Computer Algebra and Constrained Dynamics

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Abstract. In this paper we apply the algorithmic techniques of commutative computer algebra based on the use of involutive polynomial bases to finite-dimensional constrained Hamiltonian systems of polynomial type. It is shown that as well as reduced Gröbner bases involutive bases allows one to compute the complete set of constraints and separate them into the first and second classes.

1 Introduction

In paper [1] it was observed that computation of the complete set of constraints in the framework of the generalized Hamiltonian formalism invented by Dirac [2] is nothing else then completion of the initial Hamiltonian system to involution. Nowadays the Dirac approach is a main tool in investigation of gauge theories [3, 4, 5, 6] for purposes of their quantization. In so doing, Dirac classified the constraints in the first and second classes. First class constraints generate gauge degrees of freedom in the physical system under consideration, and its quantization requires gauge fixing whereas a second class constrained system does not need this. In the presence of first class constraints the general solution of the system depends on arbitrary functions. Hence, the system is underdetermined. To eliminate unphysical gauge degrees of freedom one usually imposes gauge fixing conditions whereas for elimination of other unphysical degrees of freedom occurring because of the second class constraints one can use the Dirac brackets [3, 4, 6].

Thus, to quantize a constrained Hamiltonian system one needs to know all the constraints involved and separate them into first and second classes. Dirac [2] developed a constructive method for computation of constraints which has been implemented in computer algebra software [7]. However, the original Dirac method for computation and separation of constraints is not yet an algorithm. Recently [8], we designed and implemented in Maple such an algorithm for systems which are described by polynomial Lagrangians. The algorithm combines the Dirac method with the Gröbner basis techniques which has become the most universal algorithmic tool in commutative algebra [9, 10] and algebraic geometry [11, 12].

However, in view of intrinsically involutive character of the Dirac method, it is more natural to rewrite the algorithm of paper [8] in terms of involutive polynomial bases rather than reduced Gröbner bases. Involutive polynomial bases were introduced in the pioneering paper [13] for the separation of variables into multiplicative and nonmultiplicative as used in the formal theory of partial differential equations [14]. In this case involutive bases are called Pommaret bases. A more general approach to involutive bases based on a new concept of involutive monomial division was invented in [15, 16], and it was shown that similar to Pommaret bases, which correspond to Pommaret division, every involutive polynomial basis is a Gröbner basis. Though involutive bases, as Gröbner bases, are generally redundant, they can be used for computation and separation of constraints as well as reduced Gröbner bases. Moreover, the involutive algorithms [13, 15, 16] for construction such bases are often faster then the classical Buchberger algorithm for computing reduced Gröbner bases. By now, the Buchberger algorithm built-in all the general-purpose computer algebra systems: Reduce, Mathematica, Maple, Axiom, MuPAD and many others. The involutive algorithms implemented to date in Reduce for Pommaret bases [13, 15, 16] and in Mathematica for a general involutive division [17][1].

[1]A polynomial Mathematica package is available at http://paul.math-inf.uni-greifswald.de/Invo/

In the given paper we briefly describe the concept of involutivity for systems of ordinary differential equations (Sect.2) and the notion of involutive polynomial bases (Sect.3). Then we consider the Dirac method (Sect.4) for constrained dynamics and present an involutive modification of the algorithm in [8] for computation and separation of constraints (Sect.4). This algorithm is also applicable to Lagrangian dynamical systems of polynomial type.

2 Involution of Ordinary Differential Equations

The concept of involution was invented by E.Cartan 100 years ago for systems of partial differential equations (PDEs) and led to development of powerful geometric and algebraic methods of their analysis (see historical remarks in [14, 18] and references therein). Though just for PDEs involuitive methods reveal the full power, their application to ordinary differential equations and finitely-dimensional dynamical systems is also very fruitful. The definitions taken from the formal theory of PDEs [14] and circumscribed to ODEs.

