# Machine Learning Parameter Systems, Noether Normalisations and Quasi-stable Positions

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# Abstract

We discuss the use of machine learning models for finding "good coordinates" for polynomial ideals. Our main goal is to put ideals into quasi-stable position, as this generic position shares most properties of the generic initial ideal, but can be deterministically reached and verified. Furthermore, it entails a Noether normalisation and provides us with a system of parameters. Traditional approaches use either random choices which typically destroy all sparsity or rather simple human heuristics which are only moderately successful. Our experiments show that machine learning models provide us here with interesting alternatives that most of the time make nearly optimal choices.

*Keywords:* Polynomial ideals, Pommaret bases, quasi-stable ideals, Noether normalisation, systems of parameters, machine learning, multi-class classification 2020 MSC: 13P10, 14Q15, 68T05, 68W30

# 1. Introduction

It is well known that many results in algebraic geometry and commutative algebra considerably simplify in generic coordinates. While from a theoretical point of view one may simply exploit that a random transformation (almost) always achieves a generic position, the situation is less simple from a computational point of view. Random transformations are computationally bad, as they destroy all sparsity typically present in generators of polynomial ideals. Furthermore, for many generic positions – like for example the popular GIN position in which one obtains the generic initial ideal – effective tests are either not known or prohibitively expensive.

As we have demonstrated in several articles, quasi-stable position represents an interesting alternative. It shares most of the properties of the GIN position (Hashemi et al., 2012), but can be effectively verified. It entails a Noether normalisation (Seiler, 2009b) and in quasi-stable position one obtains easily a system of parameters (Seiler,

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2012). Furthermore, in a series of articles, we developed a deterministic approach to obtain a quasi-stable position for arbitrary ideals (Hausdorf and Seiler, 2002; Seiler, 2009b; Hashemi et al., 2018). In this approach, one performs a finite sequence of very sparse transformations until quasi-stability is achieved. The efficiency depends crucially on the number of transformations required.

In each step, one typically has a choice between several possible transformations. The correctness and the termination of the whole procedure is independent of this choice. But the number of transformations required to achieve quasi-stable position can depend strongly on it. Previous computational experiments have indicated that simple human heuristics are not very successful in making consistently good choices here. Therefore we propose to apply methods from machine learning for selecting the applied transformations.

This is similar to some other proposed applications of machine learning in the context of commutative algebra. England and collaborators have studied in a larger number of articles the use of various classification methods for choosing the variable ordering for a cylindrical algebraic decomposition, see e.g. (Huang et al., 2014; England and Florescu, 2019; Florescu and England, 2019; Huang et al., 2019; Florescu and England, 2020; Pickering et al., 2023) and noted that these were better than known human heuristics. The problem of learning a selection strategy in Buchberger's algorithm applied to binomial ideals was studied in (Peifer et al., 2020; Peifer, 2021) using reinforcement learning with a 1D convolutional neural network. In all these works, one is also concerned with choices within an algorithm which do not affect its correctness or termination, but which possess a signigicant effect on its efficiency. Somewhat related is also the idea of Simpson et al. (2016) to employ machine learning for chosing the most efficient algorithm for computing resultants. By contrast, Jamshidi and Petrović (2023) presented a machine learning approach for computing Gröbner bases.

This article is structured into two parts. In the next section, we discuss the mathematical foundations: quasi-stability and Pommaret bases. We recall the necessary notions and their relevant properties. On the algorithmic side, we recall the deterministic approach from (Hashemi et al., 2018) and provide two completion algorithms for monomial Janet and Pommaret bases, respectively. The following section is concerned with applying machine learning in this context. We describe the structure of our feature vetors and how we quantitatively compare different choices. After a discussion of the training process, we present our results. Finally, some conclusions are given.

## 2. Quasi-Stability and Pommaret Bases

We will work throughout in a polynomial ring  $S = k[x_1, ..., x_n] = k[X]$  over a field k of characteristic zero<sup>3</sup> with a fixed number *n* of variables. We consider exclusively homogeneous polynomials  $f_1, ..., f_k \in S$  and the ideal  $I = \langle f_1, ..., f_k \rangle$  generated by them. A *term* is a power product  $x_1^{\mu_1} \cdots x_n^{\mu_n}$  and denoted by  $x^{\mu}$  with an exponent

<sup>&</sup>lt;sup>3</sup>In principle, we can also handle coefficient fields of positive characteristic. However, some minor adaptions are necessary. In particular, if the field is too small, a field extension is needed. We refer to (Hashemi et al., 2018) for a more detailed discussion of this situation.

vector  $\mu = (\mu_1, ..., \mu_n) \in \mathbb{N}_0^n$ . We write max  $x^{\mu} = j$ , if  $\mu_j$  is the last non-vanishing entry of  $\mu$ . We will exclusively work with the *degree reverse lexicographic order* assuming  $x_1 > \cdots > x_n$ . The *leading term* of a polynomial  $f \in S$  is written lt f. If  $\mathcal{F} \subset S$  is a finite set of polynomials, we denote by lt  $\mathcal{F}$  the set {lt  $f \mid f \in \mathcal{F}$ } of their leading terms. The set  $\mathcal{F}$  is called a *Gröbner basis* for an ideal I, if  $\mathcal{F} \subset I$  and the leading ideal satisfies lt  $I = \langle \text{lt } g \mid g \in I \rangle = \langle \text{lt } \mathcal{F} \rangle$ . We refer e. g. to (Cox et al., 2015) for more details on Gröbner bases.

#### 2.1. Quasi-Stable Ideals and Quasi-Stable Position

Quasi-stable ideals represent a special class of monomial ideals that appear in many different places and which are know under many different names like e.g. ideals of nested type (Bermejo and Gimenez, 2006), ideals of Borel type (Herzog et al., 2003) or weakly stable ideals (Caviglia and Sbarra, 2005). Many equivalent definitions are possible; we recall here the classical combinatorial one.

**Definition 2.1.** A monomial ideal  $\mathcal{J} \triangleleft S$  is *quasi-stable*, if for any term  $t \in \mathcal{J}$  and any index  $1 \leq i < j = \max t$  there exists an exponent s > 0 such that  $x_i^s t/x_j \in \mathcal{J}$ . A polynomial ideal  $\mathcal{I} \triangleleft S$  is in *quasi-stable position*, if its leading ideal lt  $\mathcal{I}$  is quasi-stable.

One readily verifies that it suffices to verify the condition in Definition 2.1 for the finitely many minimal generators of  $\mathcal{J}$ , so that quasi-stability can easily be checked effectively. If *t* is a minimal generator and for the index  $1 \le i < j = \max t$  no term of the form  $x_i^s t/x_j$  lies in  $\mathcal{J}$ , then we call the pair  $(t, x_i)$  an *obstruction to quasi-stability*. The following proposition recalls a number of well-known equivalent characterisations of quasi-stable ideals (see (Hashemi et al., 2018) for a more detailed discussion, references and some further characterisations).

**Proposition 2.2.** Let  $\mathcal{J} \triangleleft S$  be a *D*-dimensional monomial ideal. Then the following statements are equivalent:

- (i)  $\mathcal{J}$  is quasi-stable.
- (ii) Every associated prime ideal of  $\mathcal{J}$  is of the form  $\langle x_1, \ldots, x_j \rangle$  for some index  $1 \le j \le n D$ .
- (iii) The variable  $x_n$  is not a zero divisor on  $S/\mathcal{J}^{\text{sat}}$  and the variables  $x_{n-j}$  for  $1 \le j < D$  are not zero divisors on  $S/\langle \mathcal{J}, x_n, \dots, x_{n-j+1} \rangle$ .
- (iv) There is an ascending chain  $\mathcal{J}: x_n^{\infty} \subseteq \mathcal{J}: x_{n-1}^{\infty} \subseteq \cdots \subseteq \mathcal{J}: x_{n-D+1}^{\infty}$  and for each index  $1 \leq j \leq n D$  there exists a term  $x_i^{\ell_j} \in \mathcal{J}$ .
- (v) We have  $\mathcal{J}^{\text{sat}} = \mathcal{J} : x_n^{\infty}$  and for  $1 \le j < D$

$$\langle \mathcal{J}, x_n, \dots, x_{n-j+1} \rangle^{\text{sat}} = \langle \mathcal{J}, x_n, \dots, x_{n-j+1} \rangle \colon x_{n-j}^{\infty}.$$
 (2.1)

(vi) For all  $1 \le j < n$  we have

$$\mathcal{J}: x_{n-j}^{\infty} = \mathcal{J}: \langle x_1, \dots, x_{n-j} \rangle^{\infty}.$$
(2.2)

The various characterisations show that quasi-stable ideals are indeed rather special possessing many properties that do not hold for arbitrary monomial ideals and that these properties are closely related to the chosen coordinate system which here means mainly the ordering of the variables  $x_1 > \cdots > x_n$ . Seiler (2009b, 2010) furthermore showed that one can provide for quasi-stable ideals an explicit free resolution.

