Construction of adjoint symmetries for systems of second-order and mixed first- and second-order ordinary differential equations

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Abstract. We recall the notion of adjoint symmetries for second-order ordinary differential equations and sketch a recent evolution in the coordinate free description of this concept. We further indicate how the theory can be generalized to mechanical systems with non-holonomic constraints. For both cases, a theorem is presented which links a subclass of adjoint symmetries to first integrals (and Lagrangians). We then discuss how the theory can be used for a systematic construction of first integrals and how the resulting algorithm can be implemented in a computer algebra environment. The example of the last section can be used as a benchmark for testing the performance of programmes for the automatic computation of symmetries.

1 Introduction

What are adjoint symmetries and what is their potential use in the study of ordinary differential equations? For an elementary introduction to this subject, let us fix the idea by looking at the case of systems of second-order equations of the form

$$\ddot{q}^i = f^i(t, q, \dot{q}) \qquad\qquad i = 1, \ldots, n\,, \tag{1}$$

to which we can associate the partial differential operator or vector field (summation over repeated indices)

$$\Gamma = \frac{\partial}{\partial t} + \dot{q}^i \frac{\partial}{\partial q^i} + f^i(t, q, \dot{q}) \frac{\partial}{\partial \dot{q}^i}. \tag{2}$$

It is well known that the study of symmetries of differential equations is an important tool in the process of solution, or at least reduction of the problem (see e.g. [2, 10]). Many efforts have been devoted to the creation of computer algebra packages for the automatic (or "guided automatic") generation of symmetries (see [5] for a review). Roughly speaking, symmetries arise from solving the following PDE's (related to the so-called linear variational equations of (1)):

$$\Gamma^2(\mu^i) - \frac{\partial f^i}{\partial \dot q^j}\,\Gamma(\mu^j) - \frac{\partial f^i}{\partial q^j}\,\mu^j = 0, \qquad i = 1,\ldots,n\,. \tag{3}$$

Adjoint symmetries likewise correspond to solutions α_i of the adjoint equations of (3), namely

$$\Gamma^2(\alpha_i) + \Gamma\left(\frac{\partial f^j}{\partial \dot q^i}\,\alpha_j\right) - \frac{\partial f^j}{\partial q^i}\,\alpha_j = 0, \qquad i = 1,\ldots,n\,. \tag{4}$$

They are perhaps not as fundamental for the analysis of dynamical systems as symmetries are — one cannot identify a sort of direct action of adjoint symmetries on the flow of the system — but they do carry relevant information, in particular with respect to the conservation laws of the system. Specifically, the concept of adjoint symmetries provides an elegant unification of various ways of generating conserved quantities: for all systems of ordinary differential equations, there is a one-to-one correspondence between first integrals and a class of adjoint symmetries. From this point of view, one might say that the more familiar (and perhaps more appealing) duality between first integrals and symmetries, which is the content of Noether's celebrated theorem for Lagrangian systems, is mathematically speaking a mere coincidence of the fact that the availability of a Lagrangian for the system provides a mechanism for "raising the indices".

In the next two sections, we will briefly describe the theory of adjoint symmetries in its proper differential geometric setting. First we will sketch the evolution in the way we have modelled geometrically the equations (4). Secondly, we will outline a generalization of the theory to mixed systems of first- and second-order differential equations, which are important for example in the context of mechanical systems subject to non-holonomic constraints. In Sections 4 and 5, we discuss the implementation of algorithmic procedures for the construction of adjoint symmetries and for the computation of the first integrals which they may generate. The final section contains an example for which symmetries and adjoint symmetries coincide and formulates a challenge towards the computer algebra programmes for the construction of symmetries.

2 The geometrical characterization of adjoint symmetries for second-order equations

A time-dependent second-order system such as (1) is modelled by a vector field Γ on the first jet extension $J^1\tau$ of a bundle $\tau : E \to \mathbb{R}$. In natural coordinates on $J^1\tau$, Γ is of the form (2) and is characterized by the properties $\langle \Gamma, dt\rangle = 1$, $\langle \Gamma, \theta^i\rangle = 0$, where the 1-forms $\theta^i = dq^i - \dot q^i dt$ are the so-called contact forms.

