Gröbner Bases as a General Algorithmic Tool for Systems of Equations

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Introduction

Most of real-world problems are described by systems of equations rather then by an isolated single equation. Moreover, most often equations which arise in natural sciences and engineering are of polynomial type with respect to unknowns.

Thus, in development of all three computer-aided approaches

1. symbolic algebraic analysis,
2. numerical solving,
3. visualization,

one has to pay a primary attention to systems of polynomially-nonlinear equations.

Goal of symbolic algebraic analysis: given equations, extract from them as much information on solutions as possible without (generally impossible) explicit integration/solving and/or "simplify/rewrite" the equations for the further numerical solving.

Introduction (cont.)

But what can we hope to do algorithmically in the general (polynomially-nonlinear) case of equation systems?

- Check compatibility, i.e., consistency.
- Detect dimension of the solution space ("arbitrariness" in general analytical solution for DEs).
- Eliminate a subset of variables.
- Reduce the problem to (a finite set) of "simpler" problems.
- Check satisfiability of an extra equation on the solutions.
- Find Lie symmetries (DEs).
- Formulate a well-posed initial value problem (PDEs).
- Compute "hidden constraints" for dependent variables or numerical indices (ADEs).
- Rewrite into another form more appropriate for numerical solving.
- Generate finite difference schemes (for PDEs).
- ....

Introduction (cont.)

Is there a "universal" algorithmic tool for the listed subproblems?

If the system has polynomial nonlinearity in unknowns with "algorithmically computable" coefficients, then such a tool exists and based on transformation of the system into another set of equations with certain "nice" properties.

For the conventional polynomial systems and some their generalizations to noncommutative polynomials, for linear PDEs and linear finite difference equations (FDEs) / recurrence relations (RRs) such a form is canonical, i.e., uniquely defined by the initial systems and an order on the variables, and called reduced Gröbner basis (GB) (Buchberger'65).

Another "nice" canonical form is called Involutive Basis (IB) (Gerdt, Blinkov'98). IB is also GB, although (in most cases) redundant as a Gröbner one.

Introduction (cont): Simple Examples

Compatibility

$$\begin{cases} u_x + 1 = 0, \\ u_y + u = 0 \end{cases} \overset{\text{cross}-\text{derivation}}{\Longrightarrow} \begin{cases} \partial_y(u_x + 1) = 0, \\ \partial_x(u_y + u) = 0 \end{cases} \Longrightarrow u_x = 0 \Longrightarrow \boxed{1{=}0}\,(!)$$

contradiction

Solution space

$$\begin{cases} u_{xxy} = 0, \\ u_{xyy} = 0 \end{cases} \Longrightarrow u = \boxed{C}\,xy + \boxed{f_1(x)} + \boxed{f_2(y)}$$

arbitrary constant and two functions

Elimination

$$\begin{cases} u_{xxy} - u = 0, \\ u_{xyy} - u = 0 \end{cases} \overset{u_x \succ u_y}{\Longrightarrow} \begin{cases} u_x - u_y = 0, \\ \boxed{u_{yyy} - u = 0} \end{cases}$$

$\Uparrow$ u_x eliminated

Introduction (cont.)

The method of Gröbner bases has been applied successfully to:

- commutative algebra and algebraic geometry
- invariant theory
- Lie symmetry analysis of differential equations
- dynamical systems
- partial differential equations
- symbolic summation and integration
- non-commutative algebra
- robotics
- numerics (e.g. wavelets construction and difference schemes generation)
- systems theory (e.g. control theory)
- constrained dynamics (Dirac's formalism)
- reduction of loop Feynman integrals (Tarasov'98,V.Smirnov & A.Smirnov'05)
- ....

Introduction (cont.): Basic Idea

The general strategy if the Gröbner basis approach is to

- Transform a set F of equations (that describes the problem at hand) another set G of polynomials with certain "nice" properties (called a Gröbner basis) such that
- F and G are "equivalent" and G is "simple" than F.

From the theory and practice of Gröbner bases it is known:

- Because of some "nice" special properties of Gröbner bases, many problems that are difficult for general F are "easy" for Gröbner basis G
- There are algorithms and their implementations for transforming an F into G.
- The solution of the problem for G can often be easily translated back into a solution of the problem for F.