*Remark* 2.3. For a polynomial ideal  $I \triangleleft S$ , quasi-stable position is related to the better known Noether position. Part (iv) of Proposition 2.2 entails that the canonical map  $k[x_{n-d+1}, ..., x_n] \rightarrow S/I$  defines a *Noether normalisation* (see also the discussion in (Seiler, 2010)). In fact, quasi-stable position is a stronger condition than Noether position. Bermejo and Gimenez (2006) proved that an ideal is in quasi-stable position, if and only if the ideal and all primary components of its leading ideal are simultaneously in Noether position. Hashemi et al. (2018) provided a combinatorial characterisation of Noether position analogous to Definition 2.1 showing that it represents a weakened version of quasi-stability where one can simply ignore certain obstructions.

*Remark* 2.4. If the polynomial ideal  $I \triangleleft S$  is *D*-dimensional, then a maximal system of parameters consists of c = n - D ideal members  $f_1, \ldots, f_c \in I$  such that the ideal  $\tilde{I} \subseteq I$  generated by them is also *D*-dimensional. This is equivalent to  $f_1, \ldots, f_c$  defining an *S*-regular sequence in I and  $\tilde{I}$  is then a complete intersection. Such systems of parameters are relevant for many computational tasks in commutative algebra. E. g. when computing primary decompositions, their determination represents a serious bottleneck (Decker et al., 1999). It is shown in (Seiler, 2012) that in quasi-stable position those elements of a Pommaret basis of I which have a pure variable power as leading term form a maximal system of parameters. Thus in quasi-stable position the determination of a system of parameters is trivial.

It is also well-known that quasi-stable position is a generic notion (see e. g. (Seiler, 2010) for a proof). In our context, this has the following meaning given an arbitrary polynomial ideal  $I \lhd S$ . If we choose a non-singular random matrix  $A \in \mathbb{k}^{n \times n}$  and perform the coordinate transformation  $\mathbf{x} \mapsto A\mathbf{x}$ , then the transformed ideal  $I_A = A \cdot I$  will almost always be in quasi-stable position. More precisely, the set of all matrices A such that  $I_A$  is in quasi-stable position contains a Zariski open subset of  $\mathbb{k}^{n \times n}$ .

Galligo (1974) in characteristic zero and Bayer and Stillman (1987b) in positive characteristic proved for any ideal  $I \triangleleft S$  the existence of a *generic initial ideal* gin I, i.e. they showed that there exists a Zariski open subset  $\mathcal{U} \subseteq GL(n, \mathbb{k})$  such that for all  $A, B \in \mathcal{U}$  we have lt  $I_A = \operatorname{lt} I_B = \operatorname{gin} I$ . We say that I is in *GIN position*, if lt  $I = \operatorname{gin} I$ . This position is very popular among theorists, as in it many invariants of the polynomial ideal I can already be read off from the monomial ideal lt I where they are typically easier to compute. Computationally, it is very expensive to rigorously verify that an ideal is in GIN position; Hashemi et al. (2018) describe an approach based on Gröbner systems.

If an ideal  $\mathcal{I}$  is in GIN position, then its leading ideal is strongly stable and thus in particular quasi-stable. Hence GIN position entails quasi-stable position, but the converse is not true. In Hashemi et al. (2012), it is demonstrated that most of the properties of gin  $\mathcal{I}$  also hold for lt  $\mathcal{I}$  provided  $\mathcal{I}$  is in quasi-stable position. We recall here some of most important results.

**Theorem 2.5.** Let  $I \triangleleft S$  be an ideal in quasi-stable position. Then the ideals I and It I share the following invariants:

(i) *satiety* sat I = sat lt I,

(ii) projective dimension pd I = pd lt I (or equivalent depth I = depth lt I),

(iii) Casteluovo–Mumford regularity  $\operatorname{reg} I = \operatorname{reg} \operatorname{lt} I$ .

Furthermore, S/I is Cohen–Macaulay, if and only if the same is true for  $S/\operatorname{lt} I$ .

## 2.2. Pommaret Bases

Involutive bases are a special type of Gröbner bases with additional combinatorial properties and depend not only on a term order but also on a so-called involutive division, a refinement of the usual divisibility relation of terms. They were introduced by Gerdt and Blinkov (1998a) inspired by the Janet–Riquier theory of partial differential equations. The basic idea of an involutive division L is to associate with any generator h in a finite set  $\mathcal{H} \subset S$  a subset  $\chi_{L,\mathcal{H}}(h) \subseteq X$  of multiplicative variables. In linear combinations (or normal form computations), the generator h may then only be multiplied with polynomials in the subring  $\mathbb{k}[\chi_{L,\mathcal{H}}(h)] \subseteq S$ . Loosely speaking,  $\mathcal{H}$  is an involutive basis, if even with this restriction it still generates the whole ideal  $\langle \mathcal{H} \rangle$ . In contrast to the usual Gröbner bases, involutive bases are non-trivial even for monomial ideals. For an extensive introduction to theory, algorithmics and history of involutive bases, we refer to (Seiler, 2009a, 2010). We omit here the rather technical definition of an involutive division L and provide only one for L-involutive bases.

**Definition 2.6.** Let *L* be an involutive division. The *L*-involutive span of a finite set  $\mathcal{H} \subset S$  of polynomials is the k-linear space

$$\langle \mathcal{H} \rangle_L = \sum_{h \in \mathcal{H}} \mathbb{k}[X_{L,\mathcal{H}}(h)] \cdot h \subseteq \langle \mathcal{H} \rangle.$$
 (2.3)

 $\mathcal{H}$  is an *L-involutive basis* of the ideal  $\mathcal{I} = \langle \mathcal{H} \rangle$ , if (i) all elements of  $\mathcal{H}$  have different leading terms, (ii)  $\langle \mathcal{H} \rangle_L = \langle \mathcal{H} \rangle$  and (iii) the sum in (2.3) is direct.

The definition immediately implies that  $\mathcal{H}$  is an *L*-involutive basis of  $\mathcal{I}$ , if and only if lt  $\mathcal{H}$  is an *L*-involutive basis of lt  $\mathcal{I}$ . This in turn entails that any involutive basis is also a – generally non-reduced – Gröbner basis. A key difference to the theory of Gröbner bases is the requirement that any involutive basis induces a direct sum decomposition of the ideal generated by it. This fact implies for example that involutive standard representations of ideal members are unique. Most properties of involutive bases can be traced back to induced decompositions both of the (leading) ideal and its complement – for a more detailed discussion see (Seiler, 2010) and (Hashemi et al., 2022) and references therein.

*Example* 2.7. Let  $\mathcal{H}$  be a set of terms. Then the *Janet division* is defined as follows. Assume  $x^{\mu} \in \mathcal{H}$ . We have  $x_1 \in X_{J,\mathcal{H}}(x^{\mu})$ , if and only if  $\mu_1 = \max\{v_1 \mid x^{\nu} \in \mathcal{H}\}$ . For deciding whether any of the other variables are multiplicative, we must consider certain subsets of  $\mathcal{H}$  defined by initial segments of exponent vectors. Given such a segment  $(\mu_1, \ldots, \mu_j)$ , we write  $\mathcal{H}_{(\mu_1, \ldots, \mu_j)} = \{x^{\nu} \in \mathcal{H} \mid \nu_1 = \mu_1, \ldots, \nu_j = \mu_j\}$ . Now  $x_{j+1} \in X_{J,\mathcal{H}}(x^{\mu})$ , if and only if  $\mu_{j+1} = \max\{v_{j+1} \mid x^{\nu} \in \mathcal{H}_{(\mu_1, \ldots, \mu_j)}\}$ .

The Janet division has the special property that any finite set of terms is automatically involutively autoreduced, i. e. no term in the set involutively divides another term in the set. It entails that for this division the sum in (2.3) is always direct provided all elements of  $\mathcal{H}$  have different leading terms. For other divisions, one may have to perform an involutive autoreduction to ensure the directness of the sum. In the following, we will always assume that we are dealing with involutively autoreduced sets so that we will always have a direct sum in (2.3). **Definition 2.8.** Let  $\mathcal{H} \subset S$  be a finite set of polynomials and  $I = \langle \mathcal{H} \rangle$  the ideal generated by it. The *volume function* of I is the numerical function  $v_I \colon \mathbb{N}_0 \to \mathbb{N}_0$  given by  $v_I(q) = \dim_k I_q$  where  $I_q$  denotes the homogeneous component of the ideal I of degree q. If L is an involutive division for which the set  $\mathcal{H}$  is involutively autoreduced, we analogously define a *volume function* of the L-involutive span of  $\mathcal{H}$  by setting  $v_{\langle \mathcal{H} \rangle_L}(q) = \dim_k (\langle \mathcal{H} \rangle_L)_q$  where again the subscript q refers to the homogeneous component of degree q.