In our original conception (see [11, 13]), we put the following set of 1-forms in the spotlight

$$\mathcal{X}^*_\Gamma = \Big\{\phi \in \mathcal{X}^*(J^1\tau) \mid \mathcal{L}_\Gamma\big(S(\phi)\big) = \phi - \langle \Gamma, \phi\rangle\, dt\Big\}, \tag{5}$$

where

$$S = \frac{\partial}{\partial \dot{q}^i} \otimes \theta^i \tag{6}$$

is the canonically defined *vertical endomorphism* of $J^1\tau$. Adjoint symmetries in fact were defined to be 1-forms in $\mathcal{X}^*_\Gamma$, whose Lie derivative with respect to Γ belongs to the same set. Since the dt-component of an adjoint symmetry α is irrelevant, we may as well normalize it by requiring $\langle \Gamma, \alpha \rangle = 0$ (see also [3]). An adjoint symmetry then locally has the form

$$\alpha = \alpha_i\, \omega^i + \Gamma(\alpha_i)\, \theta^i, \qquad \text{with} \quad \omega^i = d\dot{q}^i - f^i dt, \tag{7}$$

where the leading coefficients α_i precisely are solutions of the PDE's (4). An alternative way of giving a coordinate free meaning to these equations is to regard adjoint symmetries as being invariant 1-forms with the same normalization of the dt-component, i.e. 1-forms β with the property $\mathcal{L}_\Gamma \beta = 0$, $\langle \Gamma, \beta \rangle = 0$. Such forms were in fact called "Γ-basic forms" in [13] and they too are determined locally by n leading coefficients satisfying (4). There is a one-to-one correspondence between both interpretations of adjoint symmetries, determined explicitly by the type (1,1) tensor field $\mathcal{L}_\Gamma S$. For a recent full account of translations of results from one picture into the image picture under $\mathcal{L}_\Gamma S$, see [9]. Note also that Ten Eikelder [17] used the term adjoint symmetries for invariant 1-forms before, in the context of first-order (and in particular Hamiltonian) dynamics.

Whatever interpretation of adjoint symmetries on $J^1\tau$ is preferred, it should be clear that it is only the leading part of the 1-form under consideration which matters (similar things in fact can be said also about symmetries of second-order equations). A more 'economical' calculus, in which redundant parts such as the second term in (7) would not occur, may therefore be expected to focus right away on the essential operations which are important for understanding the coordinate free meaning of symmetries and adjoint symmetries. Recently, such a calculus has indeed been developed (see [6, 7, 14]) and involves, for the time-dependent framework, the theory of derivations of scalar and vector-valued forms along the projection $\pi : J^1\tau \to E$. The algebra of differential forms along π, denoted by $\bigwedge(\pi)$, consists of forms which are locally spanned by the basis of forms on E, but have their coefficients in $C^\infty(J^1\tau)$ (similarly for the $C^\infty(J^1\tau)$-module $\mathcal{X}(\pi)$ of vector fields along π). What emerges from this new calculus is that two operations are essential for the description of adjoint symmetries: a derivation ∇ of degree zero, called the *dynamical covariant derivative*, and a type (1,1) tensor field Φ, called the *Jacobi endomorphism*.

For calculational purposes, it suffices to know that the action of ∇ on forms along π is determined by the following prescriptions:

$$\nabla(F) = \Gamma(F) \quad \text{for } F \in C^\infty(J^1\tau), \qquad \nabla dt = 0, \quad \nabla\theta^i = -\Gamma^i_j\, \theta^j, \tag{8}$$

where the functions

$$\Gamma^i_j = -\frac{1}{2}\frac{\partial f^i}{\partial \dot{q}^j} \tag{9}$$

are connection coefficients of a non-linear connection which is in a natural way associated to the given dynamical system Γ. The tensor Φ has the coordinate expression

$$\Phi = \Phi^i_j \frac{\partial}{\partial q^i} \otimes \theta^j, \qquad \Phi^i_j = -\frac{\partial f^i}{\partial q^j} - \Gamma^i_k \Gamma^k_j - \Gamma(\Gamma^i_j). \tag{10}$$

We can now give a geometrical formulation of adjoint symmetries in its most economical appearance: an adjoint symmetry of Γ is an element $\alpha \in \bigwedge^1(\pi)$, of the form $\alpha = \alpha_i(t, q, \dot{q})\, \theta^i$, satisfying the equation

$$\nabla^2\alpha + \Phi(\alpha) = 0. \tag{11}$$

It is of course possible to define intrinsically a map which transforms this latter notion of adjoint symmetries into any of the original ones on the full space $J^1\tau$. For the record, let us mention that symmetries in this terminology are certain vector fields X along π, which satisfy

$$\nabla^2 X + \Phi(X) = 0, \tag{12}$$

whereby the action of ∇ on $\mathcal{X}(\pi)$ follows from the rules (8) by duality with respect to the pairing between $\mathcal{X}(\pi)$ and $\bigwedge^1(\pi)$.

