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Gröbner bases of convex neural code ideals

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Abstract We present results and conjectures on the connection between the convexity of a neural code and the canonical form of its ideal. The connection is established through properties of the Gröbner basis of the neural ideal and the uniqueness of its reduced form. An efficient algorithm for identifying neural codes with unique reduced Gröbner bases is introduced.

Keywords Neural code · Neural ideal · Canonical form of neural ideal · Gröbner basis · Convexity

1 Introduction and background

Humans and animals perceive their surroundings based on previous encounters. Their brains have to store information about those encounters to be accessed in the future, and the way this information is stored and processed is the

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subject of active research in neuroscience. Great strides have also been made towards a mathematical understanding of the brain. For example, the theory of neural codes studies how the brain represents external stimulation. These codes are extracted from stereotyped stimulus-response maps, associating to each neuron a convex receptive field. An important problem confronted by the brain is to infer properties of a represented stimulus space without knowledge of the receptive fields, using only the intrinsic structure of the neural code. To understand how the brain does this, one must first determine what stimulus space features can be extracted from neural codes.

In this paper, we study neural codes through an algebraic object called a *neural ideal* which was introduced in [CIVCY13] to better understand the combinatorial structure of neural codes. More specifically, we focus on convex neural codes (and their corresponding ideals) since they have been observed experimentally in brain activity. In Section 2 we begin with a survey on what is known so far about convex neural codes. In Section 3 we discuss the structure of neural ideals and their Gröbner bases. We then introduce results on the connection between the canonical form of a neural ideal and its reduced Gröbner basis, suggesting that neural ideals which have a unique reduced Gröbner bases are of particular interest. Thus, in Section 4, we introduce a method for identifying neural codes with unique Gröbner bases. These results suggest a conjecture, stated in Section 5, that provides a characterization of convex neural codes based on their Gröbner bases.

We first review some terminology and results here (see [CIVCY13]). Given a *neural code* C written as a set of binary strings of length n (alternatively, it can be written as subsets of $[n]$), we can construct the ideal of polynomials that vanish on C:

$$I_C := \{p \in \mathbb{F}_2[x_1, \ldots, x_n] : p(c) = 0 \text{ for all } c \in C\}, \tag{1}$$

where $\mathbb{F}_2$ is the finite field of two elements (0 and 1), and $\mathbb{F}_2[x_1, \ldots, x_n]$ is the polynomial ring in n variables with coefficients in $\mathbb{F}_2$. Note that since $0^2 = 0$ and $1^2 = 1$, I_C always contains the set of Boolean relations $\mathcal{B} = \langle x_i^2 - x_i : i \in [n]\rangle$.

We can construct a generating set for the rest of the elements of I_C, via indicator functions: Given a codeword $v \in \mathbb{F}^2$, define

$$\rho_v := \prod_{i:v_i=1} x_i \prod_{j:v_j=0} (1 + x_j).$$

Note that $\rho_v(v) = 1$ and $\rho_v(c) = 0$ for $c \neq v$. From these functions, we can build the *neural ideal* of C:

$$J_C := \langle \rho_v : v \in \mathbb{F}_2^n \setminus C\rangle$$

Note that $I_C = \mathcal{B} + J_C$ ([CIVCY13]). The functions ρ_v that generate J_C are examples of *pseudo-monomials*: these are polynomials $f \in \mathbb{F}_2[x_1, \ldots, x_n]$ of the form

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

where $x_\sigma := \prod_{i\in\sigma} x_i$ and $\sigma, \tau \subseteq [n]$ with $\sigma \cap \tau = \emptyset$.

Given an ideal $J \subset \mathbb{F}_2[x_1, \ldots, x_n]$, a pseudo-monomial $f \in J$ is *minimal* if there does not exist another pseudo-monomial $g \in J$ with $\deg(g) < \deg(f)$ and $f = hg$ for some $h \in \mathbb{F}_2[x_1, \ldots, x_n]$. We define the *canonical form* of J_C to be the set of all minimal pseudo-monomials of J_C, denoted $CF(J_C)$. For any neural code C, the set $CF(J_C)$ is a generating set for the neural ideal J_C. The canonical form $CF(J_C)$ can be constructed algorithmically from the code C (see [PYK+16],[CIVCY13]).