The following assertion is a simple consequence of the assumed directness of the sum in (2.3) and elementary combinatorics. It shows that with an involutive basis it is trivial to compute the volume function (and thus also the more commonly used Hilbert function) of any ideal. Furthermore, we also obtain as a trivial corollary the well-known statement that these functions become polynomial for sufficiently high degrees.

**Lemma 2.9.** Let the finite set  $\mathcal{H} \subset S$  be involutively autoreduced for the involutive division *L*. If we denote by  $q_h$  the degree and by  $k_h$  the number of multiplicative variables of a generator  $h \in \mathcal{H}$ , then we have<sup>4</sup>

$$v_{\langle \mathcal{H} \rangle_L}(q) = \sum_{h \in \mathcal{H}} [q \ge q_h] \binom{q - q_h + k_h - 1}{k_h - 1}.$$
(2.4)

If  $\bar{q} = \max_{h \in \mathcal{H}} q_h$ , then  $v_{\langle \mathcal{H} \rangle_L}$  is a polynomial for all  $q \ge \bar{q}$ , the volume polynomial  $V_{\langle \mathcal{H} \rangle_L}$  of the involutive span. An explicit expression for it is obtained by simply dropping the Kronecker–Iversion symbol in (2.4).

In this article, mainly *Pommaret bases* are relevant. For them, the rule to determine the multiplicative variables is particularly simple, as it depends only on the polynomial h and not on the whole set  $\mathcal{H}$ , as for most other involutive divisions: if max lt h = j, then we have  $X_P(h) = \{x_j, \ldots, x_n\}$ . Thus to get as many multiplicative variables as possible, the optimal choice is to use the degree reverse lexicographic order which explains why we exclusively consider it.

While for many involutive divisions *L* (e. g. the Janet division), any ideal  $I \triangleleft S$  possesses a finite *L*-involutive basis, this is not true for the Pommaret division *P*. A trivial counterexample is the monomial ideal  $\mathcal{J} = \langle x_1 x_2 \rangle \triangleleft \Bbbk[x_1, x_2]$  where one needs the infinite set  $\{x_1^k x_2 \mid k \in \mathbb{N}\}$  to generate  $\mathcal{J}$  involutively. The following result from Seiler (2009b) relates the existence of finite Pommaret bases to quasi-stability and provides yet another characterisation of this combinatorial concept.

**Theorem 2.10.** A monomial ideal  $\mathcal{J} \triangleleft S$  has a finite Pommaret basis, if and only if it is quasi-stable. A polynomial ideal  $I \triangleleft S$  has a finite Pommaret basis, if and only if it is in quasi-stable position.

We note already above that quasi-stability is a generic property. Thus the possible non-existence of a finite Pommaret basis is only a matter of the use coordinate system:

<sup>&</sup>lt;sup>4</sup>Here, we use for notational simplicity the Kronecker-Iverson symbol [C] which is 1, if the logical statement C is true, and 0 otherwise.

after a generic linear transformation every ideal is in a position where it has finite Pommaret basis. Seiler (2009b) showed that Pommaret bases provide us with the following *effective* version of Theorem 2.5.

**Theorem 2.11.** Let  $\mathcal{H}$  be a finite Pommaret basis of the polynomial ideal  $\mathcal{I} \triangleleft S$ . Let q be the maximal degree deg h and n - d + 1 the maximal value of max h for an element  $h \in \mathcal{H}$ . Then:

- (i)  $\mathcal{I}^{\text{sat}} = \mathcal{I}: x_n^{\infty} \text{ and sat } \mathcal{I} = \max \{ \deg h \mid h \in \mathcal{H} \land \max \operatorname{lt} h = n \},$
- (ii) depth I = d,
- (iii)  $\operatorname{reg} I = q$ .

As by definition of an involutive basis, lt  $\mathcal{H}$  is a Pommaret basis of lt  $\mathcal{I}$  and as the values q and d are determined by leading terms, Theorem 2.5 becomes now an immediate corollary of Theorem 2.11. With these results, the effective computation of such key invariants like sat  $\mathcal{I}$ , depth  $\mathcal{I}$  or reg  $\mathcal{I}$  becomes trivial – provided we can efficiently determine a coordinate transformation to quasi-stable position. Despite the fact that quasi-stability is a generic property, many ideals appearing in applications are not in quasi-stable position. The only exception are zero-dimensional ideals which are always in quasi-stable position.

*Example* 2.12. A celebrated result by Bayer and Stillman (1987a) asserts that generically the maximal degree of a Gröbner basis with respect to the degree reverse lexicographic order is the Castelnuovo–Mumford regularity of the ideal. However, there is no way to effectively verify whether a given ideal is in the required generic position whereas this is trivial for quasi-stability. The difference is nicely demonstrated by the following ideal from (Seiler, 2009b, Ex. 9.9):

$$I = \langle x_1^8 - x_2^6 x_3 x_4, \ x_2^7 - x_1 x_3^6, \ x_1^7 x_2 - x_3^7 x_4 \rangle \triangleleft \mathbb{k}[x_1, x_2, x_3, x_4].$$
(2.5)

In the given coordinates, the three generators define already the reduced Gröbner basis for the degree reverse lexicographic order. Thus one might expect that reg I = 8. However, if we swap two of the coordinates and consider I as an ideal in  $k[x_1, x_3, x_2, x_4]$ , we obtain a completely different Gröbner basis for the corresponding degree reverse lexicographic order:

$$\left\{ \begin{array}{l} x_{2}^{7} - x_{1}x_{3}^{6}, \ x_{1}^{7}x_{2} - x_{3}^{7}x_{4}, \ x_{1}^{8} - x_{2}^{6}x_{3}x_{4}, \ x_{1}^{6}x_{2}^{8} - x_{3}^{13}x_{4}, \\ x_{1}^{5}x_{2}^{15} - x_{3}^{19}x_{4}, \ x_{1}^{4}x_{2}^{22} - x_{3}^{25}x_{4}, \ x_{1}^{3}x_{2}^{29} - x_{3}^{31}x_{4}, \\ x_{1}^{2}x_{2}^{36} - x_{3}^{37}x_{4}, \ x_{1}x_{2}^{43} - x_{3}^{43}x_{4}, \ x_{2}^{50} - x_{3}^{49}x_{4} \right\}.$$
(2.6)

It seems to indicate that reg I = 50. However, none of the used coordinates are generic in the sense of Bayer and Stillman (1987a). In the orginal coordinates, the ideal I is in quasi-stable position. A Pommaret basis is obtained, by adding to the Gröbner basis the polynomials  $x_1^k(x_2^7 - x_1x_3^6)$  for  $1 \le k \le 6$ . According to Theorem 2.11, we thus have reg I = 13 and we can conclude that the result by Bayer and Stillman (1987a) does not even provide either a lower or an upper bound. Without a mean to verify the genericity of the used coordinates, it is rather useless for concrete computations. Although the definitions of the Janet and the Pommaret division, respectively, look very different, the two divisions are actually closely related (see (Gerdt, 2000) for a detailed discussion). One consequence of this is the following observation that is an immediate corollary to statements in (Seiler, 2009b).

**Proposition 2.13.** Assume that the polynomial ideal  $I \triangleleft S$  is in quasi-stable position. *Then any minimal Janet basis of I is also a Pommaret basis.* 

#### 2.3. Related Algorithms

As extensively discussed in (Seiler, 2010) and references therein, the theory of involutive bases provides a direct algorithm – developed by Gerdt and Blinkov (1998a) (see also (Gerdt and Blinkov, 1998b)) – for completing an arbitrary generating set of an ideal into an involutive basis (assuming that such a basis exists) and many optimisations have been proposed for it (see e.g. (Gerdt, 2005) and references therein). Several implementations of various variants of the basic algorithm exist. Nevertheless, one must say that these are not at the same level of maturity as current implementations of algorithms for Gröbner bases. In our computational experiments, we therefore used the following strategy: we computed first reduced Gröbner bases and then completed the leading terms to an involutive basis of the leading ideal. As one can see from results like Theorem 2.5, this is sufficient for most purposes.

