Constrained Hamiltonian Systems and Gröbner Bases*

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Abstract. In this paper we consider finite-dimensional constrained Hamiltonian systems of polynomial type. In order to compute the complete set of constraints and separate them into the first and second classes we apply the modern algorithmic methods of commutative algebra based on the use of Gröbner bases. As it is shown, this makes the classical Dirac method fully algorithmic. The underlying algorithm implemented in Maple is presented and some illustrative examples are given.

1 Introduction

The generalized Hamiltonian formalism invented by Dirac [1] for constrained systems has become a classical tool for investigation of gauge theories in physics [2,3,4], and a platform for numerical analysis of constrained mechanical systems [5]. Finite-dimensional constrained Hamiltonian systems are part of differential algebraic equations whose numerical analysis is of great research interest over last decade [6] because of importance for many applied areas, for instance, multi-body mechanics and molecular dynamics.

In physics, the constrained systems are mainly of interest for purposes of quantization of gauge theories which play a fundamental role in modern quantum field theory and elementary particle physics. Dirac devised his methods to study constrained Hamiltonian systems just for those quantization purposes. Having this in mind, he classified the constraints in the first and second classes. A first class constrained physical system possesses gauge invariance and its quantization requires gauge fixing whereas a second class constrained system does not need this. The effect of the second class constraints may be reduced to a modification of a naive measure in the path integral. The presence of gauge degrees of freedom (first class constraints) indicates that 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 [2,3,7]. In some special cases one can explicitly eliminate the unphysical degrees of freedom [8].

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Unlike physics, where constrained systems are singular, as they contain internal constraints, mechanical systems are usually regular with externally imposed constraints [9]. Such a system is equivalent to a singular one whose Lagrangian is that of the regular system enlarged with a linear combination of the externally imposed constraints whose coefficients (multipliers) are to be treated as extra dynamical variables. The latter system may reveal extra constraints for the former system providing the consistency of its dynamics.

Therefore, to investigate a constraint Hamiltonian system one has to detect all the constraints involved, and separate them, for physical models, into first and second classes. In his theory [1] Dirac gave the receipt for computation of constraints which is widely known as *Dirac algorithm*, and it has been implemented in computer algebra software [10]. However, the Dirac approach, as a method for computation of constraints, is not yet an algorithm. Even computation of the primary constraints, given a singular Lagrangian, is not generally algorithmic. Moreover, in generation of the secondary, tertiary, etc., constraints by the Dirac method one must verify if a certain function of the phase space variables vanishes on the constraint manifold. Generally, the latter problem is algorithmically unsolvable. Similarly, there are no general algorithmic schemes for separation of constraints into the first and second classes. In physical literature one can find quite a number of particular methods developed for the constraint separation (see, for example, [11,12]). But all of them have non-algorithmic defects. Thereby, being successfully applied to one constrained system, those methods may be failed for another system even of a similar type.

In practice, many constrained physical and mechanical problems are described by polynomial Lagrangians that lead to polynomial Hamiltonians. In this case, as we show in the present paper, one can apply Gröbner bases which nowadays have become the most universal algorithmic tool in commutative algebra [13] and algebraic geometry [14,15]. The combination of the Dirac method with the Gröbner bases technique makes the former fully algorithmic and, thereby, allows to compute the complete set of constraints. Moreover, the constraint separation is also done algorithmically. We show this and present the underlying algorithm which we call *algorithm Dirac-Gröbner*. This algorithm has been implemented in Maple V Release 5, and we illustrate it by examples both from physics and mechanics.

2 Dirac Method

In this section we shortly describe the computational aspects of the Dirac approach to constrained finite-dimensional Hamiltonian systems [1,3].
Let us start with a Lagrangian $L(q,\dot{q}) \equiv L(q_i,\dot{q}_j)$ $(1 \le i,j \le n)$ as a function of the generalized coordinates q_i and velocities $\dot{q}_j$ [1]. If the Hessian $\partial^2 L/\partial \dot{q}_i \partial \dot{q}_j$

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

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

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

with

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{2}$$

are *singular* or *degenerate*, as not all differential equations (1) are of the second order. There are just $n - r$ such independent lower order equations. By the Legendre transformation [2]

$$H_c(p, q) = p_i q_i - L, \tag{3}$$

we obtain the *canonical Hamiltonian* with momenta p_i defined in (2). In the degenerate case there are *primary constraints* denoted by ϕ_α, which form the *primary constraint manifold* denoted by Σ_0

$$\Sigma_0 \ : \quad \phi_\alpha(p, q) = 0 \quad (1 \leq \alpha \leq n - r), \tag{4}$$

