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H–Bases II: Applications to Numerical Problems

H. Michael Möller and Thomas Sauer

Abstract. We show how H–bases can be applied to polynomial interpolation and for the solution of systems of nonlinear equations. We will give an example of a system of polynomial equations where the H–basis leads to more stable computations than with the Gröbner basis.

§1. Introduction

In the preceding paper [12], we introduced the notion of H–bases for polynomial ideals, and showed how to construct H–bases in the numerically most interesting case of a zero dimensional ideal. In this paper we consider two problems from Numerical Analysis, namely polynomial interpolation and solving systems of polynomial equations, and point out how H–bases can be applied to both. More precisely, in both cases the computation of normal forms with respect to an ideal plays a crucial role, and with the basic results from [12] available, H–bases yield a perfect replacement for the Gröbner bases which are normally and frequently used to do this job [8]. Finally, we will consider an example where a properly chosen H–basis leads to a significant stabilization of the computations in comparison with the use of Gröbner bases.

§2. Interpolation

A finite set $\Theta \subset \Pi'$ of *linearly independent* functionals on Π is said to define an ideal interpolation scheme if its kernel, $\ker \Theta \subset \Pi$, is an ideal in Π. Given an ideal interpolation scheme Θ and a polynomial $f \in \Pi$, the interpolation problem consists of finding $p \in \Pi$ such that

$$\Theta(p) = \Theta(f), \qquad \text{i.e.,} \qquad \vartheta(p) = \vartheta(f), \quad \vartheta \in \Theta. \tag{1}$$

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So far, we have put no restrictions on p; hence, there are infinitely many solutions to (1). More precisely, if p is any solution of (1), hence $f-p \in \ker\Theta$, then the set of all solutions is the equivalence class

$$[p] = p + \ker\Theta = f + \ker\Theta\,[f].$$

We denote the linear space of all equivalence classes by $\Pi/\ker\Theta$, and remark that $(\dim \Pi/\ker\Theta) = \#\Theta$. Of course, in order to compute interpolation polynomials, we must find a way to choose a specific element from the equivalence class $[f]$. A "natural" choice is to take the normal form $\mathtt{NF}\ (f,\mathcal{H})$, where $\mathcal{H}$ is an H–basis for $\ker\Theta$. Since $[f]=[g]$ implies that $f-g \in \langle\mathcal{H}\rangle$, and since $\mathtt{NF}\ (\cdot,\mathcal{H})$ is a linear operator, we have that

$$[f]=[g] \qquad \Longrightarrow \qquad \mathtt{NF}\ (f,\mathcal{H}) = \mathtt{NF}\ (g,\mathcal{H}) + \underbrace{\mathtt{NF}\ (f-g,\mathcal{H})}_{=0} = \mathtt{NF}\ (g,\mathcal{H}).$$

Hence, $\mathtt{NF}\ ([f],\mathcal{H}) = \mathtt{NF}\ (f,\mathcal{H})$, that is, the normal form is the same for any element of the same equivalence class. This algebraic approach also allows for interpolation of functionals which are only given *implicitly*, that is, by an ideal $\mathcal{I}\subset\Pi$: compute an H–basis $\mathcal{H}$ for $\mathcal{I}$ and the interpolation operator is the "remainder of division" $\mathtt{NF}\ (\cdot,\mathcal{H})$. It is worthwhile to remark that one of the oldest papers on multivariate interpolation, namely [6], starts with implicitly given interpolation nodes.

Another approach is to look for a polynomial space $\mathcal{P}\subset\Pi$ which allows for unique interpolation with respect to Θ; to restrict the number of solutions to this problem, one usually demands the interpolation operator $L_{\mathcal{P}}:\Pi\to\mathcal{P}$ to be degree reducing [3], that is,

$$\deg L_{\mathcal{P}} f \le \deg f, \qquad f\in\Pi.$$

Such an interpolation space with a degree reducing interpolation operator is called a minimal degree interpolation space. The most prominent minimal degree interpolation spaces is the least interpolation space introduced by de Boor et al in [2], and is the unique degree reducing interpolation space which satisfies the additional condition

$$\mathcal{P} = \bigcap_{q\in\ker\Theta} \ker q(D), \qquad q(D) := q\left(\frac{\partial}{\partial x_1},\dots,\frac{\partial}{\partial x_n}\right).$$

On the other hand, it is obvious that the operator $\mathtt{NF}\ (\cdot,\mathcal{H})$ is *degree reducing*, linear and interpolating, hence all the spaces $\mathcal{P} = \mathtt{NF}\ (\Pi,\mathcal{H})$, for any H–basis $\mathcal{H}$, are minimal degree interpolation spaces with interpolation operator $L_{\mathcal{P}} = \mathtt{NF}\ (\cdot,\mathcal{H})$. Moreover, it is even possible to recover known minimal degree interpolation spaces by this algebraic process.