Example 1 Given the code $C = \{000, 100, 110, 101, 001, 111\}$, there are two elements in $\mathbb{F}_2^3$ that are not in C: 010 and 011. From these, we construct the neural ideal:

$$J_C = \langle x_2(1 + x_1)(1 + x_3), x_2x_3(1 + x_1)\rangle$$

The canonical form is $CF(J_C) = \{x_2(1+x_1)\}$. Observe that if a codeword c satisfies $x_2(1 + x_1) = 0$, then whenever neuron 2 is firing ($x_2 = 1$), we must have neuron 1 firing, as well ($x_1 = 1$).

2 Convexity of neural codes

We will now investigate combinatorial codes arising from covers of a stimulus space. Let X be a topological space. A collection of non-empty open sets $\mathcal{U} = \{U_1, U_2, \ldots, U_n\}$, $U_i \subset X$, is called an *open cover*. Given an open cover $\mathcal{U}$, the *code of the cover* is the neural code defined as:

$$C(\mathcal{U}) = \{\sigma \subseteq [n] : \bigcap_{i\in\sigma} U_i \setminus \bigcup_{j\in[n]\setminus\sigma} U_j \neq \emptyset\}.$$

Given a combinatorial code C, we say that C is realized by an open cover $\mathcal{U}$ if $C = C(\mathcal{U})$. If C can be realized by $\mathcal{U}$, where $\mathcal{U} = \{U_1, \ldots, U_n\}$ with each U_i a convex subset of $\mathbb{R}^d$, then C is a *convex code* with geometric realization $\mathcal{U}$.

Not all combinatorial codes are convex. For example, the code $C = \{\emptyset, 1, 2, 13, 23\}$ cannot be realized with convex sets, as the set U_3 is the disjoint union of open sets $U_1 \cap U_3$ and $U_2 \cap U_3$, forcing it to be disconnected (and thus, non-convex). A complete condition for convexity is still unknown; we summarize here the known results.

Note that in the previous example the relationship in the receptive fields forced the non-convexity of one of the sets, and the presence of the single codeword 3 would eliminate this topological inconsistency. This is an example of a local obstruction to convexity, instrinsic to the combinatorial structure of the code itself.

Definition 1 ([CGJ+17]) Let $C = C(\mathcal{U})$ be a code on n neurons, with $\mathcal{U} = \{U_1, \ldots, U_n\}$ a realization of C. Let $U_\sigma = \bigcap_{i\in\sigma} U_i$. A *receptive field relationship* (*RF relationship*) of C is a pair (σ, τ) corresponding to the set containment

$$U_\sigma \subseteq \bigcup_{i \in \tau} U_i,$$

where $\sigma \neq \emptyset$, $\sigma \cap \tau = \emptyset$, and $U_\sigma \cap U_i \neq \emptyset$ for all $i \in \tau$. A receptive field relationship is *minimal* if no single neuron from σ or τ can be removed without destroying the containment.

In general, we can detect local obstructions via the simplicial complex of a code. Given a code C, its *simplicial complex* is $\Delta(C) := \{\sigma \subseteq [n] : \sigma \subseteq c \text{ for some } c \in C\}$. For a simplicial complex Δ, the *restriction* of Δ to σ is the simplicial complex $\Delta|_\sigma := \{\omega \in \Delta : \omega \subset \sigma\}$. For any $\sigma \in \Delta$, the *link* of σ in Δ is $Lk_\sigma(\Delta) = \{w \in \Delta : \sigma \cap w = \emptyset, \sigma \cup w \in \Delta\}$.

Definition 2 ([CGJ$^+$17]) Let (σ, τ) be a receptive field relationship, and let $\Delta = \Delta(C)$. We say that (σ, τ) is a *local obstruction* of C if $\tau \neq \emptyset$ and $Lk_\sigma(\Delta|_{\sigma\cup\tau})$ is not contractible.

Note that in $C = \{\emptyset, 1, 2, 13, 23\}$, $(\sigma, \tau) = (\{3\}, \{1, 2\})$ is a receptive field relationship ($U_3 \subseteq U_1 \cup U_2$), and $Lk_3(\Delta|_{123}) = \{1, 2\}$, which is disconnected (and thus, not contractible).

Notice that the simplicial complex of a code C is defined by its maximal codewords. A *maximal codeword* σ of a code C is maximal under inclusion in C. A code is *max intersection-complete* if it is closed under taking all intersections of its maximal codewords.

We can now state necessary and sufficient conditions for convexity:

Proposition 1 *For a neural code C:*

1. *If C is max intersection-complete, then C is convex.*
2. *If C is convex, then C has no local obstructions.*

Part 1 of Proposition 1 is due to [CGIK19], while Part 2 is due to [CGJ$^+$17] as a consequence of the Nerve Lemma.

