Multivariate polynomial interpolation with disturbed data

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Abstract

Given a finite set of points $\mathbb{X} \subset \mathbb{R}^n$, one may ask for polynomials p belonging to a subspace V, which attain given values at the points of $\mathbb{X}$. We focus on subspaces V of $\mathbb{R}[x_1, \ldots, x_n]$, generated by low order monomials. Such V were computed by the BM-algorithm, which is essentially based on an LU-decomposition. In this paper we present a new algorithm based on the numerical more stable QR-decomposition. If $\mathbb{X}$ contains only points disturbed by measurement or rounding errors, the homogeneous interpolation problem is replaced by the problem of finding (normalized) polynomials minimizing $\sum_{u \in \mathbb{X}} p(u)^2$. Such polynomials can be found as byproduct in the QR-decomposition of the new algorithm.

1 Introduction

Given a set of points $\mathbb{X} := \{u_1, \ldots, u_m\} \subset \mathbb{R}^n$, and a set of data $\{\alpha_1, \ldots, \alpha_m\} \subset \mathbb{R}$, the multivariate polynomial interpolation problem consists in finding a polynomial $p \in \mathbb{R}[x_1, \ldots, x_n]$ satisfying

$$p(u_i) = \alpha_i, \qquad i = 1, \ldots, m \ .$$

For a survey on multivariate polynomial interpolation see [7]. One major difficulty is to find for a given finite point set $\mathbb{X}$ an m-dimensional subspace $V \subset \mathbb{R}[x_1, \ldots, x_n]$ which is unisolvent, i.e., in which there is for every data set $\{\alpha_1, \ldots, \alpha_m\}$ exactly one interpolating polynomial p. We focus on arbitrarily distributed points u_i and arbitrary m. A linear algebra argument gives that V is unisolvent if and only if $V \oplus I(\mathbb{X}) = \mathbb{R}[x_1, \ldots, x_n]$, where $I(\mathbb{X})$ is the ideal of all polynomials p solving the homogeneous interpolation problem

$$p(u_i) = 0, \qquad i = 1, \ldots, m \ .$$

A polynomial set $L := \{\ell_1, \ldots, \ell_m\}$ is a basis of an unisolvent V if and only if the $\ell_i + I(\mathbb{X})$ constitute a basis of the factor ring $\mathbb{R}[x_1, \ldots, x_n]/I(\mathbb{X})$. By introducing a linear order $<_T$ among the power products (terms) $x_1^{i_1} \cdots x_n^{i_n}$, one

can have a partial order among polynomials. The BM-algorithm introduced first in [3] is based on the idea to select in every equivalence class $\ell_i + I(\mathbb{X})$ a least polynomial w.r.t. this partial order. It is used and refined in several articles in Computer Algebra like [6] and [11]. In interpolation theory, this approach has been studied by de Boor and Ron in [2]. They called their concept *least interpolation*. Later, also Sauer pursued this approach in [14] under the name *minimal interpolation with minimal monomials*.

The knowledge of $I(\mathbb{X})$, the complement of V, is also of its own interest. In the bivariate case $n = 2$ one needs sometimes to find a low order curve $p = 0$ passing through the m points u_i. For $n > 2$ the problem might be to find one or some algebraic surfaces $p_j = 0$ through the given m points. In both cases one has to determine the polynomials in the ideal $I(\mathbb{X})$ up to a certain degree. Unfortunately, in applications the problem is often that the points of $\mathbb{X}$ are only approximations to certain unknown points $\widehat{u}_i$ with $\|\widehat{u}_i - u_i\|_2 \leq \varepsilon$ for $i = 1, \ldots, m$. Hence there is possibly no low degree polynomial p vanishing in the m points $u_1, \ldots, u_m$, i.e. $p(u_i) = 0, i = 1, \ldots, m$, but a low degree $\widehat{p}$ vanishing in the unknown $\widehat{u}_1, \ldots, \widehat{u}_m$. In this case methods of Computer Algebra like [3] fail to determine $\widehat{p}$. On the other hand, in the least squares method one expects that $\widehat{p}$ or at least a good approximation to $\widehat{p}$ minimizes $\sum_{i=1}^{m} p(u_i)^2$, assumed that all polynomials p under consideration are scaled in the same way and assumed that ε is small enough. For this reason we are interested in polynomials p such that $\sum_{i=1}^{m} p(u_i)^2$ is small, called by several authors ([5], [9], [15]) "almost vanishing polynomials".

In the recent literature, the properties of the almost vanishing polynomials have been analyzed. Among the others, in [15], using the notion of H-bases, an algorithm is presented for computing a set of polynomials which generates "almost" the so called approximate ideal of accuracy ε, that is the set of all almost vanishing polynomials w.r.t. ε. In [9] an algorithm, based on the singular value decomposition, is presented for computing the "ε-approximate vanishing ideal", that is the ideal generated by a given set of almost vanishing polynomials. In [1] and [5] algorithms for computing a set of almost vanishing polynomials are introduced, following the scheme of the BM algorithm and explicitly using an estimation of the data error. An actual overview over the existing literature can be found in [12]. This thesis also contains many well described numerical programs and includes methods using singular values, while we focus on the less expensive QR-decomposition.

In the present paper, we construct at first a unisolvent $\mathbb{R}$-linear space V following the ideas of [3] assuming that the interpolation points and the computations are exact. The main tool is that we order linearly the set of terms (power products)

$$T := \{x_1^{i_1} \cdots x_n^{i_n} \mid i_1, \ldots, i_n \in \mathbb{N}_o\}$$

by a so called admissible term order $<_T$ and consider successively (for increasing terms t) the $\mathbb{R}$-linear spaces $span_{\mathbb{R}}\{\tau \in T \mid \tau \leq_T t\}$. The computation

ends when the first linear space V is found with $V \oplus I(\mathbb{X}) = \mathbb{R}[x_1, \ldots, x_n]$. Then an ideal basis for $I(\mathbb{X})$ can be computed. If the linear order is degree compatible, then we detect early low degree polynomials vanishing in the given points.

Section 3 contains two algorithms for computing such unisolvent V and a (linear) basis for it. The first one is essentially the old BM-algorithm based on successive LU-decompositions of matrices A_k, having as rows the first k evaluation vectors of a basis of V at $\mathbb{X}$. The second one uses the more stable QR-decomposition of matrices B_k, where B_k is the transposed of A_k. In both cases, the successive decompositions are realized by a recursive procedure. The QR-decomposition allows a least squares interpretation as shown in Section 4. We denote by V_t the subset of $span_{\mathbb{R}}\{\tau \in T \mid \tau \leq_T t\}$ consisting in all p which have in its term expansion $1 \in \mathbb{R}$ as cofactor of t. If M_t is the minimum of $\sum_{i=1}^m p(u_i)^2$ over all $p \in V_t$, then $\sqrt{M_t}$ is the diagonal element corresponding to t in the upper triangular matrix R of the QR-decomposition of B_m. If there is in V_t a polynomial p which has small values $|p(u_i)|$ then M_t is small. Hence the size distribution on the diagonal of R indicates where to find solutions of the homogeneous interpolation problem and basis elements for the unisolvent $\mathbb{R}$-linear space V. Section 4 ends with an upper bound for $\sum_{i=1}^m p(u_i)^2$ if p has zeros in $\widehat{u}_i$ with $\|u_i - \widehat{u}_i\|_2 \leq \varepsilon$ for $i = 1, \ldots, m$. We conclude with a series of examples.

2 The basic algorithm

In this section we begin with some elementary definitions and results from Computer Algebra. Readers who are not familiar with such techniques and results can find more details and examples in textbooks like [4].

In the following $\mathcal{P} := \mathbb{R}[x_1, \ldots, x_n]$ denotes the polynomial ring under consideration. By T we denote the set of power products (terms),

$$T := \{x_1^{i_1} \cdots x_n^{i_n} \mid i_1, \ldots, i_n \in \mathbb{N}_0\} \ .$$

A linear order in T is called admissible if it satisfies

$$\begin{array}{ll} 1 = x_1^0 \cdots x_n^0 <_T t & \text{for all } t \in T \setminus \{1\} \ , \\ t_1 <_T t_2 \Rightarrow t t_1 <_T t t_2 & \text{for all } t, t_1, t_2 \in T \ . \end{array}$$

An easy consequence is $t_1 <_T t t_1$ for arbitrary $t, t_1 \in T,\ t \neq 1$. Hence if t_1 divides properly t_2, i.e. $t_2 = t t_1$ with $t \neq 1$, then $t_1 <_T t_2$. Every admissible term order is a well-order, such that $\min T'$ exists for every non-empty subset T' of T. In the following, we fix an admissible term order $<_T$.