Needless to say, when it comes down to doing actual calculations, working out (11) in coordinates will just bring us back to the system of PDE's (4). The main advantage and motivation for the concise coordinate free description (11) is the identification of essential geometric constructions, which will help to discover interesting special requirements which can be imposed on adjoint symmetries, and which will also be a guidance for possible generalizations such as the one we will report on in the next section.

Let us now formulate the theorem which is responsible for the link between first integrals of the given system Γ and a subclass of its adjoint symmetries. To that end, we introduce one more operator, a kind of vertical exterior derivative, which on functions $F \in C^\infty(J^1\tau)$ is defined as follows:

$$d^V F = \frac{\partial F}{\partial \dot{q}^i}\, \theta^i. \tag{13}$$

What the theorem provides in the first place is the possibility of finding a Lagrangian L for the system. But there is no guarantee that this function L will satisfy the necessary regularity condition, and in fact, from the point of view of detecting first integrals, we are most interested in the very degenerate case where L happens to be zero.

Theorem. *Let $\alpha \in \bigwedge^1(\pi)$ be an adjoint symmetry of Γ which can be written as $d^V F$ for some function F. Then, the function $L = \Gamma(F)$ (provided the matrix $\left(\partial^2 L/\partial \dot{q}^i \partial \dot{q}^j\right)$ is regular) is a Lagrangian for the given system.*

This very simple statement covers a large number of results, previously discussed in the literature, concerning the generation of first integrals of Lagrangian systems (both of Noether and of non-Noether type) and the generation of alternative Lagrangians. As indicated, the case of interest in our present survey is the situation where $\Gamma(F)$ turns out to be zero, thus yielding a first integral. Note that, conversely, if F is a first integral, then $\alpha = d^V F$ is an adjoint symmetry of Γ, so that in principle all first integrals can be obtained by going through the construction of adjoint symmetries in a systematic way. Note also that in such a case, the corresponding "Γ-basic form" β, living on $J^1\tau$, is simply the exact form dF. In the particular situation where the system is known to have a Lagrangian description with corresponding Poincaré-Cartan 2-form $d\theta_L$, the mechanism of raising indices, referred to in the introduction, is the formula $X \,\lrcorner\, d\theta_L = dF$, which associates to F a symmetry vector field X (modulo Γ), thus reproducing Noether's theorem.

3 Generalization for mixed systems of first- and second-order equations

Consider now a system of ordinary differential equations of the form

$$\ddot{q}^\alpha = f^\alpha(t, q^A, \dot{q}^\beta), \qquad \alpha = 1, \ldots, k, \tag{14}$$
$$\dot{q}^a = B^a_\alpha(t, q^A)\,\dot{q}^\alpha + B^a(t, q^A), \qquad a = 1, \ldots, m. \tag{15}$$

The main motivation for investigating such systems comes from the mechanics of Lagrangian systems with non-holonomic constraints, a subject which is very much in the spotlights nowadays (see e.g. [8, 1] and the many references therein). The equations (15) are then the constraint equations in a kind of normal form — and are indeed linear in the velocity coordinates in most practical applications — whereas the second-order equations (14) are the reduced equations which emerge after elimination of the Lagrangian multipliers. Clearly, there are two sorts of coordinates involved in the above equations: those with a Greek index are in a way the free coordinates, while the ones with a lowercase Latin index are constrained in their derivatives (the uppercase index is used to cover both sets, i.e. an index like A runs from 1 to $n = k + m$). In [12], we have presented a geometrical framework for the description of such systems which involves, among other things, an intrinsic way of constructing directly the reduced set of equations (14,15) out of a given Lagrangian on the unconstrained coordinate-velocity space and the constraints. We will limit ourselves here to a sketch of the construction of all geometrical objects which are needed to discuss adjoint symmetries, in a way which is similar to the presentation at the end of the previous section. In that respect, equations (14,15) need not necessarily be thought of as coming from non-holonomic mechanics.