Consider a system of k ODEs of the order q with m unknown functions $y_1(x), \ldots, y_m(x)$ of the most general form

$$\mathcal{R}_q : \left\{ \Phi_j(x, y_\alpha, y_\alpha^{(1)}, \ldots, y_\alpha^{(q)}) = 0 \quad (1 \leq j \leq k) \right. \tag{1}$$

with $y_\alpha^{(i)} \equiv d^i y_\alpha / dx^i$. A *prolongation* of system (1) is the system of order $q+1$

$$\mathcal{R}_{q+1} : \left\{ \begin{array}{l} \Phi_j(x, y_\alpha, y_\alpha^{(1)}, \ldots, y_\alpha^{(q)}) = 0 \,, \\ \hat{D}\Phi_j(x, y^\alpha, y_\alpha^{(1)}, \ldots, y_\alpha^{(q)}) = 0 \,, \end{array} \right. \qquad (1 \leq j \leq k)$$

where $\hat{D}$ is the total derivation operator [2]

$$\hat{D} = \frac{\partial}{\partial x} + \sum_{i \geq 0} y_\alpha^{(i+1)} \frac{\partial}{\partial y_\alpha^{(i)}} \qquad (y_\alpha^{(0)} \equiv y_\alpha) \,.$$

Analogously, the r-th prolongation $\mathcal{R}_{q+r}$ of $\mathcal{R}_q$ is defined as enlargement of system (1) with all the total derivatives of its equations up order r inclusive.

An *integrability condition* of $\mathcal{R}_q$ is the equation of order $\leq q$ which is differential but not pure algebraic consequence of $\mathcal{R}_q$. In other words, the integrability conditions of $\mathcal{R}_q$, if they exist, are obtained by algebraic manipulations (by elimination of the derivatives of the order greater than q) over the prolonged systems.

As an example consider the following second order system in two unknowns $x(t), y(t)$

$$\left\{ \begin{array}{l} \dot{x} + y^2 = 0 \,, \\ \ddot{x} + x\,y + t\,x = 0 \,. \end{array} \right.$$

Here the integrability condition $2\,y\,\dot{y} - x\,y - t\,x = 0$ is obtained from the first prolongation by elimination of $\ddot{x}$.

A system (1) is called *involutive* if it has no integrability conditions. Thus, involutive systems have all integrability conditions incorporated in them. Enlargement of a system with its integrability conditions is *completion.* Any system can be *completed to involution* in finitely many steps by sequential prolongations and elimination [1, 14].

3 Involutive Polynomial Bases

Let $R = K[x_1, \ldots, x_n]$ be a ring of multivariate polynomials over a zero characteristic coefficient field K. Then a finite set $F = \{f_1, \ldots, f_m\} \subset R$ of polynomials in R is *a basis of the ideal*

$$< F > = < f_1, \ldots, f_m > = \{ \sum_{i=1}^{m} h_i f_i \mid h_j \in R \} \,.$$

[2] In this paper summation over repeated indices is we always assumed.

In the involutive approach to commutative (polynomial) algebra [15], which is a mapping of the involutivity analysis of linear PDEs [14, 18], for every polynomial in a finite set F the set variables $x_1, \ldots, x_n$ are separated into disjoint subsets of *multiplicative* and *nonmultiplicative* variables. To be self-consistent such a separation must satisfy some axioms [15], and every appropriate separation generates an *involutive monomial division* in the following sense. Fix a linear *admissible monomial order* $\succ$ such that $m \neq 1 \Longrightarrow m \succ 1$ and $m_1 \succ m_2 \iff m_1 m \succ m_2 m$ holds for any monomials (power products of the variables with integer exponents) m, m_1, m_2. Then for every polynomial f in F one can select its *leading monomial* $lm(f)$ (with respect to $\succ$). All leading monomials in F form a finite monomial set U. If $u \in U$ divides a monomial w such that all the variables which occur in w/u are multiplicative for u, then u is called *involutive divisor* of w. We shall denote by L an involutive division, which specifies a set of multiplicative (resp. nonmultiplicative) variables for every monomial u in any given finite monomial set U and write $u|_L w$ if u is ($L-$)involutive divisor of w. In the latter case we shall also write $w = u \times v$ where, by the above definition, monomial $v = w/u$ contains only multiplicative variables.