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Basic Notions

The theory of Gröbner bases is centered around the concept of ideals generated by finite sets of multivariate polynomials. Thus, to introduce the basic of Gröbner bases theory, we start our discussion by defining some related basic algebraic structures.

Definition. A ring $< R, +, \cdot >$ is a nonempty set R with the two binary operations addition $(+)$ and multiplication $(\cdot)$ on R such that $< R, + >$ is an abelian group, $(\cdot)$ is associative with an identity e $(e \cdot a = a \cdot e = a, \forall a \in R)$, and the distributive law

$$a \cdot (b + c) = a \cdot b + a \cdot c, \qquad (a + b) \cdot c = a \cdot c + b \cdot c$$

holds $\forall a, b, c \in R$. If $(\cdot)$ is commutative, then the ring is called commutative. $< R, +, \cdot >$ is called a field if every nonzero element of R has a multiplicative inverse in R.

Example. $<\mathbb{Z}, +, \cdot >$ is a commutative ring, but not a field, whereas $< \mathbb{Q}, +, \cdot >$ is a field.

Basic Notions (cont.)

Definition. Let $\mathbb{N}$ denote the nonnegative integers and let $\mu = (\mu_1, \ldots, \mu_n)$ be a power vector (multiindex) in $\mathbb{N}^n$ and let $(x_1, \ldots, x_n)$ be variables. Then a monomial $x^\mu := x_1^{\mu_1} \cdots x_n^{\mu_n}$. The total degree of x^μ is $|\mu| = \mu_1 + \cdots + \mu_n$. A polynomial f in $(x_1, \ldots, x_n)$ with coefficient in a field $\mathbb{K}$ is the finite sum

$$f(x_1, \ldots, x_n) := \sum_{\mu} a_\mu x^\mu \,, \quad a_\mu \in \mathbb{K}\,.$$

The total degree of f is $\max\{\mu \mid a_\mu \neq 0\}$.

Remark. The set of all polynomials in $(x_1, \ldots, x_n)$ over the coefficient field $\mathbb{K}$ is denoted by $\mathbb{K}[x_1, \ldots, x_n]$. It forms a commutative ring called polynomial ring.

Basic Notions (cont.)

Definition. Let $< R, +, \cdot, >$ be a commutative ring. A nonempty subset $\mathcal{I} \in R$ is called an ideal if $\mathcal{I}$ is closed under addition and is closed under inside-outside multiplication.

Definition. Let $F = \{\, f_1, \ldots, f_s \,\}$ be a set of polynomials. Then the ideal $\mathcal{I}$ generated by F, denoted also by $\mathrm{Id}(F)$, is given by

$$\mathcal{I}=\{ \sum_{i=1}^{s} h_i\, f_i \mid h_i \in \mathbb{K}[x_1, \ldots, x_n] \} \,.$$

The polynomial set F is called basis of the ideal $\mathcal{I}$. Since F is finite, $\mathcal{I}$ is finitely generated.

Hilbert Basis Theorem. Every ideal $\mathcal{I} \subseteq \mathbb{K}[x_1, \ldots, x_n]$ is finitely generated.

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Monomial Order

Obviously, there are many bases for one ideal. We can always add any linear combination of the generators, or suppress one of them if it is a linear combination of the others. However, among the different bases of an ideal stands a very useful basis: Gröbner basis (Buchberger'65).

A Gröbner basis is defined in terms of an ideal (i.e. its generating set) and a monomial order.

Definition. A total (linear) order $\succ$ on the monomials is called admissible if

$$(i)\ m \neq 1 \iff m \succ 1, \quad (ii)\ m_1 \succ m_2 \iff m_1 m \succ m_2 m$$

for any monomials m, m_1, m_2.

Given $\succ$ and $f \in F \subset \mathbb{R}$, there is the leading monomial of f denoted by $\mathrm{lm}(f)$. Correspondingly, the leading term $\mathrm{lt}(f)$ and the leading coefficients $\mathrm{lc}(f)$ are given by $\mathrm{lt}(f) := \mathrm{lc}(f) \cdot \mathrm{lm}(f)$. We shall denote the set of leading monomials in F by $lm(F)$.