Definition 2.1 *For arbitrary polynomials* $p \in \mathcal{P} \setminus \{0\}$, $p = \sum_{i=1}^{m} c_i t_i$ *with* $c_i \in \mathbb{R} \setminus \{0\}$ *and* $t_1 <_T t_2 <_T \ldots <_T t_m$, *we call* $\mathtt{lt}(p) := t_m$ *leading term,* $\mathtt{lc}(p) := c_m$ *leading coefficient of* p, *and* $\mathtt{lm}(p) := c_m t_m$ *leading monomial.*

Definition 2.2 *Let* $I \subseteq \mathcal{P}$ *be an ideal. By* $\mathtt{lt}(I)$ *we denote the set of leading terms*

$$\mathtt{lt}(I) := \{\mathtt{lt}(p) \mid 0 \neq p \in I\} \ .$$

If $\mathcal{F} \subset \mathcal{P}$ *is a finite or infinite set, then* $\langle \mathcal{F} \rangle$ *denotes the least ideal containing* $\mathcal{F}$,

$$\langle \mathcal{F} \rangle = \{\sum_{i=1}^{m} g_i f_i \mid \{f_1, \ldots, f_m\} \subseteq \mathcal{F},\ g_1, \ldots, g_m \in \mathcal{P}\} \ .$$

If $\mathcal{F}$ *is finite, then it is called basis of the ideal* $\langle \mathcal{F} \rangle$. *The set* $\{g_1, \ldots, g_r\} \subset I$ *is called a Gröbner basis of an ideal* I, *if* $\langle \mathtt{lt}(I) \rangle = \langle \mathtt{lt}(g_1), \ldots, \mathtt{lt}(g_r) \rangle$.

A Gröbner basis of an ideal I is also a basis of I, [4].

Definition 2.3 *If* $I \subset \mathcal{P}$ *is an ideal, then*

$$\mathcal{N} := \{t \in T \mid t \notin \mathtt{lt}(I)\}$$

is called normal set or set of standard monomials.

In [4], the standard monomials $t \in \mathcal{N}$ are also called *basis monomials*, because the set of cosets $\{t + I \mid t \in \mathcal{N}\}$ is a basis of the factor ring $\mathcal{P}/I$. In multivariate interpolation, the name *lower set* is used for $\mathcal{N}$. In connection with border bases, e.g. in [10], the set of terms $\mathcal{N}$ is also called *order ideal.*

Definition 2.4 *For* $\mathbb{X} := \{u_1, \ldots, u_m\} \subset \mathbb{R}^n$ *the vanishing ideal* $I(\mathbb{X})$ *is defined by*

$$I(\mathbb{X}) := \{p \in \mathcal{P} \mid p(u_i) = 0,\ i = 1, \ldots, m\} \ .$$

The following Proposition holds ([4], Th. 2.10).

Proposition 2.5 $I(\mathbb{X})$ *is an ideal. Its normal set* $\mathcal{N}$ *satisfies* $|\mathcal{N}| = |\mathbb{X}|$, *where* $|U|$ *denotes the number of elements of the set* U.

It is easily shown that a set $\mathcal{N} \subseteq T$ is the normal set of an ideal if and only if

$$t \in T, t_i \in \mathcal{N}, t | t_i \ \Rightarrow\ t \in \mathcal{N}, \tag{1}$$

where $t|t_i$ means that t divides t_i. One says that *the normal set is closed under division.* An old result of Macaulay gives that for every finite subset $\mathcal{N} \subset T$, which is closed under division, there is a point set $\mathbb{X}$ such that $\mathcal{N}$ is the normal set of $I(\mathbb{X})$, see [13].

Example 2.1 Let $\mathbb{X} := \{(0,0),(1,1),(1,-1)\}$. If $<_T$ is the `Lex`-order

$$x^i y^j <_T x^k y^\ell \text{ iff } i < k \text{ or } i = k \text{ and } j < \ell \ ,$$

then $I(\mathbb{X}) \subset \mathbb{R}[x,y]$ has as Gröbner basis $\mathcal{G} = \{y^3 - y, x - y^2\}$ and hence $\langle \mathtt{lt}(I(\mathbb{X}))\rangle = \langle y^3, x\rangle$ and $\mathcal{N} = \{1, y, y^2\}$. If $<_T$ is the `DegLex`- order,

$$x^i y^j <_T x^k y^\ell \text{ iff } i + j < k + \ell \text{ or } i + j = k + \ell \text{ and } i < k \ ,$$

then $I(\mathbb{X})$ has as Gröbner basis $\{y^2 - x, xy - y, x^2 - x\}$, hence $\mathcal{N} = \{1, y, x\}$.

Proposition 2.6 *Let $\mathcal{N}$ be the normal set of an ideal $I \subset \mathcal{P}$. Then $t^* \in \mathtt{lt}(I)$ if and only if*

$$\exists\ p \in span_{\mathbb{R}}\{t \in \mathcal{N} \mid t <_T t^*\} :\ t^* - p \in I.$$

Proof. Let $t^* \in \mathtt{lt}(I)$. Then there is a $p = \sum_i c_i t_i$ with $t_i \in \mathcal{N}$ and $c_i \in \mathbb{R}\backslash\{0\}$ such that $t^* - p \in I$, since the cosets $t + I$, $t \in \mathcal{N}$, constitute a basis of $\mathcal{P}/I$. By construction $t_i \notin \mathtt{lt}(I)$ but $\mathtt{lt}(t^* - p) \in \mathtt{lt}(I)$. Hence $t^* = \mathtt{lt}(t^* - p)$ which implies $t^* >_T t_i$. Conversely, if $t^* - p \in I$ where $p \in span_{\mathbb{R}}\{t \in \mathcal{N} \mid t <_T t^*\}$, then $\mathtt{lt}(t^* - p) = t^*$ which is in $\mathtt{lt}(I)$ because $t^* - p \in I$. □

The polynomial p in Proposition 2.6 is uniquely determined by $t^* \in \mathtt{lt}(I)$ and $\mathcal{N}$. It is called *normal form of t^**. For vanishing ideals the criterion in Proposition 2.6 can be reformulated using vectors.

Proposition 2.7 *Let $\mathbb{X} := \{u_1, \ldots, u_m\}$ and let $\mathcal{N}$ be the normal set of $I(\mathbb{X})$. Defining $t(\mathbb{X}) := (t(u_1), \ldots, t(u_m))$ for $t \in T$, then $t^* \in \mathtt{lt}(I(\mathbb{X}))$ holds if and only if*

$$t^*(\mathbb{X}) \in span_{\mathbb{R}}\{t(\mathbb{X}) \mid t \in \mathcal{N},\ t <_T t^*\} \ . \tag{2}$$

In addition, if $\mathcal{N} := \{t_1, \ldots, t_m\}$ with $t_1 <_T t_2 <_T \ldots <_T t_m$, then

$$t_k = \min_{<_T}\{t \in T \mid \dim(span_{\mathbb{R}}\{t_1(\mathbb{X}), \ldots, t_{k-1}(\mathbb{X}), t(\mathbb{X})\}) = k\} \ . \tag{3}$$

Proof. The equivalence of $t^* \in \mathtt{lt}(I(\mathbb{X}))$ and (2) holds because of Proposition 2.6 and

$$t^* - \sum_i c_i t_i \in I \Leftrightarrow t^*(\mathbb{X}) - \sum_i c_i t_i(\mathbb{X}) = 0 \ .$$

The vectors $t_1(\mathbb{X}), \ldots, t_m(\mathbb{X})$ are linearly independent because otherwise a $t_k \in \mathcal{N}$ belongs to $\mathtt{lt}(I(\mathbb{X}))$ by (2) contradicting $\mathcal{N} \cap \mathtt{lt}(I(\mathbb{X})) = \emptyset$. This together with (2) gives (3). □

If the normal set $\mathcal{N}$ of an ideal I is known, the minimal elements of $T \setminus \mathcal{N}$ w.r.t. the relation $a|b$ (a divides b) are easily determined. Let $\mathcal{M}$ be the set of these minimal elements. By Dickson's Lemma [4], $\mathcal{M}$ is finite. By

construction $\langle \mathcal{M} \rangle = \langle \mathtt{lt}(I) \rangle$ and $\langle \mathcal{M}' \rangle \neq \langle \mathtt{lt}(I) \rangle$ for every proper subset $\mathcal{M}'$ of $\mathcal{M}$, but $\langle \mathcal{M}' \rangle = \langle \mathtt{lt}(I) \rangle$ for every $\mathcal{M}' \subset T$ containing $\mathcal{M}$. For instance

$$\widetilde{\mathcal{M}} := \{\ x_i t \mid t \in \mathcal{N},\ 1 \leq i \leq n\ \} \setminus \mathcal{N}$$

contains $\mathcal{M}$ and is hence also a basis of $\langle \mathtt{lt}(I) \rangle$.
By Proposition 2.6, there is for every $t \in T \setminus \mathcal{N}$ a p in $span\mathcal{N}$ such that $t - p \in I$. Hence $\{t - p \in I \mid t \in \mathcal{M},\ p \in span\mathcal{N}\}$ and also $\{t - p \in I \mid t \in \widetilde{\mathcal{M}},\ p \in span\mathcal{N}\}$ are Gröbner bases. The first one is a so called *reduced Gröbner basis*, the latter a *border basis*.
Criterion (2) allows to decide by methods of linear algebra that $t^* \in \mathtt{lt}(I(\mathbb{X}))$ or its negation $t^* \in \mathcal{N}$ holds true, once all elements $t \in \mathcal{N}$ with $t <_T t^*$ are known. Since we consider the terms t^* in increasing order, we do not need to test a term $t \in \mathtt{lt}(I(\mathbb{X}))$, which is a proper multiple of an element of $\mathcal{M}$, because the latter is considered earlier. Therefore we deal in the following only with the finite sets $\mathcal{N}$ and $\mathcal{M}$. Then criterion (2) reduces to the test $t^* \in \mathcal{M}$ or its negation $t^* \in \mathcal{N}$. This is the central idea for the BM-algorithm, which is in the basic version as follows.