In papers [15, 16] a number of particular involutive divisions was introduced and studied (see also [17] for implementation issues). As an example we present here one of them called after M.Janet who was one of the founders of the involutive approach to PDEs and who devised the related separation of variables [19]. Given a finite set U of monomials in $\{x_1, \ldots, x_n\}$ and a monomial $u = x_1^{d_1} \cdots x_n^{d_n}$ in U, a variable x_i $(i > 1)$ is Janet multiplicative for u if its degree d_i in u is maximal among all the monomials in U having the same degrees in variables $x_1, \ldots, x_{i-1}$. As for x_1, it is *Janet multiplicative* for u if d_1 takes the maximal value among degrees in x_1 of monomials in U. If a variable is not Janet multiplicative for u in U it is considered as *Janet nonmultiplicative*.

Consider, for example, a monomial set $U = \{u = x_1 x_2, v = x_2 x_3^2, w = x_3^3\}$. Then we obtain the following Janet multiplicative variables for monomials in U: $\{x_1, x_2, x_3\}$ for u, $\{x_2, x_3\}$ for v and $\{x_3\}$ for w.

Given a finite polynomial set F, a noetherian [15] involutive division L, for instance, Janet division, and an admissible monomial order $\succ$, one can algorithmically construct [15, 16] a *minimal* $L-$*involutive basis* or $L-$basis $G \subset R$ of ideal $< F > = < G >$ such that for any polynomial f in the ideal there is a polynomial g in G satisfying $lm(g)|_L lm(f)$, and every polynomial g in G does not contain monomials having involutive divisors among the leading monomials of other polynomials in G.

If $F = \{f_1, \ldots, f_m\} \subset R$ is a polynomial set, L is an involutive division and $\succ$ is an admissible monomial order, then any polynomial p in R can be rewritten (reduced) modulo ideal $< F >$ as

$$p = h - \sum_{i=1}^{m} \sum_{j} a_{ij} f_i \times u_{ij} \tag{2}$$

where a_{ij} are elements (coefficients) of the base field K, u_{ij} are $L-$multiplicative monomials for $lm(f_i)$ such that $lm(f)\, u_{ij} \preceq lm(p)$ for all i, j, and there are no monomials occurring in h which have $L-$ involutive divisors among $\{lm(f_1), \ldots, lm(f_m)\}$. In this case h is said to be in the $L-$*normal form* modulo F and written as $h = NF_L(p, F)$.

If G is $L-$basis, then $NF_L(p, G)$ is uniquely defined for any polynomial p[3]. In this case $NF_L(p, G) = 0$ if and only if p belongs to the ideal $< G >$ generated by G. Moreover, if the ideal is *radical* for which any its element (polynomial) vanishes at the common roots of all the polynomials in G if and only if this polynomial belongs to the ideal, then it follows that the condition $NF_L(p, G) = 0$ is necessary and sufficient for vanishing p on those common roots.

It is important to emphasize that any involutive basis is a Gröbner basis, generally redundant, and can be used in the same manner as the reduced Gröbner basis [9, 11, 12]. We exploit this

[3] For other properties of involutive bases, proofs and illustrating examples see [15, 16].

fact in the below algorithm (Sect.5) which is the related modification of the algorithm of paper [8].

4 Dirac Method

In this section we shortly describe the computational aspects of the Dirac approach to constrained finite-dimensional Hamiltonian systems [2, 4].

