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Using computer algebra methods for global optimization.

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Résumé

This paper introduces computer algebra techniques for solving polynomial systems and some global optimization problems. The idea is to use these methods as preprocessing tool to separate components of different dimension and to find a simple parametrization of positive dimension components. It is then possible to use software like Global or Numerica to find the actual global minimum. As an example of the use of this method we illustrate several successful applications.

1 The problem

A global optimization problem is of the form

$$\text{minimize } \Phi(x) \quad \text{subject to } f_i(x) = 0 \ i = 1,\ldots,m \quad \text{where } \Phi : \mathbf{C}^n \longrightarrow \mathbf{R} \quad f_i : \mathbf{C}^n \longrightarrow \mathbf{C} \tag{1}$$

It is important to recall that we want the *true global* minimum and not a *local* minimum. The second point is the set of constraints

$$V_{\text{const}} = \{x \in \mathbf{C}^n \text{ s.t. } f_i(x) = 0 \ i = 1,\ldots,m\}$$

is not necessarily a compact set (not a bounded set). The last requirement is that the computations must be certified (this imply the use of exact arithmetic or interval arithmetic).
We restrict ourselves to the case where all the f_i are algebraic (possibly after some transformation see 4.2 or 4.3 for examples of such transformation). Sometimes Φ is also a polynomial equation.

2 The strategy

In order to solve the global optimization problem 1 we will use two diffirent strategy depending on whether Φ is algebraic or not.

2.1 Algebraic target function

We suppose that Φ and all the f_i are polynomials in $\mathbf{Q}[X_1,\ldots,X_n]$. We introduce a new variable F. The strategy is then to compute

$$V = V_{\text{const}} \cup \{x \text{ s.t. } \frac{\partial \Phi}{\partial x_i} = 0 \ \ i = 1,\ldots,n\} \cup \{\Phi - F\}$$

V is an algebraic variety: we will see in section 3 that it is possible to compute a decomposition into irreducible varieties $V = V_1 \cup \cdots V_k$, each V_i is an irreducible variety. Then we compute (see 3) for all i the projection $\pi(V_i)$ where $\pi : (x_1,\ldots,x_n,f) \longrightarrow f$. Now for each component V_i we compute the minimum of $\pi(V_i)$ (this is easy to compute if $\pi(V_i)$ is finite). Examples 4.1 and 4.2 have been solved by these method.

2.2 General target function

In that case we compute a decomposition into irreducible varieties of $V_{\text{const}} = V_1 \cup \cdots V_k$. For $i = 1, \ldots, k$, V_i is an irreducible variety of dimension d_i. We can consider that $x_{n-d_i}, \ldots, x_n$ are free parameters and it is possible to find $\Phi_i(x_{n-d_i}, \ldots, x_n)$ which coincides with Φ over V_i. We now use a numerical (global) optimization program to minimize Φ_i suject to V_i: we have thus reduce the number of unkwon of n to d_i. The example in section 4.3 is an illustration of this method.

3 Solving polynomial systems by Computer Algebra Method

We define a system of polynomial equations $f_1 = 0, \ldots, f_R = 0$ as a list of multivariate polynomials with rational coefficients in the algebra $\mathbf{Q}[x_1, \ldots, x_N]$. Let $F = [f_1, \ldots, f_R]$ be this list of equations. To such a system we associate $\mathcal{I}(F)$, the ideal which is generated by $f_1, \ldots, f_R$; it is the smallest ideal containing these polynomials, or equivalently $\sum_{k=1}^{R} f_k U_k$ where the U_k are in $\mathbf{Q}[x_1, \ldots, x_N]$. Since the f_k vanish exactly at points where all polynomials of $\mathcal{I}$ vanish, it is equivalent to studying the system of equations or the ideal $\mathcal{I}$. To study the solutions of the algebraic system F we define the algebraic variety of $\mathcal{I}(F)$ by $V_K(\mathcal{I}(F)) = \{z \in K \mid f_i(z) = 0 \; i = 1, \ldots, R\}$ where K is $\mathbf{R}$ the real numbers or $\mathbf{C}$ the complex numbers. From a practical point of view the main difference between the two approaches is that we keep among other things the multiplicities of the roots. For instance if $F = [x^2]$ the ideal $\mathcal{I}(F)$ is (x) but $V_K(\mathcal{I}(F)) = \{0\}$.