The distinction between the two types of coordinates geometrically means that the configuration space E, with coordinates (t, q^A) is fibred over a manifold M with coordinates (t, q^α) and, as the notations for these coordinates indicate, both spaces are fibred over $\mathbb{R}$. We denote the corresponding bundle projections as follows: $\pi : E \to M$, $\tau_0 : M \to \mathbb{R}$ and $\tau_1 : E \to \mathbb{R}$. As a result of the given constraints (15), it is clear that only a certain submanifold of the space $J^1\tau_1$ will matter this time. Geometrically, these constraints define a connection on the bundle $\pi : E \to M$, the functions $B^a_\alpha(t, q^A)$ and $B^a(t, q^A)$ being precisely the connection coefficients. One way of interpreting such a connection is that it defines a section σ of the bundle $J^1\tau_1$ over the pull back bundle $\pi^* J^1\tau_0$, expressed in coordinates by the relations (15). We thus define our velocity-state space to be the submanifold $J^1_\sigma = \sigma(\pi^* J^1\tau_0)$ of $J^1\tau_1$. Natural local coordinates on this space are the ones coming from $\pi^* J^1\tau_0$, i.e. $(t, q^\alpha, q^a, \dot{q}^\alpha)$. There are two type (1,1) tensor fields which are well defined on it, namely

$$S = \frac{\partial}{\partial \dot{q}^\alpha} \otimes \theta^\alpha, \qquad \text{and} \qquad N = \frac{\partial}{\partial q^a} \otimes \eta^a. \tag{16}$$

The forms $\theta^\alpha = dq^\alpha - \dot{q}^\alpha dt$ are the contact 1-forms inherited from $J^1\tau_0$, the $\eta^a = dq^a - B^a_\alpha dq^\alpha - B^a dt$ can be called the constraint 1-forms.

We say that a second-order system on the manifold J^1_σ is a vector field Γ, satisfying the requirements

$$\langle \Gamma, dt \rangle = 1, \quad \langle \Gamma, \theta^\alpha \rangle = 0, \quad \langle \Gamma, \eta^a \rangle = 0. \tag{17}$$

In coordinates, such a vector field is of the form

$$\Gamma = \frac{\partial}{\partial t} + \dot q^\alpha \frac{\partial}{\partial q^\alpha} + (B^a_\beta \dot q^\beta + B^a) \frac{\partial}{\partial q^a} + f^\alpha(t, q^A, \dot q^\beta) \frac{\partial}{\partial \dot q^\alpha}, \tag{18}$$

and thus precisely models differential equations such as (14,15). Similarly to the situation in the preceding section, the vector field Γ comes with its own non-linear connection on the bundle $\rho : J^1_\sigma \to E$, the most important coefficients of which are given by

$$\Gamma^\alpha_\beta = -\frac{1}{2} \frac{\partial f^\alpha}{\partial \dot q^\beta}. \tag{19}$$

Compared to the case of pure second-order equations, the model here, in some sense, becomes richer because we now have two connections at our disposal. This time, the most economical way of giving a coordinate free description of the notions of symmetries and adjoint symmetries, will make use of elements of the 'calculus along $\rho : J^1_\sigma \to E$'. An appropriate local basis of 1-forms along ρ is given by $\{dt, \theta^\alpha, \eta^a\}$. The *dynamical covariant derivative* for this theory is found to have the following action on this basis

$$\nabla(dt) = 0, \quad \nabla\theta^\alpha = -\Gamma^\alpha_\beta\, \theta^\beta, \quad \nabla\eta^a = \frac{\partial}{\partial q^b}(B^a_\beta \dot q^\beta + B^a)\, \eta^b, \tag{20}$$

and is completely determined if we further specify that on functions F, as before, we have $\nabla(F) = \Gamma(F)$. The other important operation of the preceding section, namely the *Jacobi endomorphism*, is in fact a kind of time-component of the curvature tensor of the connection involved. It will not come as a surprise therefore, that we will distinguish two type (1,1) tensor fields in the present case, namely

$$\Phi = -\Big[X_\alpha(f^\beta) + \Gamma^\gamma_\alpha \Gamma^\beta_\gamma + \Gamma(\Gamma^\beta_\alpha)\Big] X_\beta \otimes \theta^\alpha - \frac{\partial f^\beta}{\partial q^a} X_\beta \otimes \eta^a, \quad \text{where} \quad X_\alpha = \frac{\partial}{\partial q^\alpha} + B^a_\alpha \frac{\partial}{\partial q^a}, \tag{21}$$