Theorem 1. [15] *The least interpolation space is given as* $\mathtt{NF}\ (\Pi,\mathcal{H})$, *where* $\mathcal{H}$ *is an orthogonal H–basis with respect to the inner-product*

$$(p,q) = (p(D)\,q)\,(0), \qquad p,q\in\Pi.$$

§3. Polynomial System Solving

Probably the best–known and most frequent use of Gröbner bases is for solving polynomial systems of equations, where they form a core part of literally all available computer algebra systems. These systems of equations arise naturally in a geometric context, such as finding solutions of geometric constraints (for example, any Euclidean distance constraint yields a quadratic equation) or "simply" computing the intersection of algebraic curves/surfaces given in implicit form. So, given any finite set $\mathcal{F} \in \Pi$ one wants to find the associated algebraic variety $X \in \overline{\mathbb{K}}$ (some algebraic closure of our underlying field $\mathbb{K}$) such that

$$\mathcal{F}(X) = 0, \tag{2}$$

that is,

$$f(x) = 0, \qquad x \in X, \, f \in \mathcal{F}.$$

Note that the emphasis here is not on finding *one* solution (which could, at least in the case that $\#\mathcal{F} = n$, be done by a Newton method), but on finding *all* solutions and obtaining *structural* information about the variety. It is easy to see that the variety is not a property of the specific set $\mathcal{F}$, but of the ideal $\langle \mathcal{F} \rangle$:

$$\mathcal{F}(X) = 0 \qquad \Longleftrightarrow \qquad \langle \mathcal{F} \rangle (X) = 0.$$

Therefore, it may be helpful to find particular bases for $\langle \mathcal{F} \rangle$ which allow for an efficient solution of (2). The "classical" implementation in most Computer Algebra systems relies on the computation of elimination ideals, which means the computation of a basis for the subideals

$$\langle \mathcal{F} \rangle_k = \langle \mathcal{F} \rangle \cap \mathbb{K}[x_1, \ldots, x_k], \qquad k = 1, \ldots, n,$$

where $\langle \mathcal{F} \rangle_n = \langle \mathcal{F} \rangle$. In fact, this corresponds to transforming the original problem $\mathcal{F}(X) = 0$ into a *triangular* system

$$\begin{array}{llllll} g_1(& x_1 & & & &) = 0, \\ g_2(& x_1, & x_2 & & &) = 0, \\ & & & \vdots & & \\ g_m(& x_1, & x_2, & \ldots, & x_n &) = 0. \end{array} \tag{3}$$

Once such a triangular system is available, the solution strategy is obvious: determine the zeros of the univariate polynomial $g_1(x_1)$ and substitute them into $g_2(\cdot, x_2)$ which is now, for for any such zero, again a univariate polynomial in x_2, and go on with this procedure. Moreover, such a triangular basis can indeed be computed: $\mathcal{G}_{lex}$, the reduced Gröbner basis for $\langle \mathcal{F} \rangle$ with respect to the lexicographical term order where $x_1 \prec x_2 \prec \cdots \prec x_n$ has the property that

$$\mathcal{G}_k = \mathcal{G} \cap \mathbb{K}[x_1, \ldots, x_k] \subset \langle \mathcal{F} \rangle_k$$

is a Gröbner basis for $\langle \mathcal{F} \rangle_k$ (cf. [4, p. 114]).

However, as nice as this idea of successive elimination of variables sounds, there are numerous drawbacks:

(i) The complexity of computing a lexicographical Gröbner basis is tremendous, and even relatively "simple" problems still exceed the limitations of existing computing facilities.

(ii) There are often several polynomials in a certain number of variables, that is, the system is not as triangular as one would want it to be.

(iii) The degree of the polynomial g_1 is usually very high. This makes it impossible to compute its zeros exactly.