Basic BM-algorithm
Input: $\mathbb{X} := \{u_1, \ldots, u_m\} \subset \mathbb{R}^n$.
Output: The normal set $\mathcal{N}$ and the set $\mathcal{M}$ of minimal terms in $\mathtt{lt}(I(\mathbb{X}))$ w.r.t. the relation $a|b$.

Calculation:
$\mathcal{N} := \{1\};\ \mathcal{M} := \{\ \};\ L := \{x_1, \ldots, x_n\};$
while $L \neq \{\ \}$ **do**
  $t^* := \min_{<_T} L;$
  $L := L \setminus \{t^*\};$
  if $t^*(\mathbb{X}) \notin span_{\mathbb{R}}\{t(\mathbb{X}) \mid t \in \mathcal{N}\}$ % The crucial boolean expression
    then $\mathcal{N} := \mathcal{N} \cup \{t^*\};$
      for $i = 1$ **to** n **do if** no $t \in L$ divides $x_i t^*$ **then** $L := L \cup \{x_i t^*\}$
    else $\mathcal{M} := \mathcal{M} \cup \{t^*\}$
  end if
end while ;
return $\mathcal{N},\ \mathcal{M}$.

The basic BM-algorithm gives just the term sets $\mathcal{N}$ and $\mathcal{M}$ and not yet polynomials. However, the knowledge of the normal set alone is sufficient for finding an appropriate interpolation space for interpolation in $\mathbb{X} = \{u_1, \ldots, u_m\} \subset \mathbb{R}^n$. In the univariate case the situation is simple. Here, the set $\mathcal{N}$ is always generated by the terms $1, x, \ldots, x^{m-1}$. They span a linear space in which the interpolation problem in the m points is uniquely soluble. In the multivariate case, we have the following.

Theorem 2.8 *Let $\mathcal{N}$ be the normal set for the vanishing ideal $I(\{u_1,\ldots,u_m\})$ with $u_i \neq u_j$ for $i \neq j$. Then $span_{\mathbb{R}}\mathcal{N}$ is unisolvent, i.e., for arbitrary $\alpha_1,\ldots,\alpha_m \in \mathbb{R}$ there exists exactly one $p \in span_{\mathbb{R}}\mathcal{N}$ such that $p(u_i) = \alpha_i$, $i = 1,\ldots,m$.*
Let $\mathcal{N} = \{t_1,\ldots,t_m\}$ with $t_1 <_T t_2 <_T \cdots <_T t_m$. If $span_{\mathbb{R}}\{t'_1,\ldots,t'_m\}$ with $t'_1 <_T t'_2 <_T \cdots <_T t'_m$ is also unisolvent, then $t_i \leq_T t'_i$ for $i = 1,\ldots,m$.

Proof. The m vectors $t(\mathbb{X}) \in \mathbb{R}^m$, $t \in \mathcal{N}$, are linearly independent by Proposition 2.7. Hence they are a basis of $\mathbb{R}^m$. This is equivalent to the fact that the interpolation problem $p \in span_{\mathbb{R}}\mathcal{N}$, $p(u_i) = \alpha_i$, $i = 1,\ldots,m$, has always a unique solution. The remaining follows by equation (3). □

Some authors require for an interpolating polynomial p that its degree is not greater than the degree of the polynomial f which is interpolated. If the term order $<_T$ is chosen such that lower degree terms are less w.r.t. $<_T$, then this requirement results from the following.

Corollary 2.9 *Let $\mathcal{N}$ be as in Theorem 2.8 and let $f \in \mathcal{P}$. The interpolating polynomial $p \in span_{\mathbb{R}}\mathcal{N}$ with $p(u_i) = f(u_i), i = 1,\ldots,m$, satisfies $\mathtt{lt}(p) \leq_T \mathtt{lt}(f)$.*

Proof. Assume that in the contrary $\mathtt{lt}(f) <_T \mathtt{lt}(p)$. Then $\mathtt{lt}(p-f) = \mathtt{lt}(p)$. But $p - f \in I(\{u_1,\ldots,u_m\}) =: I$ such that $\mathtt{lt}(p-f) \in \mathtt{lt}(I)$ whereas $\mathtt{lt}(p) \in \mathcal{N} = T \setminus \mathtt{lt}(I)$, a contradiction. □

3 The complete BM-algorithm

The complete BM-algorithm extends the basic one by computing a reduced Gröbner basis for $I(\mathbb{X})$, a basis for $span_{\mathbb{R}}\mathcal{N}$, and modifies the criterion $t^* \notin \mathcal{M}$. We present here two variants of the complete algorithm. One is the original one of [3] and uses implicitly an LU-decomposition. The second one is based on a QR-decomposition.

When in the basic BM-algorithm the term t^* is considered, then one has already computed

$$\{t_1,\ldots,t_{s-1}\} := \{t \in \mathcal{N} \mid t <_T t^*\} \ .$$

The decision $t^* \notin \mathcal{M}$, i.e., $t^* \in \mathcal{N}$, uses equation (2) of Proposition 2.7. If we denote by A_{s-1} the $(s-1)\times m$ -matrix with rows $t_1(\mathbb{X}),\ldots,t_{s-1}(\mathbb{X})$, then A_{s-1} has full row rank $s-1$. Hence $t^* \in \mathcal{N}$ holds iff

$$rank \begin{bmatrix} A_{s-1} \\ \cdots\cdots\cdots \\ t^*(\mathbb{X}) \end{bmatrix} = s \ .$$

In the two variants of the BM-algorithm, we use the recursion $A_s = \begin{bmatrix} A_{s-1} \\ \cdots\cdots\cdots \\ t_s(\mathbb{X}) \end{bmatrix}$ and transform A_s, or its transpose A_s^T respectively, to an upper triangular matrix using that the corresponding upper triangular matrix for A_{s-1}, or A_{s-1}^T respectively, is already computed.

In [3], polynomials $q_1, \ldots, q_m$ are constructed, which can be considered as the multivariate analogous of the Newton polynomials $n_1, \ldots, n_m \in \mathbb{R}[x]$ defined by $n_k \in span\{1, \ldots, x^{k-1}\}$, $\mathtt{lc}(n_k) = 1$, and $n_k(u_{\nu_1}) = \ldots = n_k(u_{\nu_{k-1}}) = 0$. These polynomials were computed successively in the algorithm. When one considers t^* and has already found $t_1, \ldots, t_{s-1} \in \mathcal{N}$, then $q_1, \ldots, q_{s-1}$ are already computed, satisfying $q_i \in span_{\mathbb{R}}\{t_1, \ldots, t_i\}$, $\mathtt{lc}(q_i) = 1$, and

$$q_i(u_{\nu_1}) = \ldots = q_i(u_{\nu_{i-1}}) = 0, \quad q_i(u_{\nu_i}) \neq 0 \ .$$

Then one defines q recursively starting with $q^{(0)} := t^*$ and then

$$q^{(i+1)} := q^{(i)} - \frac{q^{(i)}(u_{\nu_i})}{q_i(u_{\nu_i})} q_i \qquad \text{for } i = 0, \ldots, s-1 \ .$$

$q := q^{(s)}$ has as representation $q = t^* + \sum_{i=1}^{s-1} \ell_i t_i$ with some $\ell_i \in \mathbb{R}$ and $q(u_{\nu_i}) = 0$ for $i = 1, \ldots, s-1$. If $q(u_i) = 0$ for all $i = 1, \ldots, m$, then $t^* \in \mathtt{lt}(I(\mathbb{X}))$ and q is an element of the reduced Gröbner basis. Otherwise, there is an $u_{\nu_s} \in U \setminus \{\nu_1, \ldots, \nu_{s-1}\}$ such that $q(u_{\nu_s}) \neq 0$. In this case $t_s := t^* \in \mathcal{N}$ and $q_s := q$.