and

$$\Psi = C^a_\beta \theta^\beta \otimes \frac{\partial}{\partial q^a} = \Big[\mathbf{T}(B^a_\beta) - X_\beta(B^a_\alpha \dot q^\alpha + B^a)\Big]\, \theta^\beta \otimes \frac{\partial}{\partial q^a}, \tag{22}$$

where $\mathbf{T}$ is the "total time-derivative operator"

$$\mathbf{T} = \frac{\partial}{\partial t} + \dot q^\alpha \frac{\partial}{\partial q^\alpha} + (B^a_\alpha \dot q^\alpha + B^a) \frac{\partial}{\partial q^a} \tag{23}$$

which, technically speaking, is a canonically defined vector field along ρ. For more details about all these constructions, see [12].

We are now in a position to formulate the equation for adjoint symmetries, in a way similar to (11). Consider an element $\alpha \in \bigwedge^1(\rho)$ which is of the form

$$\alpha = \overline{\alpha} + \tilde\alpha = a_\alpha \theta^\alpha + c_a \eta^a. \tag{24}$$

Note that both terms in this splitting of α have an intrinsic meaning. We say that such an α is an adjoint symmetry of Γ if it satisfies:

$$\nabla^2\overline{\alpha} - \nabla\tilde{\alpha} + (\Phi + \Psi)(\alpha) = 0. \tag{25}$$

Explicitly, this condition gives rise to the following system of mixed first- and second-order PDE's for the unknown coefficients a_α and c_a:

$$\Gamma^2(a_\alpha) = 2\Gamma(a_\beta\Gamma^\beta_\alpha) + a_\beta X_\alpha(f^\beta) - c_a C^a_\alpha, \tag{26}$$

$$\Gamma(c_a) = -a_\alpha\frac{\partial f^\alpha}{\partial q^a} - c_b\frac{\partial}{\partial q^a}(B^b_\alpha\dot{q}^\alpha + B^b). \tag{27}$$

Not surprisingly, these are also the equations which characterize the invariance under Γ of a certain 1-form on the space J^1_σ. If, by analogy with (13), we define for every $F \in C^\infty(J^1_\sigma)$

$$d^V F = \frac{\partial F}{\partial \dot{q}^\alpha}\,\theta^\alpha + \frac{\partial F}{\partial q^a}\,\eta^a, \tag{28}$$

then one can easily prove the following result.

Theorem. *Let $\alpha \in \bigwedge^1(\rho)$ be an adjoint symmetry of Γ which can be written as $d^V F$ for some function F. Then, the function $L = \Gamma(F)$ (provided the matrix $\left(\partial^2 L/\partial\dot{q}^\alpha\partial\dot{q}^\beta\right)$ is regular) is a Lagrangian for the given system.*

What is meant here by a Lagrangian for a system of equations such as (14,15), is that the second-order equations in fact are not coupled with the first-order ones and are equivalent to the Euler-Lagrange equations coming from a function $L(t, q^\alpha, \dot{q}^\alpha)$. Needless to say, we are at the moment more interested in the degenerate case of this theorem where $\Gamma(F)$ turns out to be zero: we then find a first integral of the equations (14,15) without an implication on some form of decoupling.

To conclude this survey of the theory, let us mention that work is in progress concerning a further generalization to the case of non-linear constraints, say of the form

$$\dot{q}^a = g^a(t, q^A, \dot{q}^\alpha). \tag{29}$$

Without going into details of the geometry of the problem, it looks like most results will have a straightforward generalization in the sense that they may even look formally identical, provided we make the following identifications

$$B^a_\alpha = \frac{\partial g^a}{\partial \dot{q}^\alpha}, \qquad B^a = g^a - B^a_\beta\,\dot{q}^\beta. \tag{30}$$