(iv) The tempting idea to find g_1's zeros *approximately* and substitute these values will not lead very far since it is well–known that the zeros of a polynomial are usually quite ill–conditioned with respect to its coefficients (cf. [5,17]).

So, the summary is fairly disappointing: elimination methods do not provide a good tool to tackle polynomial systems of equations. In particular, they rely too much on *symbolic* methods (with exact computations) to become a useful tool in *numerical* applications.

A different approach has been proposed quite recently by Stetter [16] (see also [10]; in [7] this method is partly attributed to Stickelberger) which is based on transforming the nonlinear system of equations into an eigenvalue problem for which a huge library of powerful routines is available. For that purpose, let us assume that the set of solutions X is *finite* (that is, the associated ideal $\langle \mathcal{F} \rangle$ is zero dimensional) and that all the common zeros are simple. The latter restriction is made to keep the presentation simple; details on how to handle multiplicities can be found in [10]. We first note that for any $f \in \Pi$, the mapping

$$\Phi_f : \begin{cases} \Pi / \langle \mathcal{F} \rangle & \to & \Pi / \langle \mathcal{F} \rangle \\ [\, p \,] & \mapsto & [\, f \cdot p \,] \end{cases}$$

is a homomorphism on the $\#X$–dimensional linear space $\Pi / \langle \mathcal{F} \rangle$. Now, suppose for a moment that we know X. Then there are polynomials $p_x \in \Pi$, $x \in X$, defined by

$$p_x(x') = \delta_{x,x'}, \qquad x, x' \in X,$$

which form a basis for $\Pi / \langle \mathcal{F} \rangle$, i.e.,

$$\Pi / \langle \mathcal{F} \rangle = \operatorname{span} \{ [p_x] : x \in X \} .$$

Obviously, for any $x \in X$, the polynomial $g_x = (f - f(x))\, p_x$ satisfies $g_x(X) = 0$, and therefore

$$[0] = [g_x] = [\, (f - f(x))\, p_x \,] = \Phi_f\, [p_x] - f(x)\, [p_x] .$$

What we have proved with this simple argument is the following crucial theorem.

Theorem 2. *The polynomials p_x, $x \in X$, are joint eigenvectors of* all *homomorphisms Φ_f, $f \in \Pi$, with respect to the eigenvalue $f(x)$.*

This result again suggests a strategy to solve polynomial systems of equations: compute a set of representers for $\Pi / \langle \mathcal{F} \rangle$, that is, a finite set $\mathcal{P} \subset \Pi$ of linearly independent polynomials such that

$$\Pi / \langle \mathcal{F} \rangle = \operatorname{span} \{ [p] : p \in \mathcal{P} \},$$

and compute the matrix M_f which describes the action of Φ_f with respect to the basis $\mathcal{P}$. The eigenvalues of such matrices yield, when combined appropriately, the solutions X. We remark that the (transpose of the) matrix M_f is called the multiplication table for f with respect to $\mathcal{P}$, and that the original goal for Buchberger's doctoral thesis (supervised by Gröbner) was not the invention of Gröbner bases but the computation of multiplication tables. Of course, the most natural approach would be to compute the multiplication tables M_{x_j}, $j = 1, \ldots, n$, for the coordinate functions and thus compute the respective coordinates of the elements of X as the eigenvalues of the multiplication table. Note that the different components are finally "glued together" by the requirement that they must correspond to the same eigenvector.

What we now have is the possibility of reducing the search for the solutions of a polynomial system of equations to an eigenvalue problem, provided that we are able to perform two operations:

(i) Given a basis $\mathcal{F}$ for an ideal $\langle \mathcal{F} \rangle$ compute a basis $\mathcal{P}$ of representers for $\Pi / \langle \mathcal{F} \rangle$.

(ii) Having this basis available and given any $f \in \Pi$, compute the multiplication table M_f with respect to $\mathcal{P}$.

Fortunately, this is where [12] enters – the answer are *normal forms*: if $\mathcal{H}$ is an H–basis for $\langle \mathcal{F} \rangle$, then any basis for $\mathtt{NF}\,(\Pi, \mathcal{H})$ is exactly the desired $\mathcal{P}$, and the action of Φ_f can be computed by expanding $\mathtt{NF}\,(f \cdot p, \mathcal{H})$ for all $p \in \mathcal{P}$, which yields the multiplication table M_f. The remaining question is "why H–bases?", and this question is justified since the computation of normal forms and thus of multiplication tables is perfectly possible with the help of Gröbner bases as well. To give a partial answer to this question, we look at an example.

