto et al.’s results [6], 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 \( \mathbb{F}_2[x_1, \ldots, x_n] \), 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 [3]: it is a well-ordering (so, \( 1 < x_i \)), and \( x_\alpha < x_\beta \) implies \( x_{\alpha \cup \gamma} < x_{\beta \cup \gamma} \).

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:

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

where (for $i = 1, \ldots, t$) 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 $\text{LT}(h_*)$. 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 $\text{LT}_{<_2}(f) = \text{LT}(h_*)$. Thus, because $g_i$ divides $h_*$, 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. 

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 $P([n]) := \mathbb{2}^{|n|}$, 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 $f = x_\sigma \prod_{i \in \tau} (1 + x_j)$ be a pseudo-monomial in $\mathbb{F}_2[x_1, \ldots, x_n]$. The hypercube of $f$, denoted by $H(f)$, is the sublattice of the Boolean lattice on $[n]$ formed by all supports of terms of $f$.

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

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

**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.

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

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

1. $g | f$,
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 $(1) \iff (2)$ is clear, and $(1) \implies (2)$ follows from the fact that $\mathbb{F}_2[x_1, \ldots, x_n]$ is a unique factorization domain. For $(2) \implies (3)$, 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 $\beta \subseteq \tau$).

$(3) \implies (4)$ is clear, so we need only show $(2) \iff (4)$. 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 $\alpha$. Indeed, let $\omega \in I$ (i.e., $\omega \in H(g)$ and $\omega \subseteq \sigma$); then, $\alpha$ 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 3.8, 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 $f = x_\sigma \prod_{i \in \tau}(1 + x_i) \in \mathbb{F}_2[x_1, \ldots, x_n]$, and let $G$ be a finite set of pseudo-monomials in $\mathbb{F}_2[x_1, \ldots, x_n]$. If some remainder on 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:

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

Figure 2. Displayed is part of the Hasse diagram of the Boolean lattice $P([4])$. The hypercube of $f = x_1x_2(1 + x_3)(1 + x_4)$ 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).
where, as in the proof of Proposition 3.3, for \( i = 1, \ldots, t \), we have \( g_i \in G \), \( h_i := \frac{LT(r_{i-1})}{LT(g_i)} g_i \), and \( r_i = f - h_1 - \cdots - h_i \) 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 \( LT(h_i) \) holds for all \( i \). We prove this claim by induction on \( i \). For the \( i = 1 \) case, \( LT(h_1) = LT(f) \). If \( i \geq 2 \), then \( LT(h_i) \) is the leading term of:

\[
\begin{align*}
    r_{i-1} &= f - h_1 - \cdots - h_{i-1}.
\end{align*}
\]

We now examine the summands in \( r_i \). As \( f \) is a pseudo-monomial, each term in \( f \) divides \( LT(f) \), and the same holds for each remaining summand \( h_i \); as noted above, its terms divide \( LT(h_i) \), and thus (by induction hypothesis) divide \( LT(f) \). So, \( LT(h_i) = LT(r_{i-1})LT(f) \), 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: \( LT(h_i) \) 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 \( LT(h_i) \) which in turn divides \( x_{\sigma \cup \tau} = LT(f) \). 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 (4) is over \( \mathbb{F}_2 \), so the polynomials \( f, h_1, \ldots, h_t \) 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, \( x_\sigma \)). 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 3.9