This is in matrix notation, using $q_i = t_i + \sum_{k=1}^{i-1} \ell_{ik} t_k$ with $\ell_{ik} \in \mathbb{R}$,

$$\begin{pmatrix} 1 & 0 & \ldots & 0 & 0 \\ \ell_{21} & 1 & & \vdots & \vdots \\ \vdots & & \ddots & 0 & 0 \\ \ell_{s-1,1} & \ldots & \ell_{s-1,s-2} & 1 & 0 \\ \ell_1 & \ldots & \ell_{s-2} & \ell_{s-1} & 1 \end{pmatrix} \begin{pmatrix} t_1(u_{\nu_1}) & t_1(u_{\nu_2}) & \ldots & t_1(u_{\nu_m}) \\ \vdots & \vdots & & \vdots \\ t_{s-1}(u_{\nu_1}) & t_{s-1}(u_{\nu_2}) & \ldots & t_{s-1}(u_{\nu_m}) \\ t^*(u_{\nu_1}) & t^*(u_{\nu_2}) & \ldots & t^*(u_{\nu_m}) \end{pmatrix}$$

$$= \begin{pmatrix} q_1(u_{\nu_1}) & q_1(u_{\nu_2}) & \ldots & q_1(u_{\nu_{s-1}}) & q_1(u_{\nu_s}) & \ldots & q_1(u_{\nu_m}) \\ 0 & q_2(u_{\nu_2}) & \ldots & q_2(u_{\nu_{s-1}}) & q_2(u_{\nu_s}) & \ldots & q_2(u_{\nu_m}) \\ \vdots & \ddots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \ldots & 0 & q_{s-1}(u_{\nu_{s-1}}) & q_{s-1}(u_{\nu_s}) & \ldots & q_{s-1}(u_{\nu_m}) \\ 0 & \ldots & \ldots & 0 & q(u_{\nu_s}) & \ldots & q(u_{\nu_m}) \end{pmatrix} .$$

At the end, for $t^* = t_m$ and $s = m$, this identity is $MA_mP = Q_m$, where P is the permutation matrix which permutes i-th and ν_i-th column, Q_m an upper triangular $m \times m$- matrix, and M a quadratic lower diagonal matrix with diagonal $(1, 1, \ldots, 1)$, such that $M^{-1}Q_m$ is the LU-decomposition of A_mP.

The number of floating point operations (flops), i.e. the number of floating point additions and multiplications, for computing the unknowns $\ell_1, \ldots, \ell_{s-1}$

is about $2sm - s^2$. If m is much greater than s, the linear increase in m indicates a good performance. This explains the success of the BM-algorithm in exact arithmetic for finding a low degree polynomial in $I(\mathbb{X})$. However, when the points $u_1, \ldots, u_m$ are only approximately known or when floating point arithmetic is used, then the decision that all $q(u_{\nu_i})$, $i = s, \ldots, m$, are zero is no more decidable and a more stable variant of the BM-algorithm should be preferred.

The QR-decomposition applied to matrices A_{s-1} can do the job. We prefer to apply the QR-decomposition to A_{s-1}^T, the transpose of A_{s-1}, because we have then a better interpretation of intermediate results. Assuming again, that the term t^* is under consideration in the basic BM-algorithm and we already have

$$\{t_1, \ldots, t_{s-1}\} := \{t \in \mathcal{N} \mid t <_T t^*\} ,$$

we define

$$B_{s-1} := A_{s-1}^T = \begin{pmatrix} t_1(u_1) & t_2(u_1) & \ldots & t_{s-1}(u_1) \\ t_1(u_2) & t_2(u_2) & \ldots & t_{s-1}(u_2) \\ \vdots & \vdots & & \vdots \\ t_1(u_m) & t_2(u_m) & \ldots & t_{s-1}(u_m) \end{pmatrix} .$$

Then B_{s-1} has full column rank. Considering now the previously introduced vectors $t(\mathbb{X})$ as column vectors, B_{s-1} has $t_1(\mathbb{X}), \ldots, t_{s-1}(\mathbb{X})$ as columns. And the criterion $t^* \in \mathcal{N}$ needed in the basic BM-algorithm is equivalent to $\text{rank}[B_{s-1} \vdots t^*(\mathbb{X})] = s$. If $B_{s-1} = Q_{s-1}R_{s-1}$ with a orthogonal matrix $Q_{s-1} \in \mathbb{R}^{m \times m}$ and an upper triangular matrix $R_{s-1} = (r_{ij}^{(s-1)}) \in \mathbb{R}^{m \times (s-1)}$, then

$$Q_{s-1}^T[B_{s-1} \vdots t^*(\mathbb{X})] = [R_{s-1} \vdots Q_{s-1}^T t^*(\mathbb{X})] = \begin{pmatrix} r_{11}^{(s-1)} & r_{12}^{(s-1)} & \ldots & r_{1,s-1}^{(s-1)} & b_1 \\ 0 & r_{22}^{(s-1)} & \ldots & r_{2,s-1}^{(s-1)} & b_2 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \ldots & 0 & r_{s-1,s-1}^{(s-1)} & b_{s-1} \\ 0 & \ldots & \ldots & 0 & b_s \\ \vdots & & & \vdots & \vdots \\ 0 & \ldots & \ldots & 0 & b_m \end{pmatrix}$$

with $b = Q_{s-1}^T t^*(\mathbb{X})$. The extended matrix $[B_{s-1} \vdots t^*(\mathbb{X})]$ has rank s iff the last $m - s + 1$ entries of b are not simultaneously 0. In this case, a column vector $w \in \mathbb{R}^m$ exists, which has the first $s - 1$ entries equal to 0 and its remaining entries are determined such that the vector

$$(I - \frac{2}{w^T w} w w^T) Q_{s-1}^T t^*(\mathbb{X})$$

has a positive s-th entry and the forthcoming entries at position $s + 1, \ldots, m$ are 0. In matrix-vector notation, there is a Householder matrix

$$H_w = I - \frac{2}{w^T w} w w^T \qquad (H_w \text{ is symmetric and orthogonal ! })$$

such that $H_w Q_{s-1}^T [B_{s-1} \vdots t^*(\mathbb{X})]$ is an upper triangular matrix R_s with full column rank. Since $Q_{s-1}H_w$ is orthogonal, $(Q_{s-1}H_w)R_s$ is the QR-decomposition of the extended matrix $B_s := [B_{s-1} \vdots t^*(\mathbb{X})]$ with $t_s = t^*$.
If the last $m - s + 1$ entries of $Q_{s-1}^T t^*(\mathbb{X})$ are simultaneously zero, then the last column $Q_{s-1}^T t^*(\mathbb{X})$ depends linearly on the columns of upper triangular matrix $Q_{s-1}^T B_{s-1} = R_{s-1}$. Backward substitution gives the solution $c := (c_1, \ldots, c_{s-1})^T$ of $R_{s-1}c = Q_{s-1}^T t^*(\mathbb{X})$. Then the polynomial

$$p := t^* - \sum_{i=1}^{s-1} c_i t_i$$

vanishes in the points $u_1, \ldots, u_m$, i.e., $p \in I(\mathbb{X})$ with $\mathtt{lt}(p) = t^*$.
Following [8], the determination of the vector w of the Householder matrix H_w requires about $3(m-s)$ flops and the multiplication about $2(m-s)^2$ flops. The complexity here is much higher than for the LU-decomposition. On the other hand, the QR-decomposition is more stable and the central key in the following least squares method.

4 The least squares method

In many applications, one is interested in a point set $\widehat{\mathbb{X}} := \{\widehat{u}_1, \ldots, \widehat{u}_m\} \subset \mathbb{R}^n$, but due to rounding or measurement errors only an approximate point set $\mathbb{X} := \{u_1, \ldots, u_m\}$ is known. Therefore it is impossible to find the vanishing ideal $I(\widehat{\mathbb{X}})$, but only polynomials p which are very close to polynomials $\hat{p} \in I(\widehat{\mathbb{X}})$. Intuitively, a polynomial p^* is close to an element of $I(\widehat{\mathbb{X}})$, if all values $p^*(u_i)$ are close to 0. We therefore make the following definition.