The converses of Part 1 and Part 2 of Proposition 1 hold for $n \leq 4$ (see [CGJ$^+$17]); however, these statements fail for $n \geq 5$. An example of a convex code which is not max intersection-complete can be seen via $C1 = \{123, 124, 145, 14, 12\}$ in Figure 1. An example of a non-convex code which has no local obstructions was found in [LSW17], which is code $C4 = \{2345, 123, 134, 145, 13, 14, 23, 34, 45, 3, 4, \emptyset\}$. The case for $n = 5$ neurons has also been fully classified; see [GP19].

3 Structure of the neural ideal

We now turn to a discussion relating convexity to the structure of the neural ideal. As we saw in Example 1 in Section 1, the canonical form encodes minimal descriptions of the relationships between the sets U_i. The following lemma given in [CIVCY13] generalizes this observation:

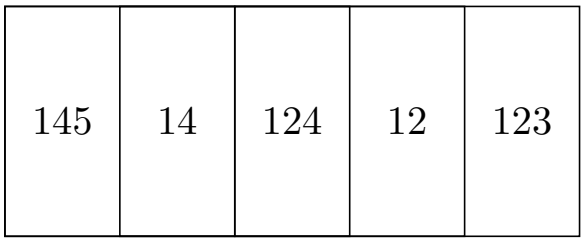

Fig. 1: Convex realization of $C1$.

Lemma 1 *Let $C = C(\mathcal{U})$ be a neural code on n neurons with neural ideal J_C. For $\sigma, \tau \in [n]$ with $\sigma \cap \tau = \emptyset$, $x_\sigma \prod_{j\in\tau}(1 + x_j) \in J_C$ if and only if (σ, τ) is an RF relationship (i.e., $U_\sigma \subseteq \bigcup_{j\in\tau} U_j$.).*

Moreover, $x_\sigma \prod_{j\in\tau}(1+x_j) \in CF(J_C)$ if and only if (σ, τ) is a minimal RF relationship.

From Example 1, the minimal pseudo-monomial $x_2(1 + x_1)$ gives us the minimal relationship $U_2 \subseteq U_1$.

3.1 Gröbner Basis of a Neural Ideal

The canonical form $CF(J_C)$ is a particular generating set for J_C that gives information about the structure of the sets U_i. Another well-known generating set for a polynomial ideal is a Gröbner basis.

Given an ideal in a polynomial ring $R = k[x_1, \ldots, x_n]$ and a monomial ordering $<$ on R, we can let $LT_<(I)$ denote the ideal generated by the leading terms of elements in I. If G is a finite subset of I whose leading terms generate $LT_<(I)$, then G is a *Gröbner basis* for I. A Gröbner basis for I is always a generating set for the ideal I. A Gröbner basis G is *reduced* if, given any element $f \in G$, f has leading coefficient 1 and no term of f is divisible by the leading term of any $g \in G$ with $g \neq f$. We often also talk about *marked* reduced Gröbner bases to emphasize that the leading term of each polynomial in a Gröbner basis is distinguished. For a given monomial order $<$, the marked reduced Gröbner basis exists and is unique.

A *universal Gröbner basis* for an ideal I is a Gröbner basis that is a Gröbner basis with respect to any monomial order. *The universal Gröbner basis* $\widehat{G}$ of an ideal I is the union of all reduced Gröbner bases of I. Since the set of all reduced Gröbner bases is finite, the universal Gröbner basis always exists and is unique.

If a set is a Gröbner basis, it is not necessarily a reduced Gröbner basis nor a universal Gröbner basis. However, it was shown in [GPK$^+$18] that if the canonical form is a Gröbner basis, then it is in fact the universal Gröbner basis for J_C. This result leads to the following proposition:

Proposition 2 *[GPK$^+$18] Let C be a neural code with neural ideal J_C. 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.*
3. *The universal Gröbner basis of J_C consists of pseudo-monomials.*

In particular, this gives a way to certify that the canonical form is not a Gröbner basis: If, for a given term order, the reduced Gröbner basis contains polynomials which are not pseudo-monomials, this implies that the canonical form is not a a Gröbner basis.