§4. When Two Ellipses Meet

In this section we consider a simple example which will show that also the eigenvalue method can encounter serious obstacles, in particular when Gröbner bases are involved. The important thing here is *simplicity*, as it will not be too surprising if extremely complicated and difficult examples cause problems.

We consider the two ellipses

$$f(x,y) = \frac{1}{3}x^2 + \frac{2}{3}y^2 - 1,$$
$$g(x,y) = \frac{2}{3}x^2 + \frac{1}{3}y^2 - 1.$$

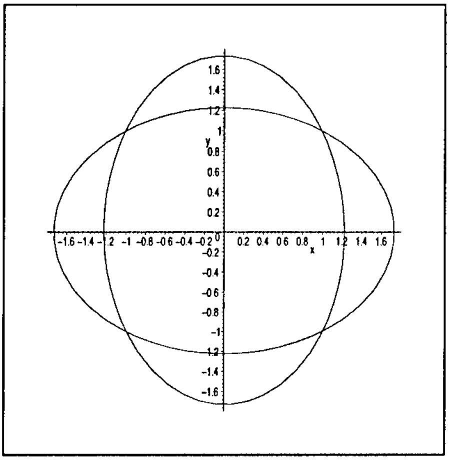

Fig. 1. The two ellipses.

Clearly, these two ellipses intersect in the four well–separated points $(\pm 1, \pm 1)$ as can be seen in Fig. 1.

Now, we are going to perturb g a little bit and replace it by $g_\phi = g\left(A_\phi(x,y)\right)$, where A_ϕ denotes the rotation

$$A_\phi(x,y) = \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}.$$

Note that we have in mind *small* values of ϕ, so the intersections should still be close to $(\pm 1, \pm 1)$ and the problem should still be well–conditioned.

Recalling that lexicographic Gröbner bases are known as troublemakers, we first try some "better" Gröbner basis, namely the one which is based on the graded lexicographic term order with $x \prec y$. Note that this ideal basis is not only a Gröbner basis, but also an H–basis. In this case the Gröbner bases $\mathcal{G}_\phi$ consists, for $\phi \neq 0$, of the three polynomials

$$\begin{aligned}
&4\sin\phi\, xy + 3\cos\phi\, x^2 - 3\cos\phi, \\
&x^2 + 2y^2 - 3, \\
&\cos\phi\left(\cos^2\phi + 8\right)\, x^3 - 3\cos\phi\left(\cos^2\phi + 2\right)\, x + 12\,\sin\phi\left(\sin^2\phi - 1\right)\, y,
\end{aligned}$$

while

$$\mathcal{G}_0 = \left\{x^2 - 1, y^2 - 1\right\}.$$

Here we already observe that some singularity must appear for $\phi = 0$, since $\mathcal{G}_0$ is not just a limit $\phi \to 0$ of $\mathcal{G}_\phi$, although the basis changes continuously with respect to ϕ. The singularity becomes more apparent if we look at the normal forms, which are

$$\mathcal{P}_\phi = \begin{cases} \left\{1, x, y, x^2\right\} & \text{if } \phi \neq 0, \\ \left\{1, x, y, xy\right\} & \text{if } \phi = 0. \end{cases}$$

Finally, the multiplication tables $M_{x,\phi}$ for the multiplication by x take the form

$$M_{x,0} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

while the multiplication table

$$M_{x,\phi} = \begin{bmatrix} 0 & 0 & \frac{3\cos\phi}{4\sin\phi} & 0 \\ 1 & 0 & 0 & -3\frac{5\cos^2\phi-8}{\cos^2\phi+8} \\ 0 & 0 & 0 & -12\frac{\sin\phi\ \cos\phi}{\cos^2\phi+8} \\ 0 & 1 & -\frac{3\cos\phi}{4\sin\phi} & 0 \end{bmatrix}, \qquad \phi \neq 0,$$