Monomial Order: Examples

Assume that $x_1 \succ x_2 \succ \cdots \succ x_n$

- Lexicographical order (Lex)
  $x^\alpha \succ_{lex} x^\beta$ if in the vector difference $\alpha - \beta = \{\alpha_1 - \beta_1, \ldots, \alpha_n - \beta_n\}$ the left-most nonzero entry is positive.
- Graduated (total degree then) lexicographical order (GradLex)
  $x^\alpha \succ_{grlex} x^\beta$ if

$$|\alpha| = \sum_{i=1}^{n} \alpha_i \succ |\beta| = \sum_{i=1}^{n} \beta_i \textit{ or if } |\alpha| = |\beta| \textit{ then } \alpha \succ_{lex} \beta.$$

- Graduated (total degree then) reverse lexicographical order (GradRevLex) or (DegRevLex) $x^\alpha \succ_{grlex} x^\beta$ if

$$|\alpha| = \sum_{i=1}^{n} \alpha_i \succ |\beta| = \sum_{i=1}^{n} \beta_i \textit{ or if } |\alpha| = |\beta|$$

and in $\alpha - \beta$ the right-most nonzero entry is negative.

Monomial Order: Examples (cont.)

In the bivariate case $x \succ y$:

- Lex

$$1 \prec x \prec x^2 \prec x^3 \prec \cdots \prec y \prec xy \prec x^2y \prec \cdots \prec y^2 \prec xy^2 \prec x^2y \prec \cdots$$

- GradLex, GradRevLex

$$1 \prec y \prec x \prec y^2 \prec xy \prec x^2 \prec y^3 \prec xy^2 \prec x^2y \prec x^3 \prec \cdots .$$

In the threevariate case $x \succ y \succ z$:

$$x^2yz^2 \succ_{grlex} xyz^3 , \qquad x^2yz^2 \prec_{grevlex} xyz^3$$

since $\alpha - \beta = \{1, 0, -1\}$.

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Gröbner Bases

Definition:. (Buchberger'65) A finite subset $G \subset \mathbb{R}$ is Gröbner basis of ideal $\mathcal{I} = \mathrm{Id}(G) \in \mathbb{R}$ if

$$\forall f \in \mathcal{I},\ \exists g \in G\ :\ \mathrm{lm}(g) \mid \mathrm{lm}(f)\,.$$

It follows that $f \in \mathcal{I}$ *is reducible modulo G*

$$f \xrightarrow[g]{} f' := f - \frac{\mathrm{lt}(f)}{\mathrm{lt}(g)}\, g, \quad f' \in \mathcal{I}, \ldots, \quad f \xrightarrow[G]{} 0\,.$$

Definition. Given a finite set $F \subset \mathbb{R}$, a polynomial $h \in \mathbb{R}$, and a monomial order $\succ$, a normal form $NF(h, F)$ of p modulo F is defined as

$$NF(h,F) = \tilde{h} = h - \sum_{ij} \alpha_{ij} m_{ij} f_j$$

with $\alpha_{ij} \in \mathbb{K},\ f_j \in F,\ m_{ij} \in \mathcal{M},\ \mathrm{lm}(m_{ij} g_j) \preceq \mathrm{lm}(h)$ and there are no monomial in $\tilde{h}$ multiple of any element in $\mathrm{lm}(F)$.

Gröbner Bases (cont.)

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Algorithms

Gröbner bases can be computed by Buchberger's algorithm (Buchberger'85) which implemented in most of modern general-purpose computer algebra systems such as Maple, Mathematica, Reduce, MuPAD, etc, or by more efficient algorithms: F_4 (Faugère'98), involutive algorithm (Gerdt'05).