The following proposition refines Proposition 2 by replacing its second statement with *"The canonical form of J_C has a unique marked reduced Gröbner basis."*

Proposition 3 *Let C be a code and J_C its neural ideal. $CF(J_C)$ is a Gröbner basis if and only if J_C has a unique marked reduced Gröbner basis.*

Proof In [DHRS19], it is shown that an ideal has a unique marked reduced Gröbner basis if and only if all marked reduced Gröbner basis generators are factor-closed, i.e., the non-leading terms of each polynomial divide its leading term. Furthermore, in [GPK$^+$18] the authors prove that if the universal Gröbner basis of J_C consists solely of pseudo-monomials, then its canonical form is a Gröbner basis. Since over $\mathbb{F}_2$ all polynomials that are factor-closed and square-free are pseudo-monomials, the result follows.

Notice that by Proposition 3, the goal of classifying codes whose neural ideals have canonical forms that are Gröbner bases becomes identical to classifying codes whose ideals of points (or neural ideals) have unique marked reduced Gröbner basis. In Section 4 we present an efficient algorithm for testing whether a code has a neural ideal with a unique marked reduced Gröbner basis.

Lemma 2 *If there is a pseudo-monomial $f \in CF(J_C)$ whose leading term is divisible by any term of another pseudo-monomial $g \in CF(J_C)$, then the canonical form is not a Gröbner basis for J_C for any monomial order.*

Proof If $f \in CF(J_C)$ has leading term that is divisible by a term of another pseudo-monomial $g \in CF(J_C)$, then the canonical form cannot be a reduced Gröbner basis, which by Proposition 2 implies that it is not a Gröbner basis.

We will utilize this fact in the next subsection.

3.2 Canonical form and Gröbner bases of J_C

Recall from Section 2 that if a code has a local obstruction, then it is not convex. Since the canonical form $CF(J_C)$ encodes information about the minimal relationships between the sets U_i, the canonical form can be used to detect certain local obstructions in the code. The following definition was introduced in [CGJ$^+$19].

Definition 3 A local obstruction (σ, τ) is CF-*detectable* if there exists a local obstruction (σ', τ') with $\sigma' \subset \sigma$ and $\tau' \subset \tau$ such that (σ', τ') is a minimal RF relationship.

The next proposition connects the convexity of C to the Gröbner basis of J_C.

Proposition 4 *Given a code C, if C has a CF-detectable local obstruction, then the canonical form of J_C is not a Gröbner basis.*

Proof By Theorem 5.4 in [CGJ+19], if C has a CF-detectable local obstruction, then there exist $\sigma, \tau \subset [n], \tau \neq \emptyset$ with $x_\sigma \prod_{i\in\tau}(1+x_i) \in CF(J_C)$ and $x_\sigma x_\tau \in J_C$. Since $x_\sigma x_\tau$ is a pseudo-monomial in J_C and $CF(J_C)$ is a generating set for J_C, there exists $x_\alpha \in CF(J_C)$ with $\alpha \subset \sigma \cup \tau$, so the canonical form is not a Gröbner basis by Proposition 5.

Thus, if a code C has a CF-detectable local obstruction, C is both not convex and its canonical form is not a Gröbner basis for J_C.

Proposition 5 *Let C be a neural code with neural ideal J_C and canonical form $CF(J_C)$. If there exist two distinct pseudo-monomials $f = x_\sigma \prod_{i\in\tau}(1+x_i)$ and $g = x_\alpha \prod_{j\in\beta}(1+x_j) \in CF(J_C)$ with $\alpha\cup\beta \subseteq \sigma\cup\tau$, then the canonical form $CF(J_C)$ is not a Gröbner basis of J_C.*

Proof For any monomial order, the leading term of f is $x_\sigma x_\tau$ while the leading term of g is $x_\alpha x_\beta$. Since $\alpha \cup \beta \subseteq \sigma \cup \tau$ implies that $x_\alpha x_\beta$ divides $x_\sigma x_\tau$, by Lemma 2 we have that the canonical form is not a Gröbner basis.

Unfortunately, the converse of Proposition 5 fails as the following example shows.

Example 2 The code
$C = \{\emptyset, 1, 2, 3, 4, 5, 134, 1234, 234, 1235, 125, 13, 15, 23, 25, 14, 24, 235, 135, 1245, 35, 123, 12345\}$
has canonical form $CF(J_C) = \{x_3x_4(1+x_1)(1+x_2), x_1x_2(1+x_3)(1+x_5), x_4x_5(1+x_1), x_4x_5(1+x_2)\}$, with leading terms $x_1x_2x_3x_4, x_1x_2x_3x_5, x_1x_4x_5, x_2x_4x_5$, none of which are divisible by the others. However, the universal Gröbner basis of J_C has the polynomial $x_4(x_1x_2 + x_1x_3 + x_2x_3 + x_3x_4 + x_3 + x_5)$, which is not a pseudo-monomial. Thus, by Proposition 2, the canonical form of this code is not a Gröbner basis.