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 \( CF(J_C) \) is a Gröbner basis, but not a reduced Gröbner basis. Then there exist \( f, g \in CF(J_C) \), with \( f \neq g \), such that \( LT(g) \) divides some term of \( f \). Thus, \( LT(g) \) divides \( LT(f) \) (because every term in a pseudo-monomial divides the leading term). Thus, \( CF(J_C) \) and \( CF(J_C) \setminus \{ f \} \) both generate the same ideal of leading terms, and hence \( CF(J_C) \setminus \{ f \} \) is also a Gröbner basis of \( J_C \). It follows that the remainder on division of \( f \) by \( CF(J_C) \setminus \{ f \} \) is 0, so by Theorem 3.9 there exists \( h \in CF(J_C) \setminus \{ f \} \) 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 $\hat{G}$ be the universal Gröbner basis of $J_C$. Then every pseudo-monomial in $\hat{G}$ 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 $\deg(h) < \deg(f)$, $h \mid f$. Then for some $g \in G$, $\text{LT}(g) \mid \text{LT}(h)$. Hence, $\text{LT}(g) \mid \text{LT}(f)$ (because $\text{LT}(h) \mid \text{LT}(f)$) 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).

Here we build on Theorem 3.1.

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)$\Leftrightarrow$(2) and (2)$\Rightarrow$(3) are clear. For (3)$\Rightarrow$(1), assume that the universal Gröbner basis $\hat{G}$ consists of pseudo-monomials. Then, by Proposition 3.12, $\hat{G}$ is contained in the canonical form of $J_C$. Thus, the canonical form contains a Gröbner basis of $J_C$ (namely, $\hat{G}$) and hence is itself a Gröbner basis.

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 $\hat{G} = \{x_3(x_4+1), x_2+1, x_1\}$, so it contains only pseudo-monomials. Thus, by Theorem 3.12, $\hat{G}$ is the canonical form.

Example 3.15. Consider the neural code $C = \{0101, 1100, 1110\}$. The universal Gröbner basis of $J_C$ is $\hat{G} = \{x_4x_3, x_3(x_1+1), x_1+x_4+1, x_2+1\}$, 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.

Table 1 displays a runtime comparison between the iterative canonical form algorithm described in [12] and a specialized Gröbner basis algorithm for Boolean rings implemented in SageMath based on the work in [2]. We report the mean time (in seconds) of 100 randomly generated codes on $n$ neurons for $n = 4, \ldots, 8$. More precisely, for each code, a number $m$ was chosen uniformly at random from $\{1, \ldots, 2^n - 1\}$ 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.
Table 1. Runtime comparison of canonical form versus Grobner basis computations.

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

For codes on a larger number of neurons, our computations indicate that in general Grobner bases computations are still more efficient than canonical form computations. However, even in the case of $n = 9$ neurons we found codes whose Grobner 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 $JC$ is the universal Grobner basis of $JC$.

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

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 Grobner basis of $JC$.

**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 $\text{supp}(C)$) [6, Lemma 4.4]. These minimal Type-1 relationships comprise the canonical form of $J_C$, and also form the universal Grobner basis of $J_C$. □

The next result gives conditions that guarantee that the canonical form is not a Grobner 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 Grobner basis of $J_C$:

1. Two proper, nonempty receptive fields coincide: $\emptyset \neq U_i = U_j \subseteq X$ 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 $\emptyset \neq U_i = U_j \subseteq X$. 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 Grobner basis. Hence, by Proposition 3.10 $\text{CF}(J_C)$ cannot be a Grobner 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 Grobner basis. □

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 $\overline{c} \in \{0, 1\}^n$ defined by $\overline{c}_i = 1$ if and only if $c_i = 0$. A neural code $C$ is complement-complete if for all $c \in C$, then $\overline{c}$ is also in $C$.

**Example 4.5.** The complement of the codeword $c_1 = 1000$ is $\overline{c_1} = 0111$, and the complement of $c_2 = 1010$ is $\overline{c_2} = 0101$. 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 \( \overline{f} = x_\tau \prod_{j \in \sigma} (1 + x_j) \).

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 \( \overline{f} \) divides \( \overline{g} \).

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

Proposition 4.8. Let \( C \) be a code on \( n \) neurons, with \( C \subseteq \{0,1\}^n \). 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 \( \overline{h} \) is also in \( J_C \).