Definition 4.1 *Let $V_{t^*} := \{p \in \mathcal{P} \mid \mathtt{lm}(p) = t^*\}$. We say that a polynomial $p^* \in V_{t^*}$ is a best approximation in the set V_{t^*} if*

$$\sum_{j=1}^{m} p^*(u_j)^2 = \min \left\{ \sum_{j=1}^{m} p(u_j)^2 \;\middle|\; p \in V_{t^*} \right\} .$$

(Note that all polynomials in V_{t^*} have leading coefficient 1.)
If one adds a polynomial q with $q(u_j) = 0$ for $j = 1, \ldots, m$ and $\mathtt{lt}(q) <_T t^*$ to a $p \in V_{t^*}$, then the square sum is unchanged, $\sum_{j=1}^m p(u_j)^2 = \sum_{j=1}^m (\, p(u_j) + q(u_j)\,)^2$. Also $p + q \in V_{t^*}$. Therefore if $\{t_1, \ldots, t_{s-1}\} := \{t \in \mathcal{N} \mid t <_T t^*\}$, we may omit all terms $t <_T t^*$ with $t \notin \{t_1, \ldots, t_{s-1}\}$ and obtain a unique $p^* \in span\{t_1, \ldots, t_{s-1}, t^*\}$ with

$$\sum_{j=1}^{m} p^*(u_j)^2 = \min \left\{ \sum_{j=1}^{m} p(u_j)^2 \;\middle|\; p \in V_{t^*} \right\} . \tag{4}$$

The finding of the optimal $p^* \in span\{t_1, \ldots, t_{s-1}, t^*\} \cap V_{t^*}$ is the least squares problem

$$\min_{c \in \mathbb{R}^{s-1}} \|B_{s-1}c - t^*(\mathbb{X})\|_2^2 = \|B_{s-1}c^* - t^*(\mathbb{X})\|_2^2, \tag{5}$$

with column vectors $c = (c_1, \ldots, c_{s-1})^T$, $c^* = (c_1^*, \ldots, c_{s-1}^*)^T \in \mathbb{R}^{s-1}$. The vector c^* is uniquely determined in (5) because B_{s-1} has full column rank, and so $p^* = t^* - \sum_{i=1}^{s-1} c_i^* t_i$. In the case $t^* \in \mathtt{lt}(I(\mathbb{X}))$ there is a $p^* = \sum c_i^* t_i$ such that $t^* - p^* \in I(\mathbb{X})$, see Proposition 2.6. The vector $c^* = (c_1^*, \ldots, c_{s-1}^*)^T$, inserted in (5), shows that the minimum is 0. These results can be summarized in the following theorem.

Theorem 4.2 *The vector c^* is the solution of the least squares problem (5) if and only if the polynomial $t^* - \sum_{i=1}^{s-1} c_i^* t_i$ is a best approximation in the set V_{t^*}. The minimum is 0 if and only if $t^* - \sum_{i=1}^{s-1} c_i^* t_i \in I(\mathbb{X})$.*

The polynomial of best approximation in the set V_{t_s} is strongly connected with the residual of the least squares problem and the QR-decomposition.

Theorem 4.3 *Let $\rho_1 := t_1(\mathbb{X})$ and, for $k = 2, \ldots, s$, let $t_k \notin \mathtt{lt}(I(\mathbb{X}))$, ρ_k be the residual of the least squares problem $\min_c \|B_{k-1}c - t_k(\mathbb{X})\|_2^2$ and p_k^* denote a polynomial of best approximation in the set V_{t_k}. Let $Q_s R_s$ be a QR-decomposition of B_s, i.e., Q_s an orthogonal $m \times m$-matrix and R_s an upper triangular matrix with positive diagonal entries. Then, for $k = 1, \ldots, s$, we have $\rho_k = (p_k^*(u_1), \ldots, p_k^*(u_m))^T$ and*

i) the k-th column of Q_s is $\frac{1}{\|\rho_k\|_2}\rho_k$,

ii) the k-th diagonal element of R_s equals $\|\rho_k\|_2$, and

iii) $\|\rho_k\|_2^2 = \sum_{j=1}^m p_k^*(u_j)^2 = \min\left\{\sum_{j=1}^m p(u_j)^2 \mid p \in V_{t_k}\right\}$.

Proof. Applying Theorem 4.2 to $t^* = t_k$ gives $p_k^* = t_k - \sum_{i=1}^{k-1} c_i^{(k)} t_i$ where the vector $c^{(k)} := (c_1^{(k)}, \ldots, c_{k-1}^{(k)})^T$ satisfies $\min_c \|B_{k-1}c - t_k(\mathbb{X})\|^2 = \|B_{k-1}c^{(k)} - t_k(\mathbb{X})\|^2$. Obviously, the j-th entry of the residual $\rho_k = t_k(\mathbb{X}) - B_{k-1}c^{(k)}$ is $t_k(u_j) - \sum_{i=1}^{k-1} c_i^{(k)} t_i(u_j) = p_k^*(u_j)$, $k = 2, \ldots, s$. For $k = 1$ we have $t_1 = 1$, $p_1^* = 1$, and $\rho_1 = (1, \ldots, 1)^T$.
The residual ρ_k is perpendicular to $W_{k-1} := span_{\mathbb{R}}\{t_1(\mathbb{X}), \ldots, t_{k-1}(\mathbb{X})\}$ and $t_k(\mathbb{X}) - \rho_k \in W_{k-1}$. By an inductive argument, $\rho_i^T \rho_k = 0$ for $1 \le i < k \le s$ and $W_k = span_{\mathbb{R}}\{\rho_1, \ldots, \rho_k\}$ for $k = 1, \ldots, s$. In addition, $\rho_k \neq 0$ since $t_k \notin \mathtt{lt}(I(\mathbb{X}))$ for $k = 1, \ldots, s$. Therefore the matrix Q_s with columns $\frac{1}{\|\rho_k\|_2}\rho_k$, $k = 1, \ldots, s$, is well defined and orthogonal. Since $t_k(\mathbb{X}) - \rho_k \in W_{k-1} = span_{\mathbb{R}}\{\rho_1, \ldots, \rho_{k-1}\}$, there is an upper triangular matrix R_s with diagonal entries $\|\rho_1\|_2, \ldots, \|\rho_s\|_2$ such that $Q_s R_s$ is the QR-decomposition of B_s. Statement iii) follows by $\rho_k = (p_k^*(u_1), \ldots, p_k^*(u_m))^T$ and the definition of p_k^*. □

The BM-algorithm in exact arithmetic can be thus considered as a succession of least squares problems or as an iterative computation of QR-decompositions

of matrices B_s, where the choice of the next t^* is as in the basic BM-algorithm. In the following we also assume that all points of $\mathbb{X}$ are scaled such that they are located in the unit hypercube $C := \{(x_1, \ldots, x_n) \in \mathbb{R}^n \mid -1 \leq x_i \leq 1\}$. This enables us to get informations on the size of the residuals ρ_k.

Theorem 4.4 *Let $t_j \in T$ divide $t_k \in T$. If all points $\{u_1, \ldots, u_m\}$ are inside C, then $\|\rho_k\|_2 \leq \|\rho_j\|_2$.*

Proof Let $p_j^* = t_j - \sum_{i=1}^{j-1} c_i^{(j)} t_i$ denote a polynomial of best approximation in V_{t_j} and let $t_k = \tau t_j$ for a $\tau \in T$. Then

$$\|\rho_k\|_2^2 = \min\left\{\sum_{i=1}^{m} p_k(u_i)^2 \mid p_k \in V_{t_k}\right\} \leq \sum_{i=1}^{m} (\tau(u_i)t_j(u_i) - \sum_{\ell=1}^{j-1} c_\ell^{(j)} \tau(u_i) t_\ell(u_i))^2$$

since $\sum_{\ell=1}^{j-1} c_\ell^{(j)} \tau t_\ell \in span\{t_1, \ldots, t_{k-1}\}$ and hence $\tau t_j - \sum_{\ell=1}^{j-1} c_\ell^{(j)} \tau t_\ell \in V_{t_k}$. The condition $u_i \in C$ implies $|\tau(u_i)| \leq 1$ for $i = 1, \ldots, m$. This gives

$$\begin{aligned} \|\rho_k\|_2^2 &\leq \textstyle\sum_{i=1}^{m} (\ \tau(u_i)t_j(u_i) - \sum_{\ell=1}^{j-1} c_\ell^{(j)} \tau(u_i) t_\ell(u_i)\ )^2 \\ &= \textstyle\sum_{i=1}^{m} (\ \tau(u_i)|^2 |t_j(u_i) - \sum_{\ell=1}^{j-1} c_\ell^{(j)} t_\ell(u_i)\ )^2 \\ &\leq \textstyle\sum_{i=1}^{m} (\ t_j(u_i) - \sum_{\ell=1}^{j-1} c_\ell^{(j)} t_\ell(u_i)\ )^2 = \|\rho_j\|_2^2\ . \end{aligned}$$

This was to be proved. □

If floating point arithmetic is used, then it is unrealistic to assume that a residual ρ_k is 0. But even if this happens and if $\mathbb{X}$ is only an approximation to $\widehat{\mathbb{X}}$, the polynomial of best approximation in V_{t_k} being then 0 in all points of $\mathbb{X}$ is possibly not the best approximating polynomial to $I(\widehat{\mathbb{X}})$ among all polynomials with leading monomial t_k. However, it is to be expected, that the greater

$$\|\rho_k\|_2^2 = \min\left\{\sum_{j=1}^{m} p(u_j)^2 \mid p \in V_{t_k}\right\}\ ,$$

the more unlikely is $t_k \in \mathtt{lt}(I(\widehat{\mathbb{X}}))$. Residuals are small, if in case $\|u_i - \widehat{u}_i\|_2 \leq \varepsilon$ there is a polynomial p zero in $\widehat{\mathbb{X}}$ as the following result shows.