Thus, the dynamics of the system is determined only on the constraint manifold (4). To take this fact into account, Dirac defined the *total Hamiltonian*

$$H_t = H_c + u_\alpha \phi_\alpha \tag{5}$$

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

$$\dot{q}_i = \{H_t, q_i\}, \;\; \dot{p}_i = \{H_t, p_i\}, \;\; \phi_\alpha(p, q) = 0 \;\; (1 \leq i \leq n, \; 1 \leq \alpha \leq n - r), \tag{6}$$

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

$$\{f, g\} = \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} - \frac{\partial g}{\partial p_i}\frac{\partial p}{\partial q_i}. \tag{7}$$

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

$$\dot{\phi}_\alpha = \{H_t, \phi_\alpha\} \stackrel{\Sigma_0}{=} 0 \quad (1 \leq \alpha \leq n - r), \tag{8}$$

where $\stackrel{\Sigma_0}{=}$ stands for the equality, called *a week equality*, on the primary constraint manifold (4). The Poisson bracket in (8) must be a linear combination of the constraint functions [3]. Given a constraint function ϕ_α, the consistency

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

condition (8), 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 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 (8) is satisfied. This is the Dirac method of the constraint computation. As shown in [16], the method is nothing else than completion of the initial Hamiltonian system to involution, and the constraints generated are just *the integrability conditions*. For general systems of PDEs, the completion process is done [17] by sequential prolongations and projections. For Hamiltonian systems, the time derivative of a constraint is its prolongation whereas projection of the prolonged constraint is realized in (8) by computing the Poisson bracket on the constraint manifold.

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

$$\Sigma \ : \quad \phi_\alpha(p,q) = 0 \quad (1 \leq \alpha \leq k). \tag{9}$$

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 constrains 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 $L_0(q,\dot{q})$ is regular with externally imposed *holonomic* constraints $\psi_\alpha(q) = 0$, the system is equivalent [5] to the singular one with Lagrangian $L = L_0 + \lambda_\alpha \phi_\alpha$ 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 Gröbner bases, as we show in the next section.

3 Algorithm Description

Here we describe an algorithm which, given a polynomial Lagrangian whose coefficients are rational numbers, computes the complete set of constraints and separates them into the first and second classes. The algorithm combines the above described Dirac method with the Gröbner bases technique. By this reason we call it algorithm Dirac-Gröbner. All the below used concepts, definitions and constructive methods related to Gröbner bases are explained, for instance, in textbooks [13,14,15].

At first we present the algorithm under assumption that a polynomial ideal generated by constraints is radical. This is true for most of real practical problems. Next, we indicate how to modify the algorithm to treat the most general (non-radical) case.

Algorithm Dirac-Gröbner

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

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 $F = \cup_{i=1}^{n}\{p_i - \partial L/\partial \dot{q}_i\}$ in variables $p, q, \dot{q}$.
   (b) Compute the Gröbner basis G of the ideal in ring $Q[p,q,\dot{q}]$ generated by F with respect to an ordering[3] which eliminates $\dot{q}$. Then compute the canonical Hamiltonian as the normal form of (3) 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 $G = \Phi$ for the Gröbner 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 (5) with multipliers u_α treated as symbolic constants (parameters).
   (c) For every element ϕ_α in Φ compute the normal form h of the Poisson bracket $\{H_t, \phi_\alpha\}$ modulo G. If $h \neq 0$ and no multipliers u_β occur in it, then enlarge set Φ with h, and compute the Gröbner 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 (8) 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] An elimination ordering which induced the degree-reverse-lexicographical one for monomials in p and q is heuristically best for efficiency reasons.

3. Separation of constraints into first and second classes:
   (a) Construct matrix M in (11) by computing the 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 set Φ_2.

The correctness of Steps 1, 2 and 3(a) of the algorithm is provided by the properties of Gröbner bases [13,14,15] and by the following facts: (i) the definition (3) of the canonical Hamiltonian implies its independence of $\dot{q}$ on the primary constraint manifold (4); (ii) whenever a multiplier u_α in (5) is differentiated when the Poisson bracket in (8) 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 termination of algorithm Dirac-Gröbner follows from the finiteness of the Gröbner basis G which is constructed at Step 2(c).