As a consequence of this strategy, we discuss here only monomial completion algorithms. The basic idea of any involutive completion algorithm is to consider what happens if a generator is multiplied with one of its non-multiplicative variables. If the thus obtained term does not lie in the involutive span, it is added to the basis. Under modest assumptions, one can show correctness and termination of such algorithms; in fact, one can even show that if the input is a minimal generating set, then the output will be a minimal involutive basis (Seiler, 2010).

Algorithm 1 allows us to compute efficiently (minimal) Janet bases, although it does not explicitly use more sophisticated data structures like Janet trees (Gerdt et al., 2001) (implicitly some ideas of such optimisations are contained in our management of the multiplicative variables). The key optimisations in this algorithm are that we keep track of the already considered non-multiplicative variables and that we do not compute the multiplicative variables from scratch after each change in the basis, but only perform some necessary adaptions. Experiments with 2000 random ideals show that such simple measures suffice to provide a rather efficient algorithm: compared with a naive completion algorithm, the runtimes were on average 10 times faster.

We do not provide a detailed proof of the correctness of Algorithm 1. It follows rather immediately from the definition of the Janet division that adding in Line 11 the new generator  $x_i \cdot h[1]$  affects the assignment of multiplicative variables only for the generators considered in Line 12. The properties of an involutive division, in particular the so-called filter axiom, ensure that the addition of a further generator can only lead to smaller sets of multiplicative variables; it is not possible that a non-multiplicative variable becomes multiplicative. One might worry that some earlier considered nonmultiplicative prolongation could then lose its Janet divisor. But it is shown in (Seiler, 2010, Sect. 4.4) that this does not affect the correctness of the algorithm.

Algorithm 1: JanetCompletion

Data:	Minimal generating set $\mathcal F$ for the monomial ideal $\mathcal J \trianglelefteq \mathcal S$					
Result	: Minimal Janet basis of ${\mathcal J}$					
1 begin						
2 H	$\longleftarrow \left\{ [f, \emptyset, \mathcal{X}_{J, \mathcal{F}}(f)] \mid f \in \mathcal{F} \right\}   $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $ $					
tr	eated non-multiplicative variables					
3 So:	rt $\mathcal H$ w.r.t. degree from the smallest to the largest one					
4 rep	peat					
5	$flag \leftarrow true$					
6	if $\exists h \in \mathcal{H}: \{x_1, \ldots, x_n\} \setminus (h[2] \cup h[3]) \neq \emptyset$ then					
7	$flag \leftarrow false$					
8	$x_i \leftarrow \text{first element of } \{x_1, \ldots, x_n\} \setminus (h[2] \cup h[3])$					
9	$h[2] \leftarrow h[2] \cup \{x_i\}$					
10	if $x_i \cdot h[1]$ has no Janet divisor in $\{h[1] \mid h \in \mathcal{H}\}$ then					
11	$\mathcal{H} \longleftarrow \mathcal{H} \cup \left\{ [x_i \cdot h[1], \emptyset, h[3] \cap \{x_1, \dots, x_{i-1}\}] \right\}$					
12	For the elements $g \in \mathcal{H}$ such that $g[1]$ and $x_i \cdot h[1]$ have the same exponents in the variables $x_1, \ldots, x_i$ , update the multiplicative variables among the variables $x_i, \ldots, x_n$ (the variable $x_i$ must be checked only for $x_i \cdot h[1]$ ).					
13	Sort $\mathcal{H}$ w.r.t. degree from the smallest to largest one					
14 un	til flag					
	$\operatorname{rurn}\left\{h[1] \mid h \in \mathcal{H}\right\}$					

If we know that the given monomial ideal is quasi-stable and hence possesses a finite Pommaret basis, then we can resort to a simpler algorithm. Recall that the Pommaret division is global, i. e. the multiplicative variables associated to a term are independent of the remaining terms in the considered set. Hence it is not necessary to manage multiplicative variables or to keep track of already considered non-multiplicative variables and we arrive at Algorithm 2 (in Line 4, any term order < may be used). Correctness and termination is extensively discussed in (Seiler, 2010).

Hashemi et al. (2018) developed a deterministic approach to achieve quasi-stable (and related) position for arbitrary ideals. This approach is based on *elementary moves*. These very sparse transformations generate the Borel group of lower triangular, non-singular matrices. Each elementary move is characterised by a pair of indices (i, j) with  $1 \le i < j \le n$  and the move  $\mu_{(i,j)}$  maps  $x_j \mapsto x_i + x_j$  and leaves all other variables unchanged. Thus in S we have a total of  $\frac{1}{2}n(n-1)$  different elementary moves.

Assume that the ideal I is not in quasi-stable position. Hence its leading ideal lt I has at least one obstruction  $(x^{\mu}, i)$  to quasi-stability. In (Hashemi et al., 2018) it is shown that if max  $x^{\mu} = j$  the transformation  $x_j \mapsto x_i + ax_j$  will remove this obstruction for almost any choice of  $a \in \mathbb{R}$  (here our assumption char  $\mathbb{R} = 0$  is crucial). We will always choose a = 1, i.e. apply the elementary move  $\mu_{(i,j)}$ . In "unlucky" situations, cancellations may allow the obstruction to persist. However, after finitely

#### Algorithm 2: PommaretCompletion

Data: Finite generating set  $\mathcal{F}$  of quasi-stable ideal  $\mathcal{J} \trianglelefteq \mathcal{S}$ Result: Pommaret basis  $\mathcal{H}$  of  $\mathcal{J}$ 1begin2 $\mathcal{H} \leftarrow \mathcal{F}; \quad \mathcal{S} \leftarrow \{x_i h \mid h \in \mathcal{H}, i < \max h\}$ 3 $\mathcal{H} \leftarrow \mathcal{F}; \quad \mathcal{S} \leftarrow \{x_i h \mid h \in \mathcal{H}, i < \max h\}$ 4 $s \leftarrow \min_{\prec} \mathcal{S}; \quad \mathcal{S} \leftarrow \mathcal{S} \setminus \{s\}$ 5if s has no Pommaret divisor in  $\mathcal{H}$  then6 $\mathcal{H} \leftarrow \mathcal{H} \cup \{s\}; \quad \mathcal{S} \leftarrow \mathcal{S} \cup \{x_i s \mid i < \max s\}$ 7return  $\mathcal{H}$ 

many iterations of  $\mu_{(i,j)}$ , it will always disappear.

These considerations lead to Algorithm 3 (in (Hashemi et al., 2018), it was given for the case of strongly stable position, but the adaption is trivial). For proving its termination and for its formulation, one needs the following ordering. Let  $\mathcal{F}$  be an autoreduced finite set of polynomials and write  $\mathcal{L}(\mathcal{F}) = (t_1, \ldots, t_\ell)$  for the tuple of leading terms of  $\mathcal{F}$  sorted such that  $t_1 <_{\text{revlex}} \cdots <_{\text{revlex}} t_\ell$  for the purely reverse lexicographic order (not the *degree* reverse lexicographic order!). Given two such sets  $\mathcal{F}$  and  $\tilde{\mathcal{F}}$  with  $\mathcal{L}(\mathcal{F}) = (t_1, \ldots, t_\ell)$  and  $\mathcal{L}(\tilde{\mathcal{F}}) = (\tilde{t}_1, \ldots, \tilde{t}_\ell)$ , we define

$$\mathcal{F} \prec_{\mathcal{L}} \tilde{\mathcal{F}} \iff \begin{cases} \exists j \le \min(\ell, \tilde{\ell}) \colon (\forall i < j \colon t_i = \tilde{t}_i) \land t_{j \prec_{\text{reviex}}} \tilde{t}_j \text{ or} \\ (\forall j \le \min(\ell, \tilde{\ell}) \colon t_j = \tilde{t}_j) \land \ell < \tilde{\ell} \end{cases}$$
(2.7)

# Algorithm 3: QSPos – Quasi-Stable Position

Γ	<b>Data:</b> Reduced Gröbner basis $\mathcal{G}$ of homogeneous ideal $I \lhd S$
F	<b>Result:</b> Linear change of coordinates $\Psi$ such that $\operatorname{lt} \Psi(\mathcal{I})$ is quasi-stable
1 b	egin
2	$\Psi \leftarrow \mathrm{id};  \mathcal{F} \leftarrow \mathcal{G}$
3	while obstruction to quasi-stability of $\langle \operatorname{lt} \mathcal{F} \rangle$ exists do
4	choose elementary move $\psi$ related to obstruction; $\Psi \longleftarrow \psi \circ \Psi$
5	$ ilde{\mathcal{F}} \longleftarrow  extsf{ReducedGr{ m obnerBasis}}(\psi(\mathcal{F}))$
6	while $\mathcal{F} \succeq_{\mathcal{L}} \tilde{\mathcal{F}}$ do
7	$\Psi \longleftrightarrow \psi \circ \Psi$
8	$ ilde{\mathcal{F}} \longleftarrow  ext{ReducedGröbnerBasis}(\psi( ilde{\mathcal{F}}))$
9	$ \mathcal{F} \leftarrow \tilde{\mathcal{F}} $
10	return Ψ

The strategy behind Algorithm 3 is quite simple. As long as obstructions exist, we apply a related elementary move. Generically, this move will eleminate at least one obstruction; in rare cases we may have to iterate the move. In (Hashemi et al., 2018), it

is shown that a given ideal I possesses modulo linear coordinate transformations only finitely many leading ideals and that after an elementary move related to an obstruction a polynomial set can never descend with respect to the ordering  $\prec_{\mathcal{L}}$ . This ensures correctness and termination of the algorithm.