Proposition 4.5 *Let $p \in \mathcal{P}$ vanish in the points of $\widehat{\mathbb{X}} = \{\widehat{u}_1, \ldots, \widehat{u}_m\} \subset \mathbb{R}^n$, and let $\mathbb{X} := \{u_1, \ldots, u_m\} \subset \mathbb{R}^n$ be close to $\widehat{\mathbb{X}}$, $\|\widehat{u}_i - u_i\|_2 \leq \varepsilon,\ i = 1, \ldots, m$. Then*

$$\sum_{i=1}^{m} p(u_i)^2 \leq \varepsilon^2 (M_1^2 + \ldots + M_m^2),$$

where

$$M_i := \max\{\|\nabla p(u)\|_2 \mid \|u - u_i\|_2 \leq \varepsilon\}\ .$$

Furthermore, $M_i^2 = \|\nabla p(u_i)\|_2^2 + O(\varepsilon)$.

Proof. The mean value theorem shows the existence of τ_i on the line between u_i and $\widehat{u}_i$ such that

$$p(u_i) = p(u_i) - p(\widehat{u}_i) = \nabla p(\tau_i)(u_i - \widehat{u}_i), \qquad i = 1, \ldots, m \ .$$

Cauchy-Schwarz gives then

$$p(u_i)^2 = (\ \nabla p(\tau_i)(u_i - \widehat{u}_i)\ )^2 \leq \|\nabla p(\tau_i)\|^2 \|u_i - \widehat{u}_i\|_2^2 \leq M_i^2 \varepsilon^2 \ .$$

The first assertion follows by summation over all i.

Furthermore, let η_i be a point such that $M_i = \|\nabla p(\eta_i)\|_2$ and $\|\eta_i - u_i\|_2 \leq \varepsilon$. Since there is a constant C_{ik} such that

$$\left| \left(\frac{\partial p}{\partial x_k}(\eta_i) \right)^2 - \left(\frac{\partial p}{\partial x_k}(u_i) \right)^2 \right| \leq C_{ik} \cdot \varepsilon$$

we have

$$M_i^2 = \|\nabla p(\eta_i)\|_2^2 = \sum_{k=1}^{n} \left(\frac{\partial p}{\partial x_k}(\eta_i) \right)^2 \leq \sum_{k=1}^{n} \left(\frac{\partial p}{\partial x_k}(u_i) \right)^2 + \varepsilon \sum_{k=1}^{n} C_{ik}$$

Hence M_i^2 equals $\|\nabla p(u_i)\|_2^2$ up to a summand of size $O(\varepsilon)$. □

Remark. Denoting by $p(\mathbb{X})$ the vector with entry $p(u_i)$ at position i, Proposition 4.5 gives that p has no zero set $\widehat{\mathbb{X}}$ close to $\mathbb{X}$ if $\|p(\mathbb{X})\|_2^2 > \varepsilon^2 \sum_{i=1}^{m} M_i^2$. If D denotes the $m \times n$ matrix with entry $\frac{\partial p}{\partial x_k}(u_i)$ at position (i,k), then $\sum_{i=1}^{m} M_i^2$ can be estimated, up to an $O(\varepsilon)$ summand, by the square of the Schur (Frobenius) norm of D. In fact $\|D\|_F^2 = \sum_{i=1}^{m} \|\nabla p(u_i)\|_2^2$ and so

$$\sum_{i=1}^{m} M_i^2 \approx \|D\|_F^2 \ . \tag{6}$$

In the examples of Section 5, we will use $\|D\|_F^2$ instead of $\sum_{i=1}^{m} M_i^2$. We expect that $\|p(\mathbb{X})\|_2^2 > \varepsilon^2 \|D\|_F^2$ allows as well to predict that p has no zero set $\widehat{\mathbb{X}}$ close to $\mathbb{X}$.

In [5] [Th. 3.5] a result analogous to Prop. 4.5 is shown, using a component-wise analysis: if there exists a set $\widehat{\mathbb{X}} = \{\widehat{u}_1, \ldots, \widehat{u}_m\}$ such that $p(\widehat{\mathbb{X}}) = 0$ and $\|\widehat{u}_i - u_i\|_\infty < \varepsilon_M$ for each $i = 1, \ldots, m$ then $|p(\mathbb{X})| < v_\varepsilon$, where the upper bounds hold component-wise. The vector v_ε can be estimated apart of an $O(\varepsilon_M^2)$ summand as follows

$$|v_\varepsilon| \approx \varepsilon_M \left| I - B(B^T B)^{-1} B^T \right| \sum_{k=1}^{n} \left| \frac{\partial p}{\partial x_k}(\mathbb{X}) \right| = \varepsilon_M \left| I - B(B^T B)^{-1} B^T \right| |D| e \tag{7}$$

with B the evaluation matrix of the terms $\{t \in \mathcal{N} \mid t <_\tau LT(p)\}$ at $\mathbb{X}$, I the identity matrix, and $e = [1, \ldots, 1]^T$. Computing the 2-norm of the estimation

of $|v_\varepsilon|$ we obtain an upper bound similar to formula (6) up to a factor $\sqrt{n}$ due to the transformation from two different norms. We have

$$\begin{aligned}&\varepsilon_M \left\| |I - B(B^TB)^{-1}B^T||D|e \right\|_2 \leq \sqrt{n}\varepsilon_M \left\| |I - B(B^TB)^{-1}B^T| \right\|_2 \left\| |D| \right\|_2 \\ &\leq \sqrt{n}\varepsilon_M \left\| I - B(B^TB)^{-1}B^T \right\|_F \|D\|_F = n\varepsilon_M \left\| I - B(B^TB)^{-1}B^T \right\|_2 \|D\|_F\end{aligned}$$

Note that, using the singular value decomposition of B, it is possible to show that $\|I - B(B^TB)^{-1}B^T\|_2 = 1$. Furthermore, if ε is the data error estimation in formula (6), we have that ε is almost equal to $\sqrt{n}\varepsilon_M$ and so

$$\varepsilon_M \left\| |I - B(B^TB)^{-1}B^T||D|e \right\|_2 \leq n\varepsilon_M \|D\|_F \approx \sqrt{n}\varepsilon \|D\|_F \quad .$$

We can conclude that upper bound (6) is more precise than the upper bound obtained computing the norm of relation (7) and we suggest to use upper bound (6) when an estimation of the norm of the data error is known while upper bound (7) when an estimation component-wise of the error is known.

This estimation of Proposition 4.5 and Theorem 4.4 suggest to compute the residuals ρ_k for increasing t_k (w.r.t. $<_T$) in the following way. If the first residual ρ_k occurs with a very small euclidean norm compared to the norm of the residuals computed before, then this t_k is the first candidate for $\mathtt{lt}(I(\mathbb{X}))$. Since $\|\rho_k\|_2 = \|p_k^*(\mathbb{X})\|_2$ by Theorem 4.3 iii), Proposition 4.5 shows when the euclidean norm of ρ_k is not small enough. If there are several residuals with small norm, but m residuals with a significantly greater norm, then the corresponding m terms, say $\{t_{r_1}, \ldots, t_{r_m}\}$, are candidates for the normal set. If all points are inside the unit hypercube C, then Theorem 4.4 gives that the set $\widetilde{\mathcal{N}} := \{t_{r_1}, \ldots, t_{r_m}\}$ is closed under division. If $\mathbb{X}$ is close to $\widehat{\mathbb{X}}$ and if only small rounding errors occur, then it is to be expected, that $\widetilde{\mathcal{N}}$ is the normal set of the ideals $I(\mathbb{X})$ and $I(\widehat{\mathbb{X}})$ and the polynomials of best approximation in V_t for every $t \in T \setminus \widetilde{\mathcal{N}}$ can be accepted as good approximations to the polynomials of $I(\widehat{\mathbb{X}})$.

5 Examples

In this section we present two examples in which, starting from a set $\mathbb{X}$ of perturbed points, the polynomials of best approximation are computed. In order to detect if a computed polynomial p^* admits a zero set close to $\mathbb{X}$, we apply Proposition 4.5, using the "simplified" upper bound, where $\sum_{j=1}^m M_j^2$ is replaced by the (squared) Frobenius norm of $D = \left(\frac{\partial p}{\partial x_k}(u_i)\right)$. All the computations are performed using MatLab and all the coefficients are rounded.

Example 5.1 Let $\widehat{\mathbb{X}} = \{\widehat{u}_1, \ldots, \widehat{u}_m\} \subset \mathbb{R}^2$ be a set of exact but "unknown" points on the unit circle $x^2 + y^2 - 1 = 0$. We consider two different cases, varying the component-wise perturbation of the points and varying m.