4 An algorithmic procedure for the construction of adjoint symmetries

Solving PDE's such as (4) or (26,27) in all generality is quite impossible, but it is usually fairly easy to obtain a few particular solutions, especially the ones for which the unknown functions are assumed to be independent of the velocity coordinates. In the context of symmetries, such a simplification would amount to constructing the point symmetries of the system. The reason why it is generally easy to do this, even by hand, is in the first place that in most practical applications, the right-hand sides f^i or f^α of the given equations will have a polynomial dependence on the velocities. As a result, coefficients of independent monomials in the PDE's under consideration have to be put separately equal to zero, yielding an overdetermined system of linear partial differential equations which becomes quite manageable. Under the same assumption on the given f^i or f^α, it is clear that one may gradually venture the construction of more complicated particular solutions, by allowing the unknown functions to have a higher-degree polynomial dependence on the velocities. In principle, this process could be carried out step by step so that at least the adjoint symmetries (or symmetries) with such a polynomial structure could be constructed in an algorithmic way. Obviously, however, with increasing degree of the polynomial expressions and increasing number of degrees of freedom, the number of conditions to be tackled rapidly grows out of hand and the only hope to pursue the procedure beyond the first step is assistance of computer algebra.

There are clearly two distinct steps which need to be implemented: the first one is 'setting up the determining equations', the second one is 'solving these equations'.

Setting up the determining equations requires a procedure which should take care of the following manipulations. After loading the data of the given system, the user should simply choose a number, reflecting the ansatz concerning the degree of polynomial dependence of the unknown coefficients of an adjoint symmetry. The programme should then take over to create the required polynomial expressions, substitute them in the master equations (4) or (26,27), single out the coefficients of all independent monomials in each of these equations and finally make a list of all resulting expressions which, when put equal to zero, will make up the set of determining equations. It is certainly helpful if this final list is put together in a clever way, meaning that the coefficients of the highest degree terms of all master equations should be on top of the list, because they usually constitute the simplest equations which one would normally solve first.

It does not really require much programming skill to write procedures which take care of such manipulations of expressions: it can all be done at the algebraic level of the computer algebra package. We have previously written such a programme in REDUCE and reported on it in [15]. That little programme, however, could greatly benefit from an update. For a start, the REDUCE environment has evolved of course, and this would allow to make the interaction with the programme more user friendly. Secondly, the old version is based on the calculus of differential forms on the full space $J^1\tau$ and makes use for that purpose of Schruefer's user package EXCALC. We would prefer to make an update which more closely links up with the calculus along $\pi : J^1\tau \to E$. Afterall, it should not be difficult to implement the action of the operators ∇ and Φ on forms and vector fields along π, the way they are determined by (8–10). There is then no need to load EXCALC first. Finally, we of course would like to build in the possibility of treating also mixed first- and second-order equations, along the lines of the theory sketched in the previous section.

Solving the determining equations is an entirely different matter and does require a great deal of programming expertise. Fortunately, the nature of this problem for adjoint symmetries is exactly the same as the corresponding one for symmetries. One may therefore hope that the many efforts which have been devoted to solving the determining equations for symmetries (see the review [5]) need not be duplicated for the study of adjoint symmetries. All one really wants is an interface which allows stepping in with ones own determining equations at the level of the solving routines of the existing software for symmetries. At the time of the submission of [15], the only programme which had such an interface (to our knowledge) was Head's muMATH package LIE (see [4]), the latest update of which is version 4.4. Since then, the situation has improved and we know at least of the REDUCE package DIMSYM by Sherring [16] which offers the same facilities and performs well. We would hope that there are similar developments in the other popular symbolic software packages.

As a final remark towards the expert programmers: it seems to me that an interesting tool for the user of the solving routines would be an option to specify that a certain set of the unknown functions should not simultaneously become zero. The reason is clear: we want to start searching for the simplest adjoint symmetries first and then gradually step up the level of complexity by increasing the degree of polynomial dependence on the velocities. In doing so, it is of course a waste of time if the programme repeats constructing the earlier obtained solutions all the time.

5 The construction of first integrals

As a preliminary remark, it should be observed that the construction of first integrals which have a polynomial structure does not necessarily require an approach via adjoint symmetries. In fact, the equation $\Gamma(F) = 0$ could itself be regarded as the master equation, from which one could generate determining equations much in the same way as explained in the previous section. However, our general theorem about the subclass of adjoint symmetries which are of the form $d^V F$ tells us that other interesting information might be obtained from adjoint symmetries. We may thus as well aim at setting up procedures which will test the possible generation of first integrals or Lagrangians at the same time. Here, we are again facing problems which anyone can implement in the computer algebra package of his choice.