3.1 Gröbner basis

Gröbner basis is a very powerful tool for solving polynomial system: the idea [2] is to find a simpler basis of the ideal $\mathcal{I}(F)$. We refer to [3] for an introduction to the subject. To define a Gröbner we need first to sort the monomials inside a polynomial (for instance the lexicographic ordering $x_1 \gg x_2 \gg \cdots \gg x_n$). Now we can define the *leading monomial* (resp. term) of a polynomial as its monomial (resp. term) with highest degree for a given ordering $<$.

Definition 1 *Let $<$ be a monomial ordering. Let G be a finite list of polynomials such that: for all $p \in \mathcal{I}$ there exist $g \in G$ such that the leading monomial of g divides the leading monomial of p. Then G is a Gröbner basis of $\mathcal{I}$ for the ordering $<$.*

Theorem 1 *For any system F of algebraic equations, and any ordering $<$ we can compute a Gröbner basis (with the Buchberger algorithm [2] or more recent algorithms F_4 [7]).*

It is important to note that all the computations are exacts since the computation of a Gröbner basis is equivalent to solve several linear systems and we can use exact arithmetic (for instance the GNU GMP package for arbitrary-precision arithmetic) to solve these systems.
It is convenient to introduce the notion of *dimension* to describe the structure of the roots. We refer to [3] for a precise mathematical definition. A meaningful interpretation of the dimension is that it corresponds to the remaining free degrees when all of the equations are satisfied.
Hence all the roots of a zero dimensional system are isolated points. The example of secttion 4.1 is a one dimensional system. The lexicographic Gröbner basis of a zero dimensional system contain a univariate polynomial in x_n.

3.2 Decomposition of ideals

One can find precise definition in [3]:

Definition 2 *A variety V is irreducible if it is not possible find non empty varieties V_1, V_2 such that $V = V_1 \cup V_2$.*

Theorem 2 *If V is an algebraic variety. There exist a unique decomposition into irreducible varieties $V = V_1 \cup \cdots V_k$*

The important point is that there exist efficient and exact algorithms for computing such decomposition (see F_7 or triangular systems [9]). On of these algorithms is implemented in an experimental software Gb and FGb ([6]) written in C/C++ (about 200 000 lines of code).
In practive we give a lexicographic Gröbner basis for each component V_i. We have thus split the initial system into several systems and each sub system is simpler. The key point is that we have separated components with isolated points , one dimensional components, ...

3.3 Finding all the roots of univariate polynomials

We have seen in previous sections that we have reduced the problem of solving polynomial system of dimension 0 to a equivalent problem with univariate polynomials. Thus it is natural to ask to solve univariate polynomials efficiently. There are two very different answer depending on whether we want to compute the real roots or the complex roots. To compute the real roots of $P(x)$ with $P \in \mathbf{Z}[x]$ we apply an efficient variant of an algorithm of Uspensky (see [5]) based on Descartes' rule of sign. The input of the algorithm is a polynomial P and integer M, the output of this algorithm is a list of intervals $\cup_{i=1}^{r}[l_i,r_i]$ of size at most 2^{-M} containing one and only one real roots.
To compute all the complex roots of $P(x)$ with $P \in \mathbf{Z}[x]$ we used the Aberth's method developed by Bini (implemented in the MPSolve program [1]). It is possible to find the complex roots with as many digits as required.