Like many algorithms in commutative algebra, Algorithm 3 is not completely specified: in Line 4, it is not said how the next elementary move should be chosen. In general, several possibilities will exist here. While the choice does not affect the correctness and the termination of the algorithm, it has an effect on the efficiency. A coarse measure for the efficiency is the number of elementary moves required until quasi-stable position is reached.

In a preparatory experiment, we compared two simple ways for performing this choice. In the "*democratic*" *strategy*, we note for each existing obstruction of quasistability for which elementary move it "votes", i. e. to which move it corresponds; the move which gets the most votes is taken. For estimating the influence of good or bad choices, we also used a *random strategy*: in each iteration of the outer while loop of Algorithm 3, we randomly pick an elementary move.

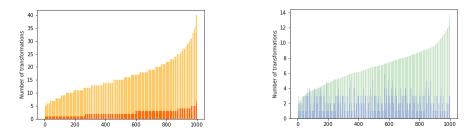


Figure 1: Performance of random choices. Left: comparison of minimal and maximal number of transformations needed to reach quasi-stable position. Right: Comparison of average number of transformations required by random strategy (green) with democratic strategy (blue).

We applied both strategies to 1000 ideals (these were a sample of 10% of a large test set of random ideals described in Section 3.2 below). The random strategy was applied to each ideal 10 times. The outcome of the experiment is shown in the two plots in Figure 1. The plot on the left shows for each ideal the minimal and the maximal number of transformations needed to reach a quasi-stable position using random choices. Obviously, the numbers differ significantly: the maximum is almost 10 times as large as the minimum in the worst cases and even in the best cases the numbers differ by a factor of five. The plot on the right compares the average number of transformations in a random strategy with the number required by the democratic strategy. The latter one needed typically between one and three elementary moves and thus was much more efficient. These observations clearly indicate that it is worth while thinking about good ways to perform the choice in Algorithm 3.

*Remark* 2.14. A natural thought is to consider only elementary moves which are related to obstructions, i. e. which obtain in the democratic strategy at least one vote. In fact, any human strategy we are aware of is based on this assumption. To our surprise, in the systematic analysis of a large set of random ideals (see Section 3.2 below), we

found cases where the optimal choice is not related to any obstruction and thus not obtainable with such strategies. However, such cases are fairly rare: we observed this phenomenon only for about 6% of the considered ideals.

## 3. Machine Learning Quasi-Stable Position

It follows from Remarks 2.3 and 2.4 that all problems mentioned in the title can be simultaneously solved by achieving quasi-stable position (for a system of parameters one needs in addition the Pommaret basis). Therefore, we will consider in the sequel only this problem. If the goal is a Noether position, then this may lead to unnecessary transformations, as it is weaker than quasi-stable position. Hashemi et al. (2019) constructed a special involutive division, called *D*-Noether division, such that a finite Noether basis exists, if and only if the ideal is in Noether position. In principle, one could adapt the approach presented here to this division and thus obtain slightly more efficient computations. As a quasi-stable position has so many further benefits, we refrain from detailing such an adaption.

We will now show how methods from supervised machine learning can successfully be applied to selecting the "right" elementary move in Line 4 of Algorithm 3. We are using a greedy approach: the models are trained to estimate which elementary move will lead to the largest Pommaret span. Following ideas used by England and collaborators for machine learning good variable orders for cylindrical algebraic decompositions (see the references in the Introduction), we consider the choice of moves as a *multi class classification problem*: each class corresponds to one possible elementary move so that we have  $\frac{1}{2}n(n-1)$  different classes.

We will compare five well established and much used classification methods:

- *k* Nearest Neighbours (*k*NN)
- Support Vector Machine (SVM)
- Decision Tree (DT)
- Multilayer Perceptron (MLP)
- Logistic Regression (LR)

Details about these methods can be found in most textbooks on machine learning; see e. g. (Aggarwal, 2015) or (Bishop, 2006). We emphasise that with the exception of the multilayer perceptron, none of them is based on a neural network. This means that training is comparatively cheap and less data are needed for it. In particular the latter point is of some relevance, as we will discuss below.

All our computations were done in PYTHON using the SCIKIT-LEARN library (Pedregosa et al., 2011). For polynomial computations, the PYTHON based computer algebra system SAGEMATH<sup>5</sup> was used. This concerns in particular the determination of Gröbner bases. For the extension to Janet or Pommaret bases, we implemented the monomial algorithms presented in Section 2.3 in SAGEMATH.

<sup>&</sup>lt;sup>5</sup>https://www.sagemath.org/

## 3.1. Features and Scoring

For applying machine learning models, the problem data must be mapped into a *feature space* of fixed dimension. This fact excludes the typical computer algebra approach of using a generating set as input: as the number of generators and the number of terms in each generator vary widely from ideal to ideal, generating sets cannot be interpreted as elements of a feature space. It also turned out that typical algebraic invariants like dimension, depth or regularity are not relevant for deciding which elementary move to choose.

Our feature vectors contain mainly what we call *statistical data* about the given generating set. This includes e.g. information about degrees (total or in individual variables) or the distribution of the variables over all terms or over the leading terms. In addition, we incorporate a *transformation part* which encodes for each elementary moves how many obstructions to quasi-stability vote for it. This makes the length of the feature vector independent of the size of the generating set, but it still depends on the number *n* of variables in the underlying polynomial ring *S* so that we must fix *n*. All experiments reported in this work have been done for n = 4. For smaller values of *n*, it is not so hard to construct by hand good coordinates. For larger values of *n*, the computational costs rapidly increasing (both for preparing the training data, but also for the learning, as the number of our features grows exponentially with *n*). Hence n = 4 seems a good choice for first experiments with different machine learning models.

Table 1 lists  $3 \cdot 2^n + 6n + 8$  statistical features, if we work in a polynomial ring with *n* variables. The second column describes the number of features each row defines. For instance, in the fourth row we have three values for each variable which gives a total of 3*n* features. For explaining the third column, we need the following notations. Let  $\mathcal{F} = \{f_1, \ldots, f_k\} \subset S$  be the considered finite generating set of an ideal I. We can write each polynomial as

$$f_i = \sum_{t=1}^{T_i} c_{i,t} x_1^{d_{i,t}^1} \cdots x_n^{d_{i,t}^n}, \quad i \in \{1, \dots, k\}.$$
(3.1)

Here  $T_i$  is the number of terms of  $f_i$ . We also write  $f_i^t$  for the term t in  $f_i$ . For the leading term, we use capital letters:

$$\operatorname{lt} f_{i} = C_{i,t} x_{1}^{D_{i,t}^{1}} \cdots x_{n}^{D_{i,t}^{n}}.$$
(3.2)

In some rows, we used the sign function to count the number of nonzero exponents and denoted by av the arithmetic mean of some values.

As one can see, this statistical part of the feature vector provides information about how the variables are distributed over all the terms, over the different generators and over the leading terms, as such information are crucial for estimating how different possible transformations may affect the size of the Pommaret span (and the sparsity) of the transformed set.