We do have the following partial converse to Proposition 5:

Proposition 6 *Let C be a neural code with canonical form $CF(J_C)$. If, for all minimal pseudomonomials $x_\sigma \prod_{i\in\tau}(1+x_i)$ and $x_\alpha \prod_{j\in\beta}(1+x_j) \in CF(J_C)$, we have $(\sigma\cup\tau)\cap(\alpha\cup\beta) = \emptyset$, then $CF(J_C)$ is a Gröbner basis for J_C.*

Proof Let $g = x_\sigma \prod_{i\in\tau}(1+x_i)$ and $h = x_\alpha \prod_{j\in\beta}(1+x_j) \in CF(J_C)$. Since the leading terms of g and h are $x_\sigma x_\tau$ and $x_\alpha x_\beta$ respectively, if $(\sigma\cup\tau)\cap(\alpha\cup\beta) = \emptyset$, then the leading terms of g and h are relatively prime. By Proposition 4 in [CLO15], this guarantees that the S-polynomial of g and h has standard representation. Since this is true for any pair of pseudo-monomials, this shows that $CF(J_C)$ is a Gröbner basis for J_C by Theorem 3 in [CLO15].

Note that the hypothesis of Proposition 6 is not a necessary condition for the canonical form to be a Gröbner basis, as will be seen in Examples 3 and 4. We now give several examples of convex and non-convex codes with their canonical forms and universal Gröbner bases $\widehat{G}$. The labeling of the codes follow the classification given in [GP19].

Example 3 The code $C4 = \{2345, 123, 134, 145, 13, 14, 23, 34, 45, 3, 4, \emptyset\}$ is non-convex, non-max intersection complete, with no local obstructions (see [LSW17]). It has canonical form $CF(C4) = \{x_5(1+x_4), x_1x_2x_4, x_2x_4(1+x_5), x_2(1+x_3), x_1x_2x_5, x_1x_3x_5, x_3x_5(1+x_2), x_1(1+x_3)(1+x_4)\}$. The universal Gröbner basis is $\widehat{G}(C4) = \{x_1x_2x_5, x_1x_2x_4, x_5(x_2+x_3), x_5(1+x_4), x_2(1+x_3), x_1(1+x_3)(1+x_4), x_1x_3x_5, x_2x_4+x_3x_5, x_2(x_4+x_5)\}$.

It was shown in [LSW17] that adding either the codeword 1 or the codewords 234 and 345 to $C4$ would make it convex. Upon adding 1, the universal Gröbner basis and the canonical form lose pseudo-monomials, but $\widehat{G}$ still does not equal the canonical form. Adding the codewords 234 and 345 instead makes the canonical form equal to the Gröbner basis: $CF = \{x_1x_2x_5, x_1x_2x_4, x_1x_3x_5, x_5(1+x_4), x_2(1+x_3), x_1(1+x_3)(1+x_4)\}$. Note that it is still not max-intersection complete.

Example 4 The code $C22 = \{145, 124, 135, 235, 125, 123, 234, 35, 1, 23, 15, 25, 5, 13, 2, 24, 3, 14, 12\}$ is convex with geometric realization in $\mathbb{R}^3$ and not max-intersection complete (see [GP19]). The universal Gröbner basis and the canonical form are the same: $CF(C22) = \{x_2x_4x_5, x_1x_2x_3x_5, x_3x_4(1+x_2), x_3x_4x_5, x_4x_5(1+x_1), x_4(1+x_1)(1+x_2)\}$.

4 Identifying neural codes with unique marked reduced Gröbner bases

Based on Proposition 3, the goal of classifying codes whose neural ideals have canonical forms that are Gröbner bases becomes identical to classifying codes whose ideals of points have unique marked reduced Gröbner basis. In this section we outline a method for testing whether a neural ideal has a unique marked reduced Gröbner basis. We begin with two relevant definitions from [BOT03].

Definition 4 A *staircase* is a set $\lambda \subseteq \mathbb{N}^d$ of nonnegative integer vectors such that $u \leq v \in \lambda$ (coordinatewise) implies $u \in \lambda$. The staircase of exponent vectors of standard monomials of an ideal I is called an *initial* staircase.