4 Applications solved by computer algebra methods

4.1 Application to the problem of R. Baker Kearfott

4.1.1 The Example

In the paper of R. Baker Kearfott [10] we found the following problem:
Find a_1,a_2,a_3,x_1,x_2 and x_3 such that $c_i = 0$ for $i = 1,\ldots,6$.

$c_1 = 0.08413\, a_1 + 0.08413\, a_2 + 0.08413\, a_3 + 0.08413 + 0.2163\, q1 + 0.0792\, q_2 - 0.1372\, q_3$

$c_2 = -0.3266\, a_1 - 0.3266\, a_2 - 0.3266\, a_3 - 0.3266 - 0.57\, q_1 - 0.0792\, q_2 + 0.4907\, q_3$

$c_3 = 0.2704\, a_1 + 0.2704\, a_2 + 0.2704\, a_3 + 0.2704 + 0.3536\, a_1\, (x_1 - x_3) + 0.3536\, a_2 \left({x_1}^2 - {x_3}^2\right) + 0.3536\, a_3 \left({x_1}^3 - {x_3}^3\right) + 0.3536\, {x_1}^4 - 0.3536\, {x_3}^4$

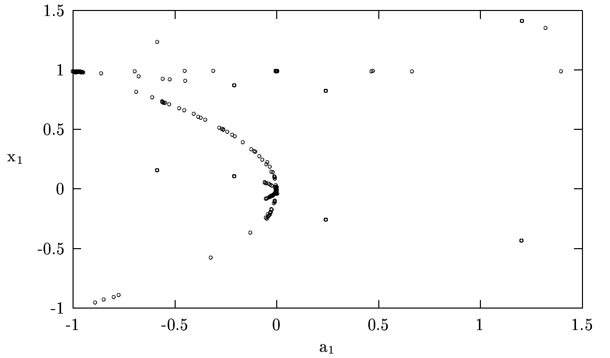
$c_4 = 0.02383\, p_1 - 0.01592\, a_1 - 0.01592\, a_2 - 0.01592\, a_3 - 0.01592 - 0.08295\, q_1 - 0.05158\, q_2 + 0.0314\, q_3$

$c_5 = -0.04768\, p_2 - 0.06774\, a_1 - 0.06774\, a_2 - 0.06774\, a_3 - 0.06774 - 0.1509\, q_1 + 0.1509\, q_3$

$c_6 = 0.02383\, p_3 - 0.1191\, a_1 - 0.1191\, a_2 - 0.1191\, a_3 - 0.1191 - 0.0314\, q_1 + 0.05158\, q_2 + 0.08295\, q_3$

where

$$i = 1,2,3 \left\{ \begin{array}{l} q_i := a_1\, x_i + a_2\, x_i^2 + a_3\, x_i^3 + x_i^4 \\ p_i := \frac{\partial q_i}{\partial x_i} = a_1 + 2\, a_2\, x_i + 3\, a_3\, x_i^2 + 4\, x_i^3 \\ r = q_i(1) = a_1 + a_2 + a_3 + 1 \end{array} \right.$$



Solution found by GlobSol

We display now the figure (4.1.1) of the Solution found by GlobSol: “A run of one hour produced 216 unverified small boxes and 12 boxes with verified feasible points” (see [10]). There are 6 equations and 6 variables but the system is not complete intersection. It is well explained in the paper [10] why it is difficult for the optimizer to find all the solutions.