Let us start with a Lagrangian $\mathcal{L}(q,\dot{q}) \equiv \mathcal{L}(q_i,\dot{q}_j)$ $(1 \le i,j \le n)$ as a function of the generalized coordinates q_i and velocities $\dot{q}_j$[4]. If the Hessian $\partial^2\mathcal{L}/\partial\dot{q}_i\partial\dot{q}_j$ has the full rank $r = n$, then the system is *regular* and it has no internally hidden constraints. Otherwise, if $r < n$, the Euler-Lagrange equations

$$\dot{p}_i = \frac{\partial \mathcal{L}}{\partial q_i} \quad (1 \le i \le n) \tag{3}$$

with

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \tag{4}$$

are *singular* or *degenerate*, as not all differential equations (3) are of the second order. There are just $n - r$ such independent lower order equations. By the Legendre transformation

$$H_c(p,q) = p_i q_i - \mathcal{L}, \tag{5}$$

we obtain the *canonical Hamiltonian* with momenta p_i defined in (4). In the degenerate case there are *primary constraints* denoted by ϕ_α, which form the *primary constraint manifold* denoted by Σ_0

$$\Sigma_0 \;:\quad \phi_\alpha(p,q) = 0 \quad (1 \le \alpha \le n - r), \tag{6}$$

Thus, the dynamics of the system is determined only on the constraint manifold (6). To take this fact into account, Dirac defined the *total Hamiltonian*

$$H_t = H_c + u_\alpha \phi_\alpha \tag{7}$$

with *multipliers* u_α as arbitrary (non-specified) functions of the coordinates and momenta. The corresponding Hamiltonian equations determine the system dynamics together with the primary constraints

$$\dot{q}_i = \{H_t, q_i\}, \quad \dot{p}_i = \{H_t, p_i\}, \quad \phi_\alpha(p,q) = 0 \;\; (1 \le i \le n,\; 1 \le \alpha \le n - r), \tag{8}$$

where the *Poisson brackets* are defined for any two functions f, g of the dynamical variables p and q as follows

$$\{f,g\} = \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i}\frac{\partial p}{\partial q_i}\,.$$

In order to be consistent with the system dynamics, the primary constraints must satisfy the conditions

$$\dot{\phi}_\alpha = \{H_t, \phi_\alpha\} \stackrel{\Sigma_0}{=} 0 \quad (1 \le \alpha \le n - r), \tag{9}$$

where $\stackrel{\Sigma_0}{=}$ stands for the equality, called *a week equality*, on the primary constraint manifold (6). The Poisson bracket in (9) must be a linear combination of the constraint functions [4]. Given a constraint function ϕ_α, the consistency condition (9), unless it is satisfied identically, may lead either to a contradiction or to a new constraint. The former case signals that the given Hamiltonian system is inconsistent. In the latter case, if the new constraint does not involve any of multipliers u_α, it must be added to the constraint set, and, hence, the constraint manifold

[4]We consider only autonomous systems, and there is no loss of generality since time t may be treated as an additional variable.

must involve this new constraint. Otherwise, the consistency condition is considered as defining the multipliers, and the constraint set is not enlarged with it.

The iteration of this consistency check ends up with the *complete set of constraints* such that for every constraint in the set condition (9) is satisfied. This is the Dirac method of the constraint computation.

It should be noted that, accordance to the definitions in Sect.2, the time derivation of constraints ϕ_α in the left hand side of (9) is their prolongation whereas elimination of the first-order derivatives is achieved by computation of the Poisson bracket in (9). The reduction to the primary constraint manifold Σ_0 in the right hand side of (9) checks whether a new independent constraint is generated.

Therefore, the Dirac method of constraint generation is just completion of system (8) to involution, and the constraints generated are nothing else than the integrability conditions.

Let now Σ be the constraint manifold for the complete set of constraints

$$\Sigma\ :\quad \phi_\alpha(p,q)=0 \quad (1\leq \alpha\leq k)\,.$$

If a constraint function ϕ_α satisfies the condition

$$\{\phi_\alpha(p,q),\phi_\beta(p,q)\} \stackrel{\Sigma}{=} 0 \quad (1\leq \beta\leq k), \tag{10}$$

it is of *the first class.* Otherwise, the constraint function is of *the second class.* The number of the second class constraints is equal to rank of the following $(k\times k)$ *Poisson bracket matrix*, whose elements must be evaluated on the constraint manifold

$$M_{\alpha\beta} \stackrel{\Sigma}{=} \{\phi_\alpha,\phi_\beta\}. \tag{11}$$

Note that matrix M has even rank because of its skew-symmetry.