Definition 5 A staircase λ is *basic* for an ideal I if the congruence classes modulo I of the monomials x^v with $v \in \lambda$ form a vector space basis for $\mathbb{Z}_p[x_1, \ldots, x_n]/I$.

As we will see in Proposition 7, if we want to find out whether $I(V)$ has a unique marked reduced Gröbner basis, we just need to check whether $I(V)$ has a unique basic staircase.

Definition 6 Given a staircase S on n variables and number of points m, let $\alpha_S = (\alpha_S^1, \cdots, \alpha_S^n)$ be an n-dimensional vector, where $\alpha_S^i = 0$ if S has zeros for all points in its ith direction. Otherwise $\alpha_S^i = 1$. We use $\sum \alpha_S$ to denote the summation of all entries in α_S, and call it the *dimension* of S.

Example 5 The following two examples illustrate the concept of staircase dimension which is needed for the algorithm at the end of this section.

1. Let $S = \{(0,0),(0,1),(0,2),(0,3)\}$. Then $\alpha_S = (0,1)$ and $\sum \alpha_S = 1$.
2. If $S = \{(0,0,0),(0,0,1),(0,1,0),(1,0,0)\}$, then $\alpha_S = (1,1,1)$ and $\sum \alpha_S = 3$.

We now construct the following matrix. Let $\lambda = \{u^1, \ldots, u^r\}$ be an r-subset of $\mathbb{Z}_p^n$ and let $V = \{v^1, \ldots, v^s\}$ be an s-subset of $\mathbb{Z}_p^n$. The *evaluation matrix* $\mathbb{X}(x^\lambda, V)$ is the s-by-r matrix whose element in position (i,j) is $x^{u^j}(v^i)$, the evaluation of x^{u^j} at v^i.

Example 6 Let $\lambda_1 = \{(0,0),(1,0)\}$, $\lambda_2 = \{(0,0),(0,1)\}$, and $V = \{(2,0),(0,1)\}$ be subsets of $\mathbb{Z}_3^2$. Then $\mathbb{X}(x^{\lambda_1}, V) = \begin{bmatrix} 1 & 2 \\ 1 & 0 \end{bmatrix}$ and $\mathbb{X}(x^{\lambda_2}, V) = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$.

Theorem 1 ([BOT03]) *Let λ and V be subsets of $\mathbb{Z}_p^n$. Then λ is basic for $I(V)$ if and only if $\mathbb{X}(x^\lambda, V)$ is invertible.*

An initial staircase must be basic, while a basic staircase might not be initial; however, if $I(V)$ has a unique initial staircase (and thus a unique reduced Gröbner basis), then $I(V)$ has a unique basic staircase. The following lemma is found in [DHSZ19] without proof.

Lemma 3 *Let x^α, x^β be monomials with $x^\alpha \nmid x^\beta$. There exists a weight vector γ and monomial order $\prec_\gamma$ such that $x^\beta \prec_\gamma x^\alpha$.*

Proof Let $x^\alpha \nmid x^\beta$. As $x^\alpha \nmid x^\beta$, $\alpha_j > \beta_j$ for some coordinate j. Take γ to be a vector in $\mathbb{R}^n$ with a sufficiently large rational value in entry j and square roots of distinct prime numbers elsewhere such that $\gamma \cdot \alpha > \gamma \cdot \beta$. Then the entries of γ are linearly independent over $\mathbb{Q}$ and so γ defines a weight order. Define $\prec_\gamma$ to be the monomial order weighted by γ. It follows that $x^\beta \prec_\gamma x^\alpha$.

Proposition 7 ([DHSZ19]) *An ideal $I(V)$ has a unique initial staircase if and only if $I(V)$ has a unique basic staircase.*

Proof Follows directly from Proposition 2.2 in [BOT03] and Lemma 3.

Based on Proposition 7, if we want to find out whether $I(V)$ has a unique marked reduced Gröbner basis, we just need to check if there exist a unique staircase $\lambda \subseteq \mathbb{Z}_p^n$ such that $\mathbb{X}(x^\lambda, V)$ is invertible.