A REDUCE-programme for running such tests and for the actual computation of the first integral or Lagrangian if the test is positive, was also presented in [15]. The same remark applies, however, concerning the need of an update which incorporates the generalizations of Section 3 and runs outside the EXCALC environment. So, let us take the situation of Section 3 to indicate briefly how such a programme can be conceived. Obviously, the first few steps will prompt the user to provide the data of the given system and of some candidate for an adjoint symmetry, either interactively or via an input file. In our present situation, the data of the system will consist of the dimensions k and m of the equations (14,15) and of the functions f^α, B^a_α, B^a in their right-hand sides. The data of an adjoint symmetry will be the coefficient functions a_α and c_a of the 1-form (24), which have been obtained via the methods described in the previous section. It cannot harm then to test first of all whether these data make sense, i.e. to verify whether the a_α, c_a satisfy the master equations (26,27). Such a test is easy to implement.

The next step is to test for the existence of a function $F(t, q^A, \dot{q}^\alpha)$, such that

$$a_\alpha = \frac{\partial F}{\partial \dot{q}^\alpha}, \qquad c_a = \frac{\partial F}{\partial q^a}. \tag{31}$$

Formally, this amounts to thinking of a 1-form which looks like $a_\alpha \, d\dot{q}^\alpha + c_a \, dq^a$, and verifying that it is closed, with the coordinates (t, q^α) treated as parametric variables. If the test turns out to be positive, the programme should say so, but should at the same time proceed to compute a corresponding function F. This can in general be done by instructing the following formula for this computation:

$$F = \dot{q}^\alpha \int_0^1 a_\alpha(t, q^\beta, sq^a, s\dot{q}^\beta) ds + q^a \int_0^1 c_a(t, q^\beta, sq^b, s\dot{q}^\beta) ds. \tag{32}$$

There are cases where this formula will not be appropriate, for example when the integrands have a singularity at the origin in the $(q^a, \dot{q}^\alpha)$ coordinates. But there are also more innocent situations in which the machine might fail to work out the integral. It will then normally be very simple to intervene and do the calculation by hand, starting from the relations (31). Once an F has been computed, the computer will certainly be happy to tell you what the corresponding function $L = \Gamma(F)$ looks like. At this point, an extra routine must be called upon to see whether we are in the situation of a first integral. Indeed, it is clear that a function F for which (31) holds is not unique and is in fact determined by (32) to within an arbitrary function f of the parametric coordinates (t, q^α). It may thus well be that $\Gamma(F)$ is not zero, even though we are in the favourable circumstances for finding a first integral. This will be the case if and only if a function $f(t, q^\alpha)$ exists, such that $\Gamma(F - f) = 0$. This in turn is equivalent to saying that $L = \Gamma(F)$ is a total time derivative and, as is well known from the calculus of variations, a necessary and sufficient condition for this to be true, is that L sits in the kernel of the Euler-Lagrange operator. In conclusion, the final stage in the automated process will be to test whether we have

$$\frac{\partial L}{\partial q^a} \equiv 0, \quad \text{and} \quad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^\alpha}\right) - \frac{\partial L}{\partial q^\alpha} \equiv 0. \tag{33}$$

If the answer is yes, we know that there exists a function $f(t, q^\alpha)$ such that

$$\frac{\partial f}{\partial q^\alpha} = \frac{\partial L}{\partial \dot{q}^\alpha}, \qquad \frac{\partial f}{\partial t} = L - \dot{q}^\beta \frac{\partial L}{\partial \dot{q}^\beta}. \tag{34}$$

Hence, f can be computed via the formula

$$f = q^\alpha \int_0^1 \frac{\partial L}{\partial \dot{q}^\alpha}(st, sq^\beta) \, ds + t \int_0^1 \left(L - \dot{q}^\alpha \frac{\partial L}{\partial \dot{q}^\alpha}\right)(st, sq^\beta) \, ds \tag{35}$$

and the first integral is given by $F - f$.