The fastest implementations are in

- Maple (library FGb implementing F_4)
- Magma (F_4)
- JB and GINV (Involutive algorithm) http://invo.jinr.ru
- Singular (Buchberger's and involutive algorithms)

Simplest Form of Buchberger's Algorithm

Algorithm: Gröbner Basis($F, \succ$)

```
Input: $F \in \mathbb{K}[x_1, \ldots, x_n] \setminus \{0\}$, a finite set; $\prec$, an order
Output: $G$, a Gröbner basis of $\mathrm{Id}(F)$
 1: $G := F$;
 2: do
 3:    choose a pair $f_1, f_2 \in G$ and compute $S(f_1, f_2)$
 4:    $h := NF(S(f_1, f_2), G)$
 5:    if $h = 0$ then
 6:       goto 3 and choose the next pair
 7:    else
 8:       $G := G \cup \{h\}$
 9:    fi
10: od while $h \neq 0$
11: return $G$
```

$S-$polynomial $S(f_1, f_2) := c_1 t_1 f_1 - c_2 t_2 f_2$. Here $c_1, c_2 \in \mathbb{K}$ and t_1, t_2 are monomials such that $c_1 t_1 lm(f_1) = c_2 t_2 lm(f_2)$.

Some Properties of GB

- Uniqueness of (inter)reduced monic GB. $Ideal(F) = Ideal(G) \Longleftrightarrow$ GB(F)=GB(G).
- Idempotency of reduced GB
  $G :=$reduced GB $\Longrightarrow$ GB(G)=G.
- Principal Ideal (generated by a single polynomial) $Ideal(F)$ is principal $\Longleftrightarrow$ GB(F) has exactly one element.
- Trivial Ideal. $Ideal(F) = K[x_1, \ldots, x_N] \Longleftrightarrow$ GB(F)={1}.
- Solvability of a system of equations F is solvable $\Longleftrightarrow 1 \notin G$.
- Finite Solvability of polynomial equations F has only finite many solutions $\Longleftrightarrow \forall\ 1 \leq i \leq n \mid \exists f \in$GB($F$) such that $lm(f)$ is a power of x_i.
- Number of Solutions of polynomial equations The number of solutions of F (with multiplicities) $=$ cardinality of $\{u \mid u \notin$ "set of multiples of lm(GB(F))"}.

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Rings of Difference Polynomials

Let $\{y^1, \ldots, y^m\}$ be the set of *difference indeterminates*, e.g. functions of $n-$variables $\{x_1, \ldots, x_n\}$, and $\theta_1, \ldots, \theta_n$ be the set of mutually commuting *difference operators (differences)*, e.g.,

$$\theta_i \circ y^j = y^j(x_1, \ldots, x_i + 1, \ldots, x_n).$$

A *difference ring R with differences $\theta_1, \ldots, \theta_n$* is a commutative ring R with a unity such that $\forall f, g \in R,\ 1 \leq i, j \leq n\ \theta_i \circ f \in R$ and

$$\theta_i\theta_j = \theta_j\theta_i,\ \theta_i \circ (f+g) = \theta_i \circ f + \theta_i \circ g,\ \theta_i \circ (f\,g) = (\theta_i \circ f)(\theta_i \circ g)$$

Similarly one defines a *difference field*.

Remark. The above and below concepts are translated to *differential algebra* if θ_i are the partial derivations

$$\theta_i \circ y^j = \partial_i y^j(x_1, \ldots, x_i, \ldots, x_n).$$

Rings of Difference Polynomials (cont.)

Let $\mathbb{K}$ be a difference field. Denote by $\mathbb{R} := \mathbb{K}\{y^1, \ldots, y^m\}$ the difference ring of polynomials over $\mathbb{K}$ in variables

$$\{\ \theta^\mu \circ y^k\ \mid \mu \in \mathbb{Z}^n_{\geq 0},\ k = 1, \ldots, m\ \}\,.$$

Denote by $\mathbb{R}_L$ the set of linear polynomials in $\mathbb{R}$ and use the notations

$$\Theta = \{\ \theta^\mu\ \mid\ \mu \in \mathbb{Z}^n_{\geq 0}\ \}\,.$$

A *difference ideal* I in $\mathbb{R}$ is an ideal $I \in \mathbb{R}$ close under the action of any operator from Θ. If $F := \{f_1, \ldots, f_k\} \subset \mathbb{R}$ is a finite set, then the smallest difference ideal containing F denoted by $\mathrm{Id}(F)$. If $F \subset \mathbb{R}_L$, then $\mathrm{Id}(F)$ is a *linear difference ideal*.