4.1.2 Decomposition into irreducible varieties

We compute a decomposition of the variety into irreducible components. We used the F_7 algorithm to compute the decomposition: it takes less than 1 minute on a PC (Pentium III - 600 Mhz).

$$V = V_1 \cap V_2 \cap V_3 \cap V_4 \cap \cdots \cap V_{12}$$

where V_i are prime ideals. Moreover $\dim(V_i) = 1$ for $i = 1,2,3$ and $\dim(V_i) = 0$ for $i = 4,\ldots,12$.
There are 26 real isolated points and 64 (pure) complex isolated points.
All the components but V_{12} are very simple. We list these solutions:
First two components parametrized by a_1 or a_2:

$$V_1 = [x_3 = x_2 = x_1 = 1, a_2 = -2\,a_1 + 1, a_3 = a_1 - 2]$$
$$V_2 = [a_3 = -a_2 - 1, x_3 = x_2 = x_1 = a_1 = 0]$$
$$V_3 = \left[a_2 - 2\,x_1 + a_1, a_3 + 2\,x_1 + 1, x_3 - x_1, x_2 - x_1, {x_1}^2 + a_1\right]$$

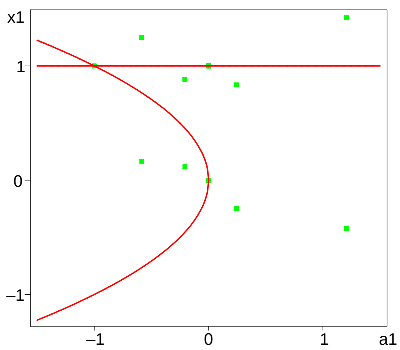
All the other components are zero dimensional (isolated points).

$$V_4 = r_1 = [a_2 = -a_3 = 3, x_3 = x_2 = x_1 = -a_1 = 1] \quad V_8 = r_5 = [a_3 = -2, a_2 = x_3 = 1, x_2 = x_1 = a_1 = 0]$$
$$V_5 = r_2 = [a_3 = -1, a_2 = a_1 = x_3 = x_2 = x_1 = 0] \quad V_9 = r_6 = [a_3 = -2, a_2 = x_3 = x_1 = 1, x_2 = a_1 = 0]$$
$$V_6 = r_3 = [a_3 = -2, a_2 = x_3 = x_2 = 1, x_1 = a_1 = 0] \quad V_{10} = r_7 = [a_3 = -2, a_2 = x_2 = x_1 = 0, x_3 = a_1 = 0]$$
$$V_7 = r_4 = [a_3 = -2, a_2 = x_1 = 1, x_3 = x_2 = a_1 = 0] \quad V_{11} = r_8 = [a_3 = -2, a_2 = x_2 = 1, x_3 = x_1 = a_1 = 0]$$

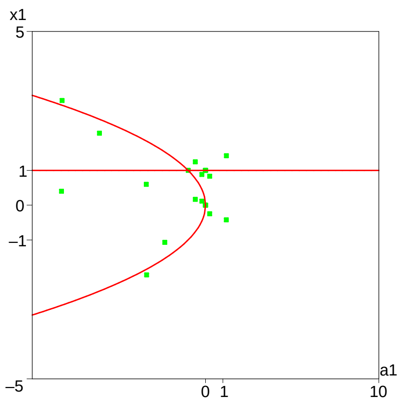
the description of V_{12} is more difficult. The shape of V_{12} is $V_{12} = [x_2 = Q_1(x_3), x_1 = Q_2(x_3), a_1 = Q_3(x_3), a_2 = Q_4(x_3), a_3 = Q_5(x_3), Q(x_3) = 0]$ where Q (resp. Q_i) is a univariate polynomial of degree 72 (resp. 71). We can show by exact (Algorithm of Uspensky implemented in F. Rouillier program RS ([5, 11]) based on Descartes rule of signs) that there are *exactly* 18 *real roots*. We give now a numerical and certified approximations of the other 18 real roots (6 digits printed):

$$r_9 = \quad [a_1 = -.616087e9, a_2 = 370507., a_3 = 2018.77, x_2 = -135.308, x_1 = 178.797, x_3 = -1426.73]$$
$$\cdots$$
$$r_{26} = \quad [a_2 = .411203e8, a_1 = -.255363e11, x_1 = 197.131, x_2 = 2255.12, a_3 = -15159.3, x_3 = 2473.72]$$