6 A benchmark example

For an instructive and illustrative example, we go back to the case of pure second-order equations as discussed in Section 2. Consider the following system with three degrees of freedom, which physically could represent the motion of a charged particle in some rather special magnetic field:

$$
\begin{aligned}
\ddot{q}^1 &= -q^1\dot{q}^3 && (36)\\
\ddot{q}^2 &= -q^2\dot{q}^3 && (37)\\
\ddot{q}^3 &= q^1\,\dot{q}^1 + q^2\,\dot{q}^2. && (38)
\end{aligned}
$$

This system in fact is self-adjoint, so that the equations (3) for symmetries and (4) for adjoint symmetries coincide. As a result, the example is well suited as a test case for existing packages for the construction of symmetries. A Lagrangian for the system is given by

$$
L = \frac{1}{2}\left[(\dot{q}^1)^2 + (\dot{q}^2)^2 + (\dot{q}^3)^2\right] - \frac{1}{2}\dot{q}^3\left[(q^1)^2 + (q^2)^2\right]. \qquad (39)
$$

Presumably, every computer algebra programme for the determination of symmetries will be happy to tell us that the system has 4 independent point symmetries corresponding to the following generators (only their leading parts are listed):

$$
\begin{aligned}
X_1 &= \frac{\partial}{\partial t} && (40)\\
X_2 &= q^2\frac{\partial}{\partial q^1} - q^1\frac{\partial}{\partial q^2} && (41)\\
X_3 &= \frac{\partial}{\partial q^3} && (42)\\
X_4 &= t\frac{\partial}{\partial t} - q^1\frac{\partial}{\partial q^1} - q^2\frac{\partial}{\partial q^2} - q^3\frac{\partial}{\partial q^3}. && (43)
\end{aligned}
$$

If we were to regard these as adjoint symmetries and submit them to the tests for the generation of first integrals (or Lagrangians), we would obtain the following results: the first three generators give rise to the following first integrals (which reflects that they are actually Noether symmetries with respect to the Lagrangian (39)),

$$
\begin{aligned}
F_1 &= \frac{1}{2}\left[(\dot{q}^1)^2 + (\dot{q}^2)^2 + (\dot{q}^3)^2\right] && (44)\\
F_2 &= q^2\,\dot{q}^1 - q^1\,\dot{q}^2 && (45)\\
F_3 &= \dot{q}^3 - \frac{1}{2}\left[(q^1)^2 + (q^2)^2\right], && (46)
\end{aligned}
$$

whereas the fourth one produces a Lagrangian, which is however simply a constant multiple of the one we already know.

Suppose now we move to the next step in our algorithmic process, namely the computation of symmetries (or adjoint symmetries) with leading coefficients which are of degree 1 in the velocities. A preliminary remark is in order here. It is well known that symmetry generators fall into equivalence classes modulo multiples of the given dynamical vector field and that one can use this freedom to pick out a representative in each class having zero $\partial/\partial t$ component. Explicitly, this amounts to replacing a generator like

$$X = \tau \frac{\partial}{\partial t} + \xi^i \frac{\partial}{\partial q^i} + \cdots \quad \text{by} \quad X = (\xi^i - \dot{q}^i \tau) \frac{\partial}{\partial q^i} + \cdots \ .$$

Up to now, this transition was tacitly assumed in our theoretical discussion: with reference to the PDE's (4), for example, the functions μ^i would precisely correspond to $\xi^i - \dot{q}^i\tau$. If the ansatz about the polynomial degree concerns the μ^i, it is clear that the generators X_1 and X_4 would in fact turn up only at the stage of 'leading coefficients, linear in the velocities'. It is, however, just as easy to implement the step by step generation of determining equations with respect to the components τ and ξ^i and this is the approach we will continue here.

Now, a little bit of thinking reveals that we should be able to find at least 12 generators at the stage of (τ, ξ^i) which are of degree 1. Indeed, the product of a symmetry generator with a first integral is again a symmetry generator and we have found two first integrals, F_2 and F_3 which are themselves linear in the velocities. Therefore, not only should we recover the 4 point symmetries, but also 8 new generators, obtained from them via multiplication with either F_2 or F_3. The question is: "Are there more than these 12 generators at that stage?".

It is our feeling that finding these 12 generators — which a theoretician will know without further computations — without interference of the user of the package, is a good challenge for the authors of code for the automatic generation of symmetries. We used this benchmark while testing beta-versions of Sherring's DIMSYM. In the end, this programme gloriously passed the test and produced in effect 13 generators. The surprise one reads:

$$X_{13} = 2t(F_3\, X_2 - F_2\, X_3) + 2(2\dot{q}^1 + q^1 q^3)\frac{\partial}{\partial q^2} - 2(2\dot{q}^2 + q^2 q^3)\frac{\partial}{\partial q^1}. \tag{47}$$

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