If a Lagrangian system $\mathcal{L}_0(q,\dot q)$ is regular with externally imposed *holonomic* constraints $\psi_\alpha(q)=0$, the system is equivalent [20] to the singular one with Lagrangian $\mathcal{L}=\mathcal{L}_0+\lambda_\alpha\phi_\alpha$ and extra generalized coordinates λ_α. Furthermore, the Dirac method can be applied for finding the other constraints inherent in the initial regular system and, hence, not involving the extra dynamical variables.

Therefore, the problem of constraint computation and separation is reduced to manipulation with functions of the coordinates and momenta on the constraint manifold. Generally, there is no algorithmic way for such a manipulation. However, for polynomial functions all the related computations can be done algorithmically by means of involutive Gröbner bases as follows from the material of Sect.3 and shown in the next section.

5 Basic Algorithm

Here we present an algorithm which, given a polynomial Lagrangian $\mathcal{L}(q,\dot q)\in Q[q,\dot q]$ whose coefficients are rational numbers, computes the complete set of constraints and separates them into the first and second classes. The algorithm combines the Dirac method with involutive polynomial bases which, as we noted in Sect.3 are also Gröbner bases. By this reason we still call it algorithm Dirac-Gröbner as in [8].

In the sequel we assume that a polynomial ideal generated by constraints obtained from (9) is radical. This is certainly true for most of real practical problems, and the ideal generated by the primary constraints is always radical since they are linear in momenta by linearity of (4). For those cases, which are rear in occurrence, when a non-radical ideal is generated in the course of the below algorithm one can always extent the latter by inclusion of an additional subaglorithm. This subalgorithm, given a basis of the non-radical ideal, outputs an involutive basis of its radical. There are special algorithms for construction of a basis, and, hence, a Gröbner basis or involutive basis of the radical of a given ideal, which are built-in some computer algebra systems (see [9, 11, 12] for more details and references).

Algorithm Dirac-Gröbner

Input: $\mathcal{L}(q, \dot{q})$, a polynomial Lagrangian ($\mathcal{L} \in Q[q, \dot{q}]$)

Output: Φ_1 and Φ_2, sets of the first and second class constraints, respectively.

1. Computation of the canonical Hamiltonian and primary constraints:

   (a) Construct the polynomial set $F = \cup_{i=1}^{n} \{p_i - \partial\mathcal{L}/\partial\dot{q}_i\}$ in variables $p, q, \dot{q}$.

   (b) Choose a noetherian involutive division L to be fixed for the next steps and compute the $L-$ basis G of the ideal in ring $Q[p, q, \dot{q}]$ generated by F with respect to an ordering[5] which eliminates $\dot{q}$. Then compute the canonical Hamiltonian as the $L-$normal form $NF_L(H_c, G)$ of (5) modulo G.

   (c) Find the set Φ of primary constraint polynomials as $G \cap Q[p, q]$. If $\Phi = \emptyset$, then stop since the system is regular. Otherwise, go to the next step.

2. Computation of the complete set of constraints:

   (a) Take $G = \Phi$ as an $L-$basis G of the ideal generated by Φ in $Q[p, q]$ with respect to the ordering induced by that chosen at Step 1(b). Fix this ordering in the sequel.

   (b) Construct the total Hamiltonian in form (7) with multipliers u_α treated as symbolic constants (parameters).

   (c) For every element ϕ_α in Φ compute the $L-$normal form $h = NF_L(H_t, \phi_\alpha, G)$. If $h \neq 0$ and no multipliers u_β occur in it, then enlarge set Φ with h, and compute the $L-$basis G for the enlarged set.

   (d) If $G = \{1\}$, stop because the system is inconsistent. Otherwise, repeat the previous step until the consistency condition (9) is satisfied for every element in Φ irrespective of multipliers u_α. This gives the complete set of constraints $\Phi = \{\phi_1, \ldots, \phi_k\}$.