provides us with difficulties. Not only does this matrix *not* converge to $M_{x,0}$ for $\phi \to 0$, but some entries in this matrix even *diverge* to $\pm\infty$, respectively. Indeed, if one tries to compute the eigenvalues and eigenvectors of this matrix for small values of ϕ, things become disastrous: A `Maple` computation with 10 digits worked until about $\phi \sim 10^{-5}$, where an error message reported that the QR algorithm did not work. For smaller values, like $\phi \sim 10^{-6}$, `Maple` invented *complex* zeros with an imaginary part of the magnitude 0.5×10^{-5} which by far exceeds any negligible machine number. On the other hand, `Octave`, a free `Matlab` clone whose Linear Algebra facilities are based on `LAPACK` [1], reproduced the eigenvalues correctly, but gave eigenvectors which were practically 0.

Hence, we end up with some kind of paradox which is due to a singularity at $\phi = 0$: though the original problem of solving the polynomial system of equations is very well–conditioned, the graded lexicographical Gröbner basis is extremely sensitive to *very small* perturbations ($|\phi| \leq 10^{-5}$), but by far not so sensitive to relatively "large" ($|\phi| > 10^{-5}$) perturbations.

Similar problems appear when we replace the graded lexicographical Gröbner basis by a purely lexicographical one with $x \prec y$ which yields the normal forms

$$\mathcal{P}_\phi = \begin{cases} \{1, x, x^2, x^3\} & \text{if } \phi \neq 0, \\ \{1, x, y, xy\} & \text{if } \phi = 0. \end{cases}$$

Though the components of the multiplication table $M_{x,\phi}$ at least are continuous functions in ϕ and remain bounded in this case, the limit $\phi \to 0$ again is not $M_{x,0}$. But the multiplication tables $M_{y,\phi}$ with respect to the purely lexicographical Gröbner basis is even worse: its entries are either zero or diverge for $\phi \to 0$.

The behavior of the Gröbner bases at $\phi = 0$ raises the question of whether this singularity is *systematic*, that is, intrinsic to the problem, or if it is a *representation singularity* generated by the Gröbner bases. Systematic singularities appear, for example, if several zeros "collapse" into one multiple zero which leads to extremely intricate problems in the multivariate case [9]. Here, however, the good separation of the zeros suggests the conjecture that we only face a representation singularity.

Indeed, since H–bases leave more degrees of freedom, we can try another one which is now based on orthogonalization. For this purpose, we use the inner-product

$$(p,q) = (p(D)\,q)\,(0)$$

and recall from [11, Theorem 5.3] that the set $\{f, g_\phi\}$ is already an H–basis. Moreover, the normal form space, which is, according to Theorem 1, the least interpolation space, is spanned by

$$\mathcal{P}_\phi^* = \left\{1, x, y, 2\sin\phi\, x^2 - 3\cos\phi\, xy - \sin\phi\, y^2\right\}$$

and depends *continuously* on ϕ with

$$\lim_{\phi\to 0} \mathcal{P}_\phi^* = \mathcal{P}_0 = \{1, x, y, xy\}\,.$$

Then one can compute the respective multiplication table as

$$M_{x,\phi}^* = \begin{bmatrix} 0 & 1+\varepsilon_1(\phi) & \varepsilon_2(\phi) & \varepsilon_3(\phi) \\ 1 & 0 & 0 & \varepsilon_4(\phi) \\ 1 & 0 & 0 & 1+\varepsilon_5(\phi) \\ 0 & \varepsilon_6(\phi) & 1+\varepsilon_7(\phi) & \varepsilon_8(\phi) \end{bmatrix},$$

where $\varepsilon_j\,(\cdot)$, $j = 1,\dots,8$, are continuous functions which vanish at the origin. In particular, $M_{x,\phi}^* \to M_{x,0}$ as $x \to 0$ and the computation of eigenvalues and eigenvectors of $M_{x,\phi}^*$ can now be done with sufficient accuracy. However, we remark that the fact that the matrices $M_{x,\phi}^*$ and $M_{y,\phi}^*$ have two approximately double eigenvalues ± 1, requires some extra care when connecting these individual values in the final determination of the intersections.

§5. Summary

We have given examples of numerical applications which can be reduced to the computation of normal forms with respect to a certain polynomial ideal, an operation which is usually performed using a Gröbner basis. On the other hand, H–bases could as well be used for normal form computations, and their greater flexibility may yield stabilizing effects which are highly desired in numerical computations.

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