To see this, let \( S \) be the set of all degree-\( n \) pseudo-monomials in \( \mathbb{F}_2[x_1, \ldots, x_n] \) that are multiples of \( h \) (so, \( S \subseteq J_C \)). Degree-\( n \) pseudo-monomials in \( \mathbb{F}_2[x_1, \ldots, x_n] \) are characteristic functions \( \rho_v \), so, every element of \( S \) is some \( \rho_v \), where \( v \notin C \). Thus, every element of \( S := \{ \overline{f} \mid f \in S \} \) has the form \( \overline{\rho_v} = \rho_{c \cdot v} \) where \( v \notin C \), which is equivalent to \( c \not\in C \), as \( C \) is complement-complete. So, \( S \subseteq J_C \).

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

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

Example 4.9. Consider again the complement-complete code \( C = \{1000, 0111, 1010, 0101\} \) from Example 3.5. 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 \( \overline{f} = x_4(x_2 + 1) \) 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 \( f + \overline{f} = x_2 + x_4 + 1 \) 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 \( U = \{U_i\}_{i=1}^n \) be a collection of sets in a stimulus space \( X \). Let \( C = C(U) \) 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 \( 1 \leq i_1 < i_2 < \cdots < i_m \leq n \), with \( m \geq 2 \), we have RF relationships as follows:

Type 4: \( x_{i_1} \prod_{i \in \tau_1} (1 + x_i) + x_{\sigma_2} \prod_{j \in \tau_2} (1 + x_j) \in J_C \Rightarrow U_{\sigma_1} \cap (\bigcap_{i \in \tau_1} U_i^c) = U_{\sigma_2} \cap (\bigcap_{j \in \tau_2} U_j^c) \).

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

Type 6: \( x_{i_1} + \cdots + x_{i_m} + 1 \in J_C \Rightarrow \bigcup_{k=1}^m U_{i_k} = X \).
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 \( W_1 := U_{\sigma_1} \cap (\bigcap_{i \in \tau_1} U_i^c) \), and let \( W_2 := U_{\sigma_2} \cap (\bigcap_{j \in \tau_2} U_j^c) \). 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 \( g := x_{i_1} + \cdots + x_{i_m} \). By symmetry, we need only show that \( U_{i_1} \subseteq \bigcup_{i=2}^{m} U_{i_i} \). 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 \( F_2 \):

\[
0 = g(c(p)) = c(p)_{i_1} + c(p)_{i_2} + \cdots + c(p)_{i_m} = 1 + c(p)_{i_2} + \cdots + c(p)_{i_m} .
\]

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

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 \( 0 = g(c(q)) = 1 + \cdots + 1 = m \), which contradicts the hypothesis that \( m \) is odd. So, \( \bigcap_{k=1}^{m} U_{i_k} = \emptyset \).

**Type 6.** Let \( h := x_{i_1} + \cdots + x_{i_m} + 1 \). 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 \( 0 = h(c(p)) = c(p)_{i_1} + \cdots + c(p)_{i_m} + 1 \). Thus, for some \( k \in \{m\} \), we have \( c(p)_{i_k} = 1 \), i.e., \( p \in U_{i_k} \). Hence, \( p \in \bigcup_{k=1}^{m} U_{i_k} \).

**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 \( \hat{G} = \{x_4 x_3, x_3(x_1 + 1), x_1 + x_4 + 1, x_2 + 1\} \). 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 \( x_1 x_4 \), which encodes a Type 1 relationship: \( U_1 \cap U_4 = \emptyset \). We conclude that \( U_1 \cup U_4 = U_2 \).

**Example 5.4.** Consider the code \( C = \{00, 11\} \). The universal Gröbner basis of \( C \) is \( \hat{G} = \{x_1(1 + x_1), x_1 + x_2, x_2(1 + x_2)\} \). 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 stimulus space 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, we now know that 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 computed efficiently. 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. Canonical-form algorithms, therefore, can be made more efficient by first computing the universal Gröbner basis and then, if necessary, proceeding to compute the canonical form.
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