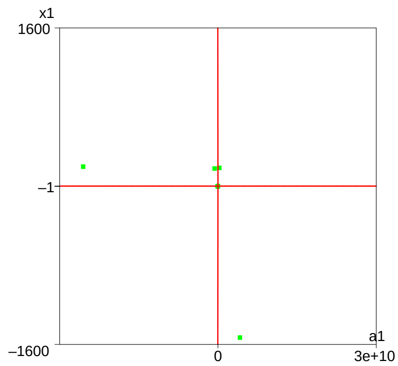
Hence we have found explicitely $(r_i)_{i=1,\ldots,26}$ all the real isolated roots of the system.



$a_1 \in [-\frac{3}{2}, \frac{3}{2}]$



$a_1 \in [-10, 10]$



all (real) solutions

Be careful that on all these figures it is impossible to see the component V_2 and the vertical line is not a vertical line but a parabola.

4.2 Breguet Formula

The goal (problem submitted by ONERA) is to *maximize* the Breguet endurance formula $\psi = \psi_1 \psi_2$. The Breguet endurance give the endurance of plane in function of the length (L) and the area (S) of the wings (all the other variables are parameters: for instance m_{init} is the initial mass, $g = 9.806, \ldots$).

$$\psi_1 = \frac{1}{\sqrt{\begin{array}{l} K_r\ (k_f + k_e + k_t + k_{cu})\sqrt{S}L^{3/2} + \frac{\sqrt{2}\mu_{mot}\, g^{3/2}\, Cx_0\, \sqrt{S}}{\nu_{prop}\, \sqrt{\rho}{C_z}^{3/2}\sqrt{m_{init}}} + \frac{\sqrt{2}\mu_{mot}\, g^{3/2}\, K_r\, Cx_0\, SL^{3/2}}{\nu_{prop}\, \sqrt{\rho}{C_z}^{3/2}\sqrt{m_{init}}} \\ + \frac{m_s\, S}{m_{init}} + \frac{\sqrt{2}\mu_{mot}\, g^{3/2}\sqrt{C_z}K_r\, S\sqrt{L}}{\nu_{prop}\, \sqrt{\rho}\sqrt{m_{init}}\pi} + \frac{\sqrt{2}\mu_{mot}\, g^{3/2}\sqrt{C_z}\sqrt{S}}{\nu_{prop}\, \sqrt{\rho}\sqrt{m_{init}}\pi\, L} + k_f + k_e + k_t + k_{cu} \end{array}}} - 1$$

$$\psi_2 = \sqrt{S}\left(1/2\, \frac{C_{x0}\ C_{sp}\, g^{3/2}\sqrt{m_{init}}\sqrt{2}}{\nu_{prop}\, \sqrt{\rho}{C_z}^{3/2}} + 1/2\, \frac{\sqrt{C_z}\, C_{sp}\, g^{3/2}\sqrt{m_{init}}\sqrt{2}}{\pi\, \nu_{prop}\, \sqrt{\rho}L}\right)^{-1}$$

It is not difficult to transform the target function inton a rational fraction. We found in a few seconds 96 complex solution and it is easy to plug these values into ψ to find the global solution. It should be noticed that the solution found by numerical methods was not correct (a linearization of the equation ψ was first computed).

4.3 Design of filter bank

This problem was supply to us by French Telecom (we refer to [8] for a complete description of the problem and the solutions we found). The design of two-dimensional filter banks yielding orthogonality and linear-phase filters, and generating regular wavelet bases is a difficult task involving algebraic properties of multivariate polynomials. Using cascade forms implies dealing with global non-linear optimization. We turn the issue of optimizing the orthogonal linear-phase cascade by Vetterli and Kovacevic into a polynomial problem and solve it using Gröbner basis techniques and computer algebra. This leads to a complete description of maximally flat wavelets among the orthogonal linear-phase family proposed by Vetterli and Kovacevic.
More precisely, let K be a given integer (in practice k = 7,8,9). Let $(\alpha_i)_{i=1,\ldots,K)}$ and β_i are free parameters (real numbers). For $z = (z_1, z_2)$, we first define the 4×4 polyphase matrix $\mathcal{H}(z)$:

$$\mathcal{H}(z) = R_1 W P \prod_{i=2}^{K} (D(z_1,z_2) P W R_i W P)$$

$\mathcal{H}_{i,j}$ denotes the (i,j) component of the matrix $\mathcal{H}(z)$. We can now define the polynomial

$$H_i(z) = \mathcal{H}_{i,0}(z_1^2,z_2^2) + \mathcal{H}_{i,1}(z_1^2,z_2^2)z_1 + \mathcal{H}_{i,2}(z_1^2,z_2^2)z_2 + \mathcal{H}_{i,3}(z_1^2,z_2^2)z_1 z_2$$

where

$$R_i = \begin{bmatrix} \cos\alpha_i & -\sin\alpha_i & 0 & 0 \\ \sin\alpha_i & \cos\alpha_i & 0 & 0 \\ 0 & 0 & \cos\beta_i & -\sin\beta_i \\ 0 & 0 & \sin\beta_i & \cos\beta_i \end{bmatrix} \quad W = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \quad P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad D(z_1,z_2) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & z_1 & 0 & 0 \\ 0 & 0 & z_2 & 0 \\ 0 & 0 & 0 & z_1 z_2 \end{bmatrix}$$

The goal is to find the maximum integer N such that for all $k_1,k_2,k_1+k_2 \leq N$

$$\frac{\partial^{k_1+k_2} H_0}{\partial z_1^{k_1}\partial z_2^{k_2}} = 0 \text{ at } (1,-1),(-1,-1),(-1,1) \qquad \frac{\partial^{k_1+k_2} H_1}{\partial z_1^{k_1}\partial z_2^{k_2}} = 0 \text{ at } (1,-1),(1,1),(-1,1)$$

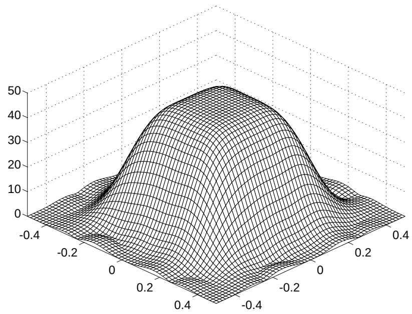
$$\frac{\partial^{k_1+k_2} H_2}{\partial z_1^{k_1}\partial z_2^{k_2}} = 0 \text{ at } (1,1),(-1,-1),(-1,1) \qquad \frac{\partial^{k_1+k_2} H_3}{\partial z_1^{k_1}\partial z_2^{k_2}} = 0 \text{ at } (1,-1),(-1,-1),(1,1)$$

$$\min\{\text{Energy Compaction}(\alpha_i,\beta_i)\} \tag{2}$$

It is obvious that we can transform all the equations except (2) into polynomials by adding new variables $c_i = cos(\alpha_i)$, $s_i = sin(\alpha_i)$ and a new equation $c_i^2 + s_i^2 = 1$ (the same for the β_i).

The first task is to find the maximum N for a given K. This is done with gröbner bases methods: for a given K we try successively $N = 1,2,3$ until we found no solution. We find:

K	3	4	5	6	7	8
maximal N	2	2	3	3	4	5
dimension	0	2	2	4	2	2



For a given K, say $K = 7$, we have a two dimensional system. In other words, we have two free parameters, for instance α_1,β_1, and we can express all the other variables α_i,β_i as rational functions of α_1,β_1. We use now a "standard" optimizer to optimize the criteria (2) but with respect to only two parameters.

5 Conclusion

The association of two methods, Computer Algebra algorithms as a preprocessing tool and rigorous global search engine (such as GlobSol [4]) seems a very promising tool to find global optimization problem.

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