Now consider the most general case when the constraints obtained from (8) lead to a non-radical ideal. It should be noted that the ideal generated by the primary constraint polynomials (Step 1) is always radical. This is provided by linearity of (2) in momenta. However, already the first secondary constraint added may destroy this property of the ideal. Therefore, the algorithm 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 normal form modulo G. All the elements with zero normal forms are eliminated from the set. The extra step is also algorithmic. There are algorithms for construction of a basis, and, hence, a Gröbner basis, of the radical of a given ideal, which are built-in in some computer algebra systems (see [13,14,15] for more details and references). One can also check the radical membership of h at Step 2(c) before its adding to Φ. This check is easily done [13,14], but in any case Step 2, for the correctness of Step 3, must end up with the radical sets Φ and G.

We implemented algorithm Dirac-Gröbner, as it presented above for the radical case, in Maple V Release 5. The implementation is relied on the built-in system facilities for computation and manipulation with Gröbner bases and for linear algebra. Using our 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.

4 Examples

In this section we illustrate, by examples from physics and mechanics, the application of algorithm Dirac-Gröbner.

Example 1. $SU(2)$ Yang-Mills mechanics in $0+1$ dimensional space-time [8]. This is a constrained physical model with gauge symmetry. The model Lagrangian is given by $L = \frac{1}{2}(D_t)_i(D_t)_i$, $(D_t x)_i = \dot{x}_i + g\epsilon_{ijk}y_j x_k$ $(1 \le i,j,k \le 3)$. Here x_i and y_i are the generalized coordinates and tensor ϵ_{ijk} is antisymmetric in its indices with $\epsilon_{123} = 1$. Respectively, the primary constraints and the canonical Hamiltonian are $p^y_i = 0$ and $H_c = \frac{1}{2} - \epsilon_{ijk}x_j p_k y_i$ with the momenta given by $p^y_i = \partial L/\partial \dot{y}_i$ and $p_i = \partial L/\partial \dot{x}_i$. The other constraints in the complete set computed by the algorithm are $\phi_i = \epsilon_{ijk}x_j p_k = 0$, and all the six constraints found are of the first class.

Example 2. Point particle of mass m moving on the surface of a sphere (rigid rotator). The movement is described by the regular Lagrangian $L_0 = \frac{1}{2}m^2({\dot{q}_1}^2 + {\dot{q}_2}^2 + {\dot{q}_3}^2)/2 \equiv \frac{1}{2}m^2\dot{q}^2$ with the externally imposed holonomic constraint $\phi(q) = q^2 - 1 = 0$. This system is equivalent to the singular Lagrangian system $L = L_0 + \lambda\phi$, where λ is an extra coordinate. There is the only primary constraint $p_\lambda = 0$ $(p_\lambda = \partial L/\partial\lambda)$, and the canonical Hamiltonian is $H_c = \frac{1}{2}m^2p^2 - \lambda\phi(q)$ $(p_i = \partial L/\partial q_i)$. The complete set of constraint polynomials for the singular system contains four second class polynomials $\{p_\lambda, \phi(q), p_i q_i, 2m\lambda + p^2\}$. Coming back to the initial regular system, the first and the last polynomials in the set must be omitted since they determine the extra dynamical variables.

Example 3. Singular physical system with both first and second class constraints[4]. The system Lagrangian is $L = q_1(\dot{q}_2 - q_3) - \dot{q}_1 q_2$. There are three primary constraint polynomials $\{p_1 + q_2, p_2 - q_1, p_3\}$. The canonical Hamiltonian is $H_c = q_1 q_2$. One more constraint polynomial q_1 is found by the Dirac-Gröbner algorithm. The sets Φ_1 and Φ_2 of the first and second classes are $\{p_2 + q_1, p_3\}$ and $\{p_1 + q_2, q_1\}$, respectively. Note that this system has no physical degrees of freedom (c.f. [16]).

Example 4. Inconsistent singular system [4]: $L = \frac{1}{2}\dot{q}_1^2 + q_2$. There is the single primary constraint $p_2 = 0$. The canonical Hamiltonian is $H_c = p_1^2/2 - q_2$. At Step 2(c) of algorithm Dirac-Gröbner the inconsistency $\dot{p}_2 = 1$ occurs. The algorithm detects this inconsistency and stops.

The above examples are rather small and can be treated by hand. With our Maple code we have already tried successfully much more nontrivial examples. For instance, we computed and separated the constraints for the $SU(2)$

[4] A.Burnel. Private communication.

Yang-Mills mechanics in $3+1$ dimensional space-time [8]. Surprisingly, this computation took only a few seconds on an Pentium 100 personal computer though the model Lagrangian and the canonical Hamiltonian are rather cumbersome polynomials of the 4th degree in 21 variables.

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