In addition, we have a smaller *transformation part* in the feature vector consisting of  $\frac{1}{2}n(n-1)$  entries: we store for each elementary move how many obstructions vote for it. A natural human strategy – the democratic strategy mentioned above – is based

Table 1: Used statistical features

Description	#	Formula
Number of generators	1	k
total number of terms	1	$\sum_i T_i$
Min/max/average total degree of	3	$\min_i \sum_{j=1}^n d_{i,t}^j$ , $\max_i \sum_{j=1}^n d_{i,t}^j$ and
generators		$\frac{\operatorname{av}_{i} \sum_{j=1}^{n} d_{i,t}^{j}}{\min_{i} d_{i,t}^{j}, \max_{i} d_{i,t}^{j} \operatorname{and} \operatorname{av}_{i} d_{i,t}^{j} \operatorname{for}}$
Min/max/average degree in single	3 <i>n</i>	$\min_i d_{i,t}^j$ , $\max_i d_{i,t}^j$ and $\operatorname{av}_i d_{i,t}^j$ for
variable of generators		$j \in \{1, \ldots, n\}$
Min/max/average degree in single	3 <i>n</i>	$\min_i D_i^j$ , $\max_i D_i^j$ and $\operatorname{av}_i D_i^j$ for
variable of leading terms		$j \in \{1, \ldots, n\}$
Min/max/average number of	3	$\min_i T_i$ , $\max_i T_i$ and $\operatorname{av}_i T_i$
terms in generators		
Number of generators containing	$2^{n} - 1$	$\sum_{i} \operatorname{sgn}\left(\sum_{t} \prod_{x_{i} \in \bar{X}} \operatorname{sgn}\left(d_{i,t}^{j}\right)\right)$ for
certain variables		$\emptyset \neq \bar{X} \subseteq X$
Number of terms containing	$2^{n} - 1$	$\sum_{i,t} \prod_{x_i \in \bar{X}} \operatorname{sgn}(d_{i,t}^j) \text{ for } \emptyset \neq \bar{X} \subseteq X$
certain variables		· · ·
Number of leading terms	$2^{n} - 1$	$\sum_{i} \prod_{x_i \in \bar{X}} \operatorname{sgn}(D_i^j)$ for $\emptyset \neq \bar{X} \subseteq X$
containing certain variables		, <u> </u>
Sum of total degrees of generators	1	$\sum_i \deg(f_i)$
Number of pure variable powers	1	$\sum_{i} T_{i} - \sum_{i,t,j} \operatorname{sgn}\left( d_{i,t}^{j} - \operatorname{deg}\left(f_{i}^{t}\right) \right)$
among terms		
Number of pure variable powers	1	$k - \sum_{i,t,j} \operatorname{sgn}\left( D_{i,t}^j - \operatorname{deg} f_i \right)$
among leading terms		μ - <del>3</del> -

exclusively on these values. The total number of features is thus  $3 \cdot 2^n + \frac{1}{2}(n^2 + 11n) + 8$  which leads for n = 4 to 86 features.

England and Florescu (2019) used 11 similar statistical features in their work on learning good variables orderings for cylindrical algebraic decomposition. Later, they proposed in (Florescu and England, 2019) a brute force approach to automatically generate new features. They generated algorithmically almost 2000 features (in a polynomial ring with n = 3 variables) to extract in the end with a statistical variance analysis 78 relevant and independent ones. We believe that we understand our problem sufficiently well to be able to select the relevant features by hand and refrained from such an automatised approach. The results presented below seem to indicate that this belief is not unjustified.

Given a finite polynomial set  $\mathcal{F} \subset S$  generating an ideal  $I \triangleleft S$ , our final goal is to put I into quasi-stable position and to obtain a Pommaret basis  $\mathcal{H}$  of I. We first compute a reduced Gröbner basis  $\mathcal{G}$  out of  $\mathcal{F}$  so that lt  $\mathcal{G}$  is the minimal generating set of lt I. For determining the transformation part of the feature vector, we need the obstructions to quasi-stability of lt  $\mathcal{G}$ . If no obstructions exist, I is already in quasi-stable position and we can determine a Pommaret basis (of its leading ideal) with Algorithm 2.

If obstructions exist, then we need a more quantitative measure for assessing how

far away from quasi-stable position we are. Taking lt *G* as input for Algorithm 1, we determine a minimal Janet basis  $\mathcal{H}$  of lt  $\mathcal{I}$  and read off from it the volume polynomial  $V_{\mathcal{I}}$  via Lemma 2.9. With the same lemma, we can also compute the volume polynomial  $V_{\langle \mathcal{H} \rangle_P}$  of the Pommaret span of  $\mathcal{H}$ . In quasi-stable position, these two polynomials are identical, as then the Janet basis is simultaneously a Pommaret basis by Proposition 2.13 and thus  $\langle \mathcal{H} \rangle_P = \text{lt } \mathcal{I}$ . Otherwise, we have for all sufficiently large degrees q that  $V_{\langle \mathcal{H} \rangle_P}(q) < V_{\mathcal{I}}(q)$ .

The formula in Lemma 2.9 expresses the volume polynomials as a sum of binomial coefficients. But it is of course trivial to expand these explicitly into the standard form of a univariate polynomial

$$V(q) = v_{n-1}q^{n-1} + v_{n-2}q^{n-2} + \dots + v_1q + v_0$$
(3.3)

and it also follows immediately from Lemma 2.9 that the maximal degree of any volume polynomial is n - 1. We associate with each volume polynomial written in the form (3.3), its coefficient vector  $v = (v_{n-1}, \ldots, v_1, v_0) \in \mathbb{Q}^n$ . Given two volume polynomials, we can compare their coefficient vectors using a lexicographic ordering. The volume polynomial with the larger vector will have the stronger asymptotic growth, i. e. from some degree on it will always produce larger values. For example, if we are not in quasi-stable position, then  $v_{\langle H \rangle p} <_{lex} v_I$ .

Based on this observation, we can compare the effect of different elementary moves. Let  $\mu_{(i,j)}$  and  $\mu_{(k,\ell)}$  be two moves. Applying each of them to the generating set  $\mathcal{F}$ , we obtain two new polynomial sets  $\mathcal{F}_{(i,j)}$  and  $\mathcal{F}_{(k,\ell)}$ , respectively. Out of them, we compute first reduced Gröbner bases  $\mathcal{G}_{(i,j)}$  and  $\mathcal{G}_{(k,\ell)}$  and then complete their leading terms to Janet bases  $\mathcal{H}_{(i,j)}$  and  $\mathcal{H}_{(k,\ell)}$ . If now  $v_{\langle \mathcal{H}_{(i,j)} \rangle_{\mathcal{P}}} \prec_{\text{lex}} v_{\langle \mathcal{H}_{(k,\ell)} \rangle_{\mathcal{P}}}$ , then we consider the elementary move  $\mu_{(k,\ell)}$  as the better choice in Algorithm 3.

Obviously, it is very costly to analyse all possible elementary moves in this way, in particular for a larger number n of variables. One may say that we try to bypass this expensive computation by using machine learning. The task of the different models is to predict the best move purely on the basis of the above described features – without actually applying any transformation and without computing any Gröbner basis.

# 3.2. Producing Training Data

A fundamental problem in the application of tools from machine learning to commutative algebra is the lack of a sufficiently large repository of polynomial ideals. Available collections contain typically some dozens of examples with different numbers of variables, whereas the training of a typical machine learning model will require at least a few thousand examples (and in our case all with the same number of variables). Hence we must resort to *random ideals*. It is well known that the properties of polynomial ideals appearing in applications often differ from random ideals, but we are not aware of any alternative.

Instead of relying on some built-in functions of SAGEMATH, we wrote our own random generator for homogeneous ideals to have full control over all relevant parameters like degrees, number of generators or number of terms. It uses a *Poisson distribution* for choosing these parameters. Hence like in many applications, most generators have rather small degrees and a low number of terms, but some generators may have fairly high degrees or a larger number of terms.

An important goal is that most generated ideals are not in quasi-stable position, as only these are useful for our purposes. Furthermore, the dimension of the ideals is important. Any zero-dimensional ideal is automatically in quasi-stable position<sup>6</sup> and for ideals of dimension n - 1, i. e. hypersurfaces, it is usually easy to find by hand good coordinates. Thus we chose the parameters of the Poisson distributions in such a way that many ideals of intermediate dimensions are produced.

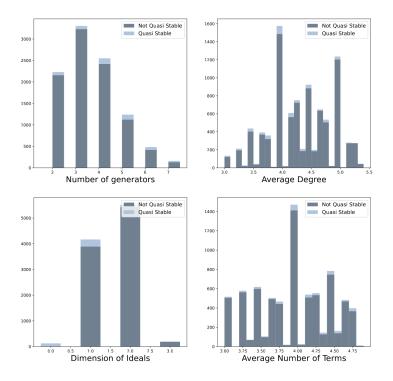


Figure 2: Some statistics of the 10.000 generated random ideals and their generating sets

With this random generator, we produced 10.000 ideals in a polynomial ring with 4 variables over the rational numbers. About 95% of them, 9.509 to be precise, were not in quasi-stable position and we only used these ideals for our experiments. The histograms in Figure 2 show some key properties of the generated polynomial sets and their ideals. The first histogram of the number of generators shows the typical shape of a Poisson distribution with most of the sets containing two to four generators. The second and the fourth histogram depicts the average degree and the average number of

<sup>&</sup>lt;sup>6</sup>Unfortunately, many of the ideals in available collections are zero-dimensional which further reduces the amount of training data available from real applications.

terms in a generator. The third histogram plots the dimensions of the generated ideals. It shows that most ideals have their dimension in the desired intermediate range.

*Remark* 3.1. We used the occasion of having so many ideals available to do some statistics on their properties and on their bases. More precisely, we were interested in comparing the number of generators and the maximal degree of a generator in the original generating set, in the reduced Gröbner basis and in the Janet basis as an empirical way to assess the practical complexity of the latter two types of bases.

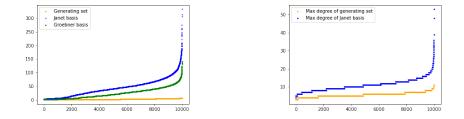


Figure 3: Sizes (left) and maximal degrees (right) of the original generating sets, the reduced Gröbner bases and the Janet bases of the random ideals

The left diagram in Figure 3 concerns the sizes of the different types of generating sets. Each curve contains one point for each of the 10.000 random ideals and each curve is separately sorted by size. It thus makes no sense to compare individual points, as they will typically belong to different ideals. One clearly see that for the vast majority of ideals the size of the Gröbner and Janet bases, respectively, grow only moderately; only for a very small fraction of the ideals large bases with more than one hundred elements occur. As Janet bases are non-reduced Gröbner bases, they contain of course more generators, but on average they seem to be larger by a relatively modest factor.

The right diagram in Figure 3 shows the maximal degree of a generator; we omitted here a curve for the reduced Gröbner bases, as it is indistinguishable from the one for the Janet bases. As already mentioned, Bayer and Stillman (1987a) proved that generically the maximal degree of a Gröbner basis with respect to the degree reverse lexicographic order is the Castelnuovo–Mumford regularity of the ideal. But as we demonstrated in Example 2.12, this degree is neither a lower nor an upper bound of the regularity. In (Albert et al., 2015), it is shown that the degree of a Janet basis is always at least the Castelnuovo–Mumford regularity and thus represents an upper bound. The diagram confirms a well-known empirical fact: although the Castelnuovo–Mumford regularity may grow double exponentially with the number n of variables and the degree d of the generating set, this rarely occurs in practise. In other words, our random ideals exhibit here again the same behaviour as ideals appearing in applications.

Hashemi et al. (2021, Ex. 7.7) exhibited a family of ideals in an arbitrary number of variables such that the difference between the degree of the Janet basis and the Castelnuovo–Mumford regularity can become arbitrarily large (based on an example in three variables from (Albert et al., 2015)). The benchmarks presented in (Albert et al., 2015) indicate, however, that in practise large differences are rare. Our 10.000 random ideals seem to confirm this observation: 5.863 have a Janet basis with exactly

the same degree as the Gröbner basis, 4.081 Janet bases have a degree which is one higher and 56 a degree which is two higher; larger differences do not occur. Thus, although the Janet bases are typically considerable larger, the additional generators do not increase noticably the maximal degree.

To each of the not quasi-stable ideals, we applied each of the six possible elementary moves and determined which move yields the largest Pommaret span in the sense that the coefficient vector of the volume polynomial is maximal for the lexicographic ordering. We sorted the elementary moves as (2, 1), (3, 1), (3, 2), (4, 1), (4, 2) and (4, 3) and labelled the corresponding classes as  $0, 1, \ldots, 5$ . Figure 4 shows how the ideals distribute over the six different classes. Obviously, the distribution is very uneven: almost

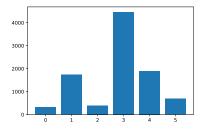


Figure 4: Distribution of classes in data set

half of the ideals belong to class 3, whereas the classes 0 and 2 are very rare. As a consequence, we used for the determination of the hyperparameters of the different models a *stratified* cross-validation. It is an interesting question whether this unevenness is an artefact of working with random ideals or whether it can also be observed in ideals from applications.

## 3.3. Experimental Results

We determined the hyperparameters of the different used machine learning models by a grid search with a 5-fold stratified cross-validation. Thus we separated our data set into five parts of equal size taking care that the distribution of the ideals over the different classes remains the same in each part. Then always four parts were used for training and one part for testing. The values obtained for the various hyperparameters of the different models are shown in Table 2.

As the different models depend on different numbers of hyperparameters and also the possible ranges of values for the various hyperparameters can be very different (sometimes a finite number of discrete values, sometimes a real interval), it makes no sense to directly compare the computation times for the determination of the hyperparameters. We only mention that the multilayer perceptron required by far the longest time and the decision trees were the fastest model in this respect.

Working with the thus determined hyperparameters, we observed for the five different models investigated the accuracies reported in Table 3 (these are the *average* accuracies over the five different test sets in the 5-fold cross-validation). Even the worst model, *k* nearest neighbours, achieved an accuracy of 74%, while the best model, the multilayer perceptron, reached 94%. For comparison: England and Florescu (2019) reported for their use of machine learning in the context of cylindrical algebraic decomposition accuracies around 60% for all tested models. This seems to indicate that our problem is very well suited for the use of machine learning. However, one should take into account that because of the stratification of our data set, always answering class 3 yields already an accuracy of almost 50%.

Model	Hyperparameter	Value
<i>k</i> -NN	k	20
K-ININ	Weights	Inv. proport. distance
	Algorithm	KDtree
SVM	Regularisation param. C	0.1
SVM	Kernel	Linear
DT	Criterion	Gini impurity
	Maximum depth	5
	Hidden layer size	100
MLP	Activation function	logistic sigmoid
FILF	Optimizer	Quasi-Newton method
	Regularisation param. $\alpha$	1.0
	Class	Multinomial
LR	Max. iterations	1.000
	Solver	Stoch. average gradient
	Penalty	L1

Table 2: Hyperparameters determined by a grid search with 5-fold stratified cross-validation

Model	k-NN	SVM	DT	MLP	LR	Demo.	Random
Accuracy	0.74	0.90	0.78	0.94	0.88	0.43	0.17
Time (sec.)	16.49	15.32	30.44	34.94	146.98	740.32	0.29

Table 3: A	ccuracy of	f the diff	erent models
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In the last two columns of Table 3, we contrast the accuracies with a human strategy – the democratic strategy mentioned above – and a simple random approach. For the random approach, we used a uniform random generator, as in real application situations the uneven distribution of the classes shown for our data in Figure 4 is not known. Somewhat surprisingly, we observed for random choices an accuracy of 17% which is exactly the value one would expect for a uniform distribution. Not surprising is the fact that this is by far the lowest value in the table. The democratic strategy as one of the most natural human strategies achieved only an accuracy of 43% which is even worse than always saying class 3 and far inferior to any used machine learning model. Thus this human strategy cannot be considered as very successful.

The last row in Table 3 provides for each model and the two other strategies the time required to determine the accuracy. For the machine learning models, this means the time needed to perform a 5-fold stratified cross-validation. Trivially, the random strategy is the fastest. As the democratic strategy requires to determine all obstructions, it is by far the slowest. Among the machine learning models, k nearest neighbours and support vector machine were the fastest; decision trees and multilayer perceptrons required roughly double the time and the logistic regression even the tenfold time.

For a more detailed accuracy analysis, we compare in Figure 5 the confusion matrices (based on all 9.509 test ideals not in quasi-stable position) for two models: the decision tree as an example of a model which did not work so well on our data and the multilayer perceptron as the winner among the considered models in terms of accuracy. One sees the biggest differences in the relatively rare classes 0 and 2 and in the class 1 which is apparently difficult to recognise. The multilayer perceptron classified the vast majority of ideals in these three classes correctly, whereas the decision tree put most of ideals in the wrong classes 3 and 4.

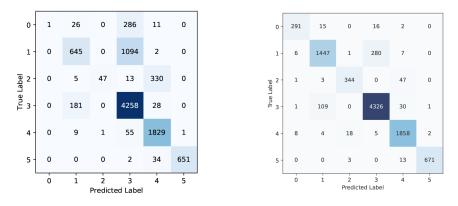


Figure 5: Confusion matrices for two models: decision tree (left) and multilayer perceptron (right)

A comparison based on accuracies and similar measures like sensitivity, precision or specifity is "binary": if the model does not predict the *optimal* move, its answer is considered as false. However, it might be that the move selected by the model has almost the same effect on the Pommaret span as the optimal one. We therefore computed for each model for each ideal where it did not predict the optimal move a "volume ratio", i. e. the ratio  $V_{\text{pred}}(\bar{q})/V_{\text{opt}}(\bar{q})$  where  $V_{\text{pred}}$  denotes the volume polynomial of the Pommaret span after the predicted move,  $V_{\text{opt}}$  the volume polynomial of the Pommaret span after the optimal move and the degree  $\bar{q}$  was chosen as ten times the degree of the Janet basis of the original ideal, i. e. so high that it approximates well the asymptotic behaviour. As one can clearly see in Figure 6, in many cases the predicted move was actually not much worse than the optimal move with a volume ratio above 90%. For the multilayer perceptron the volume ratio was really bad for less than 100 ideals out of almost 10.000. By comparison, the decision tree classified more than 1.000 ideals really badly, i. e. more than 10 times as many.

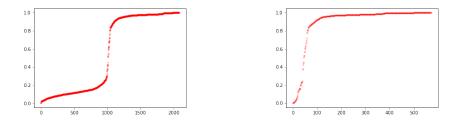


Figure 6: Volume ratios for two models: decision tree (left) and multilayer perceptron (right)

## 3.4. Complete Determination of Quasi-Stable Position

So far, we have only been concerned with one intermediate step of Algorithm 3, the choice of the next elementary move in Line 4. In principle, it is straightforward to embed machine learning into the algorithm: in Line 4, the choice of the next move is done by a trained model. Note, however, the following difference: in Algorithm 3, the next move is chosen among all moves related to an obstruction, whereas our machine learning models always consider *all* possible elementary moves. As discussed in Remark 2.14, in a small number of cases the optimal move is not related to an obstruction and hence it appears useful to allow also such moves. On the other hand, the termination proof in (Hashemi et al., 2018) does not take such moves into account.

Algorithm 4: QSPosML – Quasi-Stable Position with ML				
<b>Data:</b> Reduced Gröbner basis $\mathcal{G}$ of homogeneous ideal $I \triangleleft S$				
<b>Result:</b> Linear change of coordinates $\Psi$ such that lt $\Psi(I)$ is quasi-stable				
1 begin				
$2 \qquad \Psi \longleftarrow \mathrm{id};  \mathcal{F} \longleftarrow \mathcal{G}$				
3 $\mathcal{M} \leftarrow \{\text{elem. moves related to obstr. to quasi-stability of } \langle \text{lt} \mathcal{F} \rangle \}$				
4 while $\mathcal{M} \neq \emptyset$ do				
5 $ \mathbf{i}\mathbf{f} \mathcal{M}  = 1$ then				
$6 \qquad \qquad \psi \leftarrow \mathcal{M}[1];$				
7 else				
8 let ML model choose elementary move $\psi$				
9 $\tilde{\mathcal{F}} \leftarrow$ ReducedGröbnerBasis $(\psi(\mathcal{F}))$				
10 <b>if</b> $(\psi \notin \mathcal{M}) \land (\mathcal{F} \succeq_{\mathcal{L}} \tilde{\mathcal{F}})$ then				
11 $\psi \leftarrow$ move in $\mathcal{M}$ with most votes				
12 $\tilde{\mathcal{F}} \leftarrow \text{ReducedGröbnerBasis}(\psi(\mathcal{F}))$				
13 $\Psi \leftarrow \psi \circ \Psi$				
14 while $\mathcal{F} \geq_{\mathcal{L}} \tilde{\mathcal{F}}$ do				
15 $\Psi \leftarrow \psi \circ \Psi$				
15 $\Psi \leftarrow \psi \circ \Psi$ 16 $\tilde{\mathcal{F}} \leftarrow$ ReducedGröbnerBasis $(\psi(\tilde{\mathcal{F}}))$				
17 $\mathcal{F} \leftarrow \tilde{\mathcal{F}}$				
18 $\mathcal{M} \leftarrow \{\text{elem. moves related to obstr. to quasi-stability of } \langle \text{lt} \mathcal{F} \rangle \}$				
19 return $\Psi$				

In our experiments, it turned out that these moves may inded lead to termination problems. We encountered surprisingly often situations where only a very small number of elementary moves was related to an obstruction, but the selected machine learning model proposed another move. Unfortunately, this move did not change the leading ideal and thus the algorithm ran into an infinite loop. We therefore designed Algorithm 4 which is modified in two respects. (i) If only one elementary move is related to an obstruction, it always applies this move without asking the machine learning model. This reflects that in such a situation one can expect that after this move a quasi-stable position will be reached and thus the question of choosing a move does not arise. (ii) If the machine learning model proposes a move which is *not* related to an obstruction, then the algorithm uses this move only tentatively. This means that it checks afterwards whether the move has lead to a new set of leading terms which is larger than the old one with respect to the ordering  $<_{\mathcal{L}}$  introduced in (2.7). Only if this is the case, it continues with the transformed set. Otherwise, it rejects the move and instead uses the democratic strategy to choose the next move. This modification makes the algorithm consistent with the termination proof in (Hashemi et al., 2018) – which is based on producing a sequence of leading ideals which is strictly increasing with respect to the ordering  $<_{\mathcal{L}}$  – and thus ensures termination of the adapted algorithm.

We applied Algorithm 4 to the 9.509 test ideals not in quasi-stable position and counted for each how many elementary moves were necessary to reach a quasi-stable position. In this experiment, we used the support vector machine as machine learning model, as it has almost the same accuracy as the multilayer perceptron, but requires less computation time. Figure 7 shows a histogram depicting how many ideals needed how many transformations to reach a quasi-stable position. 90% of the ideals require at most four transformations with 55% needing two or three; more than eight transformations were never nec-

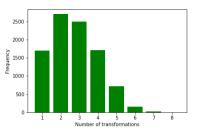


Figure 7: Number of transformations required to achieve a quasi-stable position.

essary. This indicates that most of our test ideals are not far away from a quasi-stable position. We also monitored the effect of the modifications introduced in the design of Algorithm 4. About two thirds of the ideals reached a situation where only one elementary move was related to an obstruction; one may conjecture that this typically happens for the last transformation. Given the observation from Remark 2.14 that moves not related to obstructions are rarely optimal, it is surprising that it happened also for about two thirds of the ideals that the support vector machine proposed in at least one iteration such a move. But on average only about every fourth such move could be accepted.

# 4. Conclusions

Our preliminary experiments already indicate that the problem of obtaining a quasistable position is well suited for the use of machine learning models and definitely better than the coarse human heuristics used so far. This is not very surprising, as the latter ones are based only on an analysis of the leading terms, whereas our feature vector takes the complete support of all generators into account.

Of course, the here presented results still have to be confirmed by further experiments with polynomials in a larger number of variables, say n = 5 and n = 6. Such experiments will also provide some information how our approach scales with n. It is clear that both the preparation of the training data and the determination of the hyperparameters will become significantly more expensive with an increasing number of variables and features. But once the models are trained, the costs of applying them should be neglectable compared to the costs of the required Gröbner bases.

The performance of both Algorithm 4 and the machine learning models are not yet completely satisfactory. In particular, the large number of instances where the machine learning model proposes a move which is not related to an obstruction to quasi-stability is surprising and requires further study. As currently only about one fourth of these moves can be accepted, they lead to a considerable waste of computation time.

We have not yet analysed how good our choice of the used features is. Only support vector machines offer here a simple possibility by looking at the support vectors defining the hyperplanes separating the different classes. While one can observe there differences in the relative importance of the various features, it turned out that at least for this model all features are relevant and used for the classification. Thus it seems that our choice of features was not so bad, but we plan to confirm this in the future with a more rigorous statistical analysis of all used models. Hopefully, such an analysis will also provide some insight into the inner working of the models, i. e. offer some explanations how they reach their decisions. This in turn may allow us to come up with better human heuristics applicable for an arbitrary number of variables.

Recall from the discussion in the Introduction that a key aspect in determining a quasi-stable position is to preserve as much sparsity as possible during the transformations, as otherwise all subsequent computations are getting rather expensive. Currently, this additional goal is neglected in our scoring which is solely based on the size of the Pommaret span. As we could see in Figure 6, sometimes two different moves provide Pommaret spans of almost the same size. In such a situation, the move producing the slightly smaller span might preserve more sparsity and thus might be preferable from the point of view of the full process of determining a quasi-stable position. We plan to include sparsity considerations into the scoring and to perform a multi-objective optimisation in the training phase. In fact, our features have already been selected in such a way that they should provide the necessary information for estimating also the sparsity of the transformed ideal.

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