First case. Let $\widehat{\mathbb{X}}$ be the "exact" set of $m = 8$ points, where $\widehat{\alpha} = \sqrt{2}/2$,

$$\widehat{\mathbb{X}} = \{(1,0),(0,1),(-1,0),(0,-1),(\widehat{\alpha},\widehat{\alpha}),(-\widehat{\alpha},\widehat{\alpha}),(-\widehat{\alpha},-\widehat{\alpha}),(-\widehat{\alpha},\widehat{\alpha})\} \ .$$

The vanishing ideal $I(\mathbb{X})$ is generated by the `DegLex`-Gröbner basis

$$g_1 = x^2 + y^2 - 1 \quad g_2 = xy^3 - 0.5xy \quad g_3 = y^5 - 1.5y^3 + 0.5y \ .$$

Let $\mathbb{X} = \{u_j \mid j = 1,\ldots,8\}$ be the set of points obtained perturbing all the coordinates of the points in $\widehat{\mathbb{X}}$ by component-wise errors less than 10^{-2}:

$$\mathbb{X} = \{(0.9986, 0.0032),\ (0.7146, 0.7117),\ (0.0053, 1.0044),\ (-0.698, 0.7052),\ (-0.9972, 0.0028),\ (-0.7155, -0.7130),\ (0.0063, -0.9963),\ (0.7149, -0.7155)\} \ .$$

In this case $\|u_j - \widehat{u}_j\|_2 < 1.5 \cdot 10^{-2} =: \varepsilon$. In the `DegLex`-order, the first eight terms are $1 < y < x < y^2 < xy < x^2 < y^3 < xy^2$. Let the k-th term be denoted by t_k and let $R(k,k)$ denote the k-th diagonal element in the QR-decomposition of $B_8 = (t_1(\mathbb{X}),\ldots,t_8(\mathbb{X}))$. Then $\min_c\{\|B_{k-1}c - t_k(\mathbb{X})\|_2\} = R(k,k)$ where $B_{k-1} = (t_1(\mathbb{X}),\ldots,t_{k-1}(\mathbb{X}))$ by Theorem 4.3. The QR-decomposition gives the following (rounded to four decimal places).

t_k			$R(k,k)$		
y^3			0.3438		
y^2	xy^2		1.0008	0.4336	
y	xy		2.0064	1.0112	
1	x	x^2	2.8284	2.0031	0.0312

Table 1: Terms and diagonal entries in a two-dimensional scheme each

The gap between the element $R(6,6) = 0.0312$, associated to $t_6 = x^2$, and the other seven diagonal elements suggests that p_6^*, the polynomial of best approximation in V_{x^2}, is close to a polynomial of $I(\widehat{\mathbb{X}}) \cap V_{x^2}$. The coefficients of p_6^* are the solution of the least squares problem $B_5 c = t_6(\mathbb{X})$,

$$p_6^* = x^2 - 0.0148xy + 0.9946y^2 - 0.0070x + 0.0035y - 1.0020 \ .$$

p_6^* is similar to g_1 and satisfies the "simplified" upper bound of Proposition 4.5:

$$\begin{aligned} &\textstyle\sum_{u\in\mathbb{X}} p_6^*(u)^2 = R(6,6)^2 && \approx 9.7495 \cdot 10^{-4} \\ <\quad &\varepsilon^2 \textstyle\sum_{u\in\mathbb{X}} \|\nabla p_6^*(u)\|_2^2 && \approx 31.98 \cdot \varepsilon^2 = 7.196 \cdot 10^{-3}. \end{aligned}$$

Now we consider the first 8 terms in the `DegLex`-order, omitting multiples of x^2, that is $1 < y < x < y^2 < xy < y^3 < xy^2 < y^4$ (and denote them again by $t_1 < \ldots < t_8$). The diagonal elements $R(k,k)$ of R in the QR-decomposition of $B_8 = (t_1(\mathbb{X}),\ldots,t_8(\mathbb{X}))$ are now

t_k		$R(k,k)$	
y^4		0.3538	
y^3		0.4961	
y^2	xy^2	1.0008	0.5067
y	xy	2.0064	1.0112
1	x	2.8284	2.0031

Table 2: Terms and diagonal entries in a two-dimensional scheme each

Since there are no large gaps between these values, we expect that $\{1, y, x, y^2, xy, y^3, xy^2, y^4\}$ is the normal set $\mathcal{N}$ for $I(\widehat{\mathbb{X}})$. Best approximating polynomials in V_{xy^3} and V_{y^5} resp. are

$$\begin{aligned} p_9^* &= xy^3 + 0.0034y^4 + 0.0028xy^2 - 0.0013y^3 - 0.5061xy - 0.0033y^2 \\ &\quad +0.0015x - 0.0016y + 0.0001 \ , \\ p_{10}^* &= y^5 - 0.0053y^4 + 0.0017xy^2 - 1.5067y^3 + 0.0023xy + 0.0028y^2 \\ &\quad -0.0001x + 0.5063y - 0.0015 \quad . \end{aligned}$$

The similarity to g_2 and g_3 is apparent.

Finally, the following table shows that the "simplified" upper bound of Proposition 4.5 is not satisfied by any polynomial of best approximation p_k^* corresponding to $t_k \in \mathcal{N}$, since $\|p_k^*(\mathbb{X})\|_2^2 > \varepsilon^2 \|\nabla p_k^*(\mathbb{X})\|_2^2$, $k = 1, \ldots, 8$.

k	$\|p_k^*(\mathbb{X})\|_2^2$	$>$	$\varepsilon^2 \|\nabla p_k^*(\mathbb{X})\|_2^2$
1	8	$>$	0
2	4.0256	$>$	$1.8000 \cdot 10^{-3}$
3	4.0124	$>$	$1.8000 \cdot 10^{-3}$
4	1.0017	$>$	$3.6234 \cdot 10^{-3}$
5	1.0226	$>$	$1.8091 \cdot 10^{-3}$
6	0.2461	$>$	$3.0624 \cdot 10^{-3}$
7	0.2568	$>$	$1.2571 \cdot 10^{-3}$
8	0.1252	$>$	$1.8165 \cdot 10^{-3}$

We conclude that there is no set $\widehat{\mathbb{X}}$, close to $\mathbb{X}$ by less than ε, such that $p_k^*(\widehat{\mathbb{X}}) = 0$. Hence the terms $\{1, y, x, y^2, xy, y^3, xy^2, y^4\}$ form a normal set.

Second case. Let $\widehat{\mathbb{X}}$ be a set of $m = 40$ points on the circle $x^2+y^2-1 = 0$ and let $\mathbb{X}$ be a set of points obtained by perturbing the coordinates of each point $\widehat{u}_i \in \widehat{\mathbb{X}}$ by less than 10^{-2}. Then $\|\widehat{u}_i - u_i\|_2 < \sqrt{2}\|\widehat{u}_i - u_i\|_\infty < \sqrt{2} \cdot 10^{-2} =: \varepsilon$ for $i = 1, \ldots, 40$. Following the same strategy and using the same notation as in the first case, we consider the first six terms $1 < y < x < y^2 < xy < x^2$ in the `DegLex`-order. Let the k-th term be denoted by t_k and let $R(k,k)$ denote the k-th diagonal element in the QR-decomposition of $B_6 = (t_1(\mathbb{X}), \ldots, t_6(\mathbb{X}))$. Then $\min_c\{\|B_{k-1}c - t_k(\mathbb{X})\|_2\} = R(k,k)$ where $B_{k-1} = (t_1(\mathbb{X}), \ldots, t_{k-1}(\mathbb{X}))$

by Theorem 4.3. The QR-decomposition gives the following (rounded to four decimal places).

t_k			$R(k,k)$		
y^2			1.8669		
y	xy		4.8953	2.2102	
1	x	x^2	6.3241	3.7284	0.0620

Table 3: Terms and diagonal entries in a two-dimensional scheme each

Since the element $R(6,6)$ is considerably smaller than the other ones, we expect $\{1, y, x, y^2, xy\} \subset \mathcal{N}$. The term x^2 is the leading term of the best approximating polynomial $p_6^* \in V_{x^2}$:

$$p_6^* = x^2 - 0.0029xy + 1.0032y^2 - 0.0005x + 0.0007y - 1.0037$$

Polynomial p_6^* satisfies the "simplified" upper bound of Proposition 4.5, since $\sum_{u\in\mathbb{X}} p_6^*(u)^2 \approx 3.844 \cdot 10^{-3}$ and

$$\begin{aligned}\varepsilon^2 \sum_{u\in\mathbb{X}} \|\nabla p_6^*(u)\|_2^2 &= \varepsilon^2 \sum_{(x,y)\in\mathbb{X}} (2x - 0.0029y - 0.0005)^2 \\ &+(-0.0029x + 2.0064y + 0.0007)^2 = 160.96 \cdot \varepsilon^2 \approx 3.22 \cdot 10^{-2}\end{aligned}$$

and so its is possible that a zero set of p_6^* close to $\mathbb{X}$ by less than ε exists. Finally we consider the first 40 terms w.r.t. the `DegLex` term ordering omitting the multiples of x^2,

$$\{t_k \mid k = 1, \ldots, 40\} = \{1, y\} \cup \{xy^j, y^{j+2} \mid j = 0, \ldots, 18\} \ .$$

