An introduction to symmetry methods in the solution of differential equations that occur in chemistry and chemical biology

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Synopsis

This paper is a short overview of the main ways in which symmetries can be used to obtain exact information about differential equations. It is written for a general scientific audience; readers do not need any previous knowledge of symmetry methods. The information yielded by symmetry methods may include the general solution of a given differential equation, special 'invariant solutions' (such as similarity solutions), and conservation laws. Several symmetry methods have been implemented as computer algebra packages, which can be used by nonspecialists.

Towards the end of the paper, there is a brief outline of some recent developments in symmetry methods that await translation into symbolic algebra.

Key words

Symmetry, differential equation, computer algebra, difference equation, invariant.

1 Introduction

In the second half of the 19th century, the Norwegian mathematician Sophus Lie began to create a remarkable body of work that unified virtually all known methods of solving differential equations. He discovered that symmetries of differential equations can be found and exploited systematically. Over many years,