The above paragraph is the basis of the following method we propose for identifying if a set of points has an ideal with a unique marked reduced Gröbner basis: Given a set of points V, the algorithm goes over all possible staircases

with $|V|$ elements and checks if the corresponding evaluation matrix is invertible. Notice that no Gröbner basis computation is required. Unfortunately, finding all staircases is equivalent to the NP-complete integer partitioning problem [Hay02] but there are pseudo-polynomial time dynamic programming solutions. For example, one can use the Sherman-Morrison formula [SM50]: Given an invertible matrix $A \in \mathbb{R}^{n\times n}$, and two column vectors $u, v \in \mathbb{R}^n$, $A + uv^T$ is invertible if and only if $1 + v^T A^{-1} u \neq 0$.

The following algorithm is based on the theory summarized in this section. Its goal is to identify data sets $V \subseteq Z_p^n$ of fixed size, dimension, and finite field cardinality having an ideal with a unique marked reduced Gröbner basis. Before we present it, we need one last definition.

Definition 7 ([DHSZ19]) For $V_1, V_2 \subset \mathbb{Z}_p^n$ with $|V_1| = |V_2|$, we say V_1 is a *linear shift* of V_2, if there exists $\phi = (\phi_1, \cdots, \phi_n) : \mathbb{Z}_p^n \to \mathbb{Z}_p^n$ such that $\phi(V_1) = V_2$ and for each $i \in \{1, \cdots, n\}$, $\phi_i(x_i) = a_i x_i + b_i : \mathbb{Z}_p \to \mathbb{Z}_p$ with $a_i \in (\mathbb{Z}_p \backslash \{0\})$ and $b_i \in \mathbb{Z}_p$.

The linear shift is a bijection between two data sets, defining an equivalence relation. We note that by a "good" representative of an equivalence class E we mean one of the data sets with smallest total Euclidean distance to the origin among all data sets in E.

4.1 Data preparation

Input: n (dimension), p (characteristic of finite field), m (number of points in the data set)
Purpose: Prepare the data for use in the main iterations
Steps:

1. Generate all staircases $\{S\}$ and their corresponding dimensions $\{\alpha_S\}$.
2. For each S, calculate all evaluation matrices $\{\mathbb{X}(x^S, S)\}$ and their inverses $\{\mathbb{X}(x^S, S)^{-1}\}$.
   Note: Since $\{\mathbb{X}(x^S, S)\}$ is a square Vandermonde matrix and S is a set of distinct points, $\{\mathbb{X}(x^S, S)\}$ is invertible.
3. Find "good" representatives $\{E_\ell\}$, for all the equivalence classes.

Note: The number of staircases has an upper bound of $O(m(\log m)^{n-1})$ [BOT03].

4.2 Main iterations

Input: $\{S\}, \{\alpha_S\}, \{\mathbb{X}(x^S, S)\}, \{\mathbb{X}(x^S, S)^{-1}\}, \{E_\ell\}$.
Output: Good representatives of equivalence classes in which an ideal of the data sets have unique reduced Gröbner bases.

Create a list called storage to store all the previous results
for $\ell \in \{E_\ell\}$ **do**
  create an empty vector called flag = [ ]

for $S \in \{S\}$ **do**
if ℓ and S are only different in one point **then**
compute $D = \mathbb{X}(x^S, \ell) - \mathbb{X}(x^S, S)$
decompose $D = uv^T$, where $u, v \in \mathbb{F}_p^m$ are two column vectors
if $1 + v^T \mathbb{X}(x^S, S)^{-1} u = 0 \in \mathbb{Z}_p$ **then**
flag.append(False)
else
flag.append(True)
end if
else if $\sum \alpha_S < n$ and storage has the result of ℓ' such that ℓ' have exactly the same value of ℓ at non-zero entries in α_S **then**
flag.append(the previous result)
else if $\det(\mathbb{X}(x^S, \ell)) \neq 0 \in \mathbb{Z}_p$ **then**
flag.append(True)
else
flag.append(False)
end if
if there are two Trues in flag **then**
use storage to store flags
break the inside loop
end if
end for
use storage to store flags
if flag has only one T **then**
print ℓ
end if
end for

5 Discussion and future work

We explored convex neural codes by considering the canonical forms and Gröbner bases of their ideals. While we still do not have a complete algebraic characterization of convex codes, the results we presented lead us to believe that there is a strong connection between convexity of a code and the number of the marked reduced Gröbner bases of its ideal. In particular, it would seem that the relations among the U_i from Definition 1 cannot be too "contradictory" for the canonical form of a neural ideal to be a Gröbner basis. From the comparisons and computations of canonical forms and Gröbner bases for convex and non-convex codes thus far, the authors make the following conjecture to strengthen Proposition 4:

Conjecture 1 Given a neural code C with neural ideal J_C, if the canonical form $CF(J_C)$ is a Gröbner basis, then the code C is convex.