3. Separation of constraints into first and second classes:

   (a) Construct matrix M in (11) by computing the $L-$normal forms of its elements modulo G, and determine rank r of M. If $r = k$, stop with $\Phi_1 = \emptyset$, $\Phi_2 = \Phi$. If $r = 0$, stop with $\Phi_1 = \Phi$ and $\Phi_2 = \emptyset$. Otherwise, go to the next step.

   (b) Find a basis $A = \{a_1, \ldots, a_{k-r}\}$ of the null space (kernel) of the linear transformation defined by M. For every vector a in A construct a first class constraint as $a_\alpha\phi_\alpha$. Collect them in set Φ_1.

   (c) Construct $(k-r) \times k$ matrix $(a_j)_\alpha$ from components of vectors in A and find a basis $B = \{b_1, \ldots, b_r\}$ of the null space of the corresponding linear transformation. For every vector b in B construct a second class constraint as $b_\alpha\phi_\alpha$. Collect them in Φ_2.

The correctness of Steps 1, 2 and 3(a) of the algorithm is provided by the properties of $L-$bases as Gröbner bases [9, 11, 12] and by the following facts: (i) the definition (5) of the canonical Hamiltonian implies its independence of $\dot{q}$ on the primary constraint manifold (6); (ii) whenever a multiplier u_α in (7) is differentiated when the Poisson bracket in (9) is evaluated, the corresponding term vanishes on the constraint manifold. The correctness of Steps 3(b) and 3(c) follows from definition (10) of the first class constraints and the correctness of Step 3(a). The

[5] An elimination ordering which induced the degree-reverse-lexicographical one for monomials in p and q is heuristically best for efficiency reasons.

termination of algorithm Dirac-Gröbner follows from the finiteness of the $L-$basis G which is constructed at Step 2(c). The finiteness is guaranteed by noetherity of L [15, 16].

As we mentioned above, the algorithm generally needs one more step, namely, Step 2(e), where the Gröbner basis G of the radical ideal for the polynomial set Φ is computed. Next, every constraint polynomial in Φ is replaced by its $L-$normal form modulo G. All the elements with zero normal forms are eliminated from the set. One can also check the radical membership of h at Step 2(c) before its adding to Φ. This check is easily done [9, 11], but in any case Step 2, for the correctness of Step 3, must end up with the radical sets Φ and G.

To illustrate the algorithm consider an example of constrained gauge system which is known as non-Abelian Christ and Lee model [21, 22]

$$\mathcal{L} = \frac{1}{2}\,(D_t x)_i (D_t x)_i - \frac{1}{2}(x_i x_i)^2 \qquad (1 \le i, j \le 3)\,,$$

where $(D_t x)_i = \dot{x}_i + g\epsilon_{ijk} y_j x_k$ is the covariant derivative and dynamical variables x_i, y_i are the components of three-dimensional vector. The canonical Hamiltonian computed at Step 1(b) is given by

$$H_c = \frac{1}{2}\,p_i p_i - \epsilon_{ijk} y_i x_j p_k + \frac{1}{2}(x_i x_i)^2\,, \quad p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = \dot{x}_i + g\,\epsilon_{ijk} y_j x_k\,.$$

The primary constraints computed at Step 1(c) are $\{p^y_1, p^y_2, p^y_3\}$ where momenta p^y_i are canonically conjugate to y_i. The complete set of constraints computed at Step 2(c) is

$$\{p^y_1, , p^y_2, p^y_3, p_2 x_1 - p_1 x_2, p_3 x_1 - p_1 x_3, p_3 x_2 - p_2 x_3\}\,.$$

The computations of Step 3(a) give that all these constraints are of the first-class.

The version of algorithm Dirac-Gröbner based on the use of reduced Gröbner bases was implemented in Maple V Release 5 [8]. The implementation is relied on the built-in system facilities for computation and manipulation with Gröbner bases and for linear algebra. Using that Maple code for different examples from physics and mechanics, we experimentally observed that in those infrequent cases when the constraint ideals are non-radical this can easily be detected from the structure of the output set.

An efficient implementation of the involutive polynomial algorithms is in progress both in Mathematica and C, and we plan to implement the above algorithm Dirac-Gröbner in these platforms.

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