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Ranking

A total ordering $\prec$ over the set of $\theta_\mu y^j$ is a *ranking* if it satisfies

1. $\theta_i \theta^\mu \circ y^j \succ \theta^\mu \circ y^j$
2. $\theta^\mu y^j \succ \theta^\nu \circ y^k \quad \Longleftrightarrow \quad \theta_i \theta^\mu \circ y^j \succ \theta_i \theta^\nu \circ y^k \quad \forall\, i, j, k, \mu, \nu.$

If $\mu \succ \nu \Longrightarrow \theta_\mu \circ y^j \succ \theta_\nu \circ y^k$ the ranking is *orderly*.
If $i \succ j \Longrightarrow \theta_\mu \circ y^j \succ \theta_\nu \circ y^k$ the ranking is *elimination*.

Given a ranking $\succ$,

- every linear polynomial $f \in \mathbb{R}_L \setminus \{0\}$ has the *leading term* $a\,\theta \circ y^j$, $\theta \in \Theta$;
- $\mathrm{lc}(f) := a \in \mathbb{K} \setminus \{0\}$ is the *leading coefficient*;
- $\mathrm{lm}(f) := \theta \circ y^j$ is the *leading monomial*.

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Gröbner Bases

Given nonzero linear difference ideal $I = \mathrm{Id}(G)$ and term order $\succ$, its generating set $G = \{g_1, \ldots, g_s\} \subset \mathbb{R}_L$ is a *Gröbner basis* (GB) (Kondratieva,Levin,Mikhalev,Pankratiev'99) of I if

$$\forall f \in I \cap \mathbb{R}_L \setminus \{0\}\ \exists g \in G, \theta \in \Theta\ :\ \mathrm{lm}(f) = \theta \circ \mathrm{lm}(g)\,.$$

It follows that $f \in I$ *is reducible modulo G*

$$f \underset{g}{\longrightarrow} f' := f - \mathrm{lc}(f)\,\theta \circ (g/lc(g)), \quad f' \in I, \ldots, \quad f \underset{G}{\longrightarrow} 0\,.$$

Some Computer Algebra Systems and Packages

Software	Commutative algebra	PDE	LFDE	Language
Maple	+	diffalg	Ore_algebra	Maple
		Rif		Maple
	Gb			C
	FGb			C
Mathematica	+	–	–	C
Reduce	+	–	–	Lisp
OreModules	–	LPDE	LFDE	Maple
Janet	–	LPDE	–	Maple
LDA	–	–	LFDE	Maple
GINV	+	–	–	Pyton/C++
JB	+	–	–	C

Reduction of 1-loop Integral

Consider a simple one-loop propagator type scalar integral with one massive and another massless particle studied, for example, in Tarasov'98,Smirnov'04

$$f(k,n) := \frac{1}{i\pi^{d/2}} \int \frac{d^d s}{P^k_{s-q,m} P^n_{s,0}}.$$

Here we apply the Gröbner basis method, as implemented in our package LDA (Gerdt,Robertz'05), directly to the recurrence relations:

$$[d - 2k - n - 2m^2 k\mathbf{1}^+ - n\,\mathbf{2}^+(\mathbf{1}^- - q^2 + m^2)]\, f(k+1, n+1) = 0,$$

$$[n - k - k\,\mathbf{1}^+(q^2 + m^2 - \mathbf{2}^-) - n\mathbf{2}^+(\mathbf{1}^- - q^2 + m^2)]\, f(k+1, n+1) = 0.$$

Here

$$\mathbf{1}^{\pm} f(k,n) = f(k\pm 1, n), \quad \mathbf{2}^{\pm} f(k,n) = f(k, n\pm 1).$$

Conclusions

- GB are the most universal algorithmic tool for the multivariate equation systems of polynomial type. In particular for multivariate recurrence relations with symbolic indices.
- GB have found numerous applications in many areas of science and technology.
- There are efficient algorithms for computing polynomial GB. Their extension to differential and difference systems is in progress.
- There are many different implementations of the Gröbner basis algorithms into computer algebra systems and software packages.
- In practice, efficiency of constructing GB strongly depends on the order chosen. Heuristically, reverse lexicographical order is best.
- Complexity of computing GB is at least exponential in the number of variables.
- Blowing-up of intermediate (especially parametric) coefficients is one of the main computational obstacles.

Some References

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  http://www.ricam.oeaw.ac.at/Groebner-Bases-Bibliography
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