Notice that in light of Proposition 3, the above conjecture can also be stated as "Given a neural code C with neural ideal J_C, if J_C has a unique marked reduced Gröbner basis, then the code C is convex."

In addition, Section 4 of [GPK+18] gives three examples of families of codes whose canonical forms are Gröbner bases, which we can verify will always be convex codes, thus further suggesting that Conjecture 1 is worth future work:

1. C is a simplicial complex: then C is intersection complete, so C is convex.
2. C is the singleton $C = \{(c_1, \ldots, c_n)\}$. Then $U_i = X$ for $c_i = 1$, and $U_j = \emptyset$ for $c_j = 0$. If X is chosen to be convex, then the code will be convex.
3. C is missing one codeword from $[n]$. If $11\cdots1 \in C$, then C is convex (see [CGJ+17]). If $C = \{0,1\}^n \setminus \{11\cdots1\}$, then C is a simplicial complex, which is convex by (1).

In [DHSZ19] we characterize geometrically a family of codes whose ideals have a unique marked reduced Gröbner basis and the codes above are in that family. By Proposition 3, the above conjecture would imply that all codes in the family are convex which remains to be verified. Furthermore, in [DHRS19], we show that if the neural ideal of a code has a unique marked reduced Gröbner basis, so does the neural ideal of its complement. It remains to be verified if convex codes whose neural ideals have unique marked reduced Gröbner bases always have convex complements.

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References

BOT03. E. Babson, S. Onn, and R. Thomas. The Hilbert zonotope and a polynomial time algorithm for universal Gröbner bases. *Advances in Applied Mathematics*, 30(3):529–544, 2003.

CGIK19. J. Cruz, C. Giusti, V. Itskov, and Bill Kronholm. On open and closed convex codes. *Discrete & Computational Geometry*, 61(2):247–270, 2019.

CGJ+17. C. Curto, E. Gross, Jack Jeffries, K. Morrison, M. Omar, Z. Rosen, A. Shiu, and N. Youngs. What makes a neural code convex? *SIAM Journal on Applied Algebra and Geometry*, 1:222–238, 2017.

CGJ+19. C. Curto, E. Gross, J. Jeffries, K. Morrison, Z. Rosen, A. Shiu, and N. Youngs. Algebraic signatures of convex and non-convex codes. *Journal of Pure and Applied Algebra*, 223(9):3919–3940, 2019.

CIVCY13. C. Curto, V. Itskov, A. Veliz-Cuba, and N. Youngs. The neural ring: an algebraic tool for analyzing the intrinsic structure of neural codes. *Bulletin of Mathematical Biology*, 75:1571–1611, 2013.

CLO15. D. A. Cox, J. Little, and D. O'Shea. *Ideals, Varieties, and Algorithms*. Springer, New York City, 4 edition, 2015.

DHRS19. E. S. Dimitrova, Q. He, L. Robbiano, and B. Stigler. Small Gröbner fans of ideals of points. *Journal of Algebra and Its Applications*, 2019.

DHSZ19. E. S. Dimitrova, Q. He, B. Stigler, and A. Zhang. Geometric characterization of data sets with unique reduced Gröbner bases. *Bulletin of Mathematical Biology*, 2019.

GP19. S. A. Goldrup and K. Phillipson. Classification of open and closed convex codes on five neurons, 2019.

GPK+18. R. Garcia, L. D. García Puente, R. Kruse, J. Liu, D. Miyata, E. Petersen, K. Phillipson, and A. Shiu. Gröbner bases of neural ideals. *International Journal of Algebra and Computation*, 28(4):553–571, 2018.

Hay02. B. Hayes. Computing science: The easiest hard problem. *American Scientist*, 90(2):113–117, 2002.

LSW17. C. Lienkaemper, A. Shiu, and Z. Woodstock. Obstructions to convexity in neural codes. *Advances in Applied Mathematics*, 85:31–59, 2017.

PYK+16. E. Petersen, N. Youngs, R. Kruse, D. Miyata, R. Garcia, and L. D. García Puente. Neural ideals in sagemath, 2016.

SM50. J. Sherman and W. J. Morrison. Adjustment of an inverse matrix corresponding to a change in one element of a given matrix. *Ann. Math. Statist.*, 21(1):124–127, 03 1950.