Computation gives that there is no a large gap between the diagonal elements $R(k,k)$ of R in the QR-decomposition of $B_{40} = (t_1(\mathbb{X}), \ldots, t_{40}(\mathbb{X}))$. For detecting the elements of the normal set we apply Proposition 4.5 to each best approximating polynomial $p_k^* \in V_{t_k}$, $k = 1, \ldots, 40$. The generic term t_k can be added to the normal set if p_k^* does not satisfy the "simplified" upper bound of Proposition 4.5, that is if

$$\sum_{u\in\mathbb{X}} p_k^*(u)^2 > \varepsilon^2 \sum_{u\in\mathbb{X}} \|\nabla p_k^*(u)\|_2^2$$

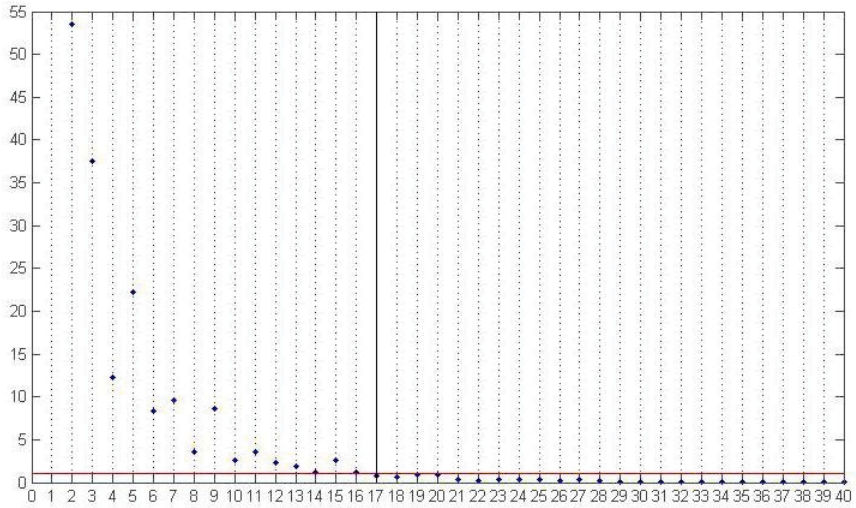
or equivalently if

$$\mu_k^2 := \frac{\sum_{u\in\mathbb{X}} p_k^*(u)^2}{\varepsilon^2 \sum_{u\in\mathbb{X}} \|\nabla p_k^*(u)\|_2^2} > 1 \ .$$

In the following figure we display the values μ_k, $k = 1, \ldots, 40$. For $k \leq 16$ the μ_k are greater than 1 (represented by the horizontal line) and so the terms

$$\{t_1, \ldots, t_{16}\} = \{1, y\} \cup \{xy^j, y^{j+2} \mid j = 0, \ldots, 6\}$$

can be added to the normal set. For the terms $t_k, k > 16$, the error ε is not small enough to predict $t_k \in \mathcal{N}$.



Example 5.2 The twisted cubic is the curve $\widehat{\mathbb{X}} := \{(t^3, t^2, t) \mid t \in \mathbb{R}\}$. Its vanishing ideal $I(\widehat{\mathbb{X}})$ is generated by the `DegLex`-Gröbner basis

$$z^2 - y, \quad yz - x, \quad y^2 - xz \ .$$

The problem is here that the twisted cubic is no zero dimensional variety. The BM-algorithm only applies to zero-dimensional varieties. But if there are enough good approximations to points of the twisted cubic, then one can get good approximations for the low degree polynomials in $I(\widehat{\mathbb{X}})$. Let $\mathbb{X} := \{u_1, \ldots, u_5\}$ be the following set

$$\begin{aligned}\mathbb{X} \ = \ & \{(-0.999912, 1.000029, -1.000039),\ (-0.124925, 0.249976, -0.499998),\\ & (0.00001, 0.000062, 0.000002),\ (0.125025, 0.250007, 0.500063),\\ & (1.000017, 0.99997, 1.000059)\}\end{aligned}$$

whose points are close to the set $\{\widehat{u}_1, \ldots, \widehat{u}_5\} \subset \widehat{\mathbb{X}}$, consisting of

$$\{(-1, 1, -1), (-0.125, 0.25, -0.5), (0, 0, 0), (0.125, 0.25, 0.5), (1, 1, 1)\}$$

In this case $\|u_j - \widehat{u}_j\|_2 \leq 1.5 \cdot 10^{-4} =: \varepsilon$, $j = 1, \ldots, 5$. In the `DegLex`-order, the first five terms are $1 < z < y < x < z^2$. Let the k-th term be denoted by t_k and let $R(k,k)$ denote the k-th diagonal element in the QR-decomposition of $B_5 = (t_1(\mathbb{X}), \ldots, t_5(\mathbb{X}))$. Then $\min_c\{\|B_{k-1}c - t_k(\mathbb{X})\|_2\} = R(k,k)$ where $B_{k-1} = (t_1(\mathbb{X}), \ldots, t_{k-1}(\mathbb{X}))$ by Theorem 4.3. The QR-decomposition gives the following (rounded to four decimal places).

t_k	1	z	y	x	z^2
$R(k,k)$	2.2361	1.5812	0.9354	0.4744	0.0001

The terms $\{1, z, y, x\}$ are inserted into $\mathcal{N}$ and the best approximating polynomial $p_5^* \in V_{z^2}$, with leading term $t_5 = z^2$, is computed solving the least

squares problem $B_4 c = t_5(\mathbb{X})$,

$$p_5^* = z^2 - 0.00002x - 1.000126y - 0.00003z + 0.00002 \ .$$

Analogously, considering the next term $t_6 = yz$ in the `DegLex`-order, the QR-decomposition of the matrix $(t_1(\mathbb{X}), \ldots, t_4(\mathbb{X}), t_6(\mathbb{X}))$ gives the following (rounded to four decimal places)

t_k	1	z	y	x	yz
$R(k,k)$	2.2361	1.5812	0.9354	0.4744	$8.2 \cdot 10^{-6}$

and so the best approximating polynomial $p_6^* \in V_{yz}$ is computed,

$$p_6^* = yz - 1.0000363x + 0.000057y - 0.000048z + 0.000016 \ .$$

The normal set can be completed adding to $\mathcal{N}$ the term $t_7 = xz$ chosen following the `DegLex`-order, since the diagonal elements of R of the QR-decomposition of the matrix $(t_1(\mathbb{X}), \ldots, t_4(\mathbb{X}), t_7(\mathbb{X}))$ are

t_k	1	z	y	x	xz
$R(k,k)$	2.2361	1.5812	0.9354	0.4744	0.1792

The "simplified" upper bound of Proposition 4.5 shows that there is no set of points close to $\mathbb{X}$ at which the best approximating polynomial $p_k^* \in V_{t_k}$, $t_k \in \mathcal{N}$, vanish. In fact we have that

$$\sum_{u \in \mathbb{X}} p_k^*(u)^2 \geq \varepsilon^2 \sum_{u \in \mathbb{X}} \|\nabla p_k^*(u)\|_2^2 \qquad \forall \ t_k \in \mathcal{N}$$

as reported in the following table

k	$\|p_k^*(\mathbb{X})\|_2^2$	$>$	$\varepsilon^2 \|\nabla p_k^*(\mathbb{X})\|_2^2$
1	5	$>$	0
2	2.5002	$>$	$1.1250 \cdot 10^{-7}$
3	0.8750	$>$	$1.1250 \cdot 10^{-7}$
4	0.2251	$>$	$1.9377 \cdot 10^{-7}$
7	0.0321	$>$	$2.3987 \cdot 10^{-7}$

Let $t_8 = y^2$ be the next term in the `DegLex`-order; solving the linear system $(t_1(\mathbb{X}), \ldots, t_4(\mathbb{X}), t_7(\mathbb{X}))c = t_8(\mathbb{X})$ the coefficient vector of polynomial p_8, with leading term t_8, is computed:

$$p_8 = y^2 - 0.99996xz + 1.05 \cdot 10^{-4}x - 2.85 \cdot 10^{-5}y + 1.63 \cdot 10^{-5}z - 3.14 \cdot 10^{-9}$$

Note that p_8 is vanishing at $\mathbb{X}$ (apart of floating point errors). Furthermore, the necessary condition given by Proposition 4.5 for the existence of a set of

points close to $\mathbb{X}$ at which p_5^* and p_6^* vanish, is satisfied. In fact, if each M_j^2 is approximated by $\|\nabla p_5^*(u_j)\|_2^2$ for p_5^* or by $\|\nabla p_6^*(u_j)\|_2^2$ for p_6^*, we have

$$\sum_{u\in\mathbb{X}} p_5^*(u)^2 \approx 10^{-8} < \varepsilon^2 \sum_{u\in\mathbb{X}} \|\nabla p_5^*(u)\|_2^2 \approx 3.34\cdot 10^{-7} \ ,$$
$$\sum_{u\in\mathbb{X}} p_6^*(u)^2 \approx 6.8\cdot 10^{-11} < \varepsilon^2 \sum_{u\in\mathbb{X}} \|\nabla p_6^*(u)\|_2^2 \approx 2.17\cdot 10^{-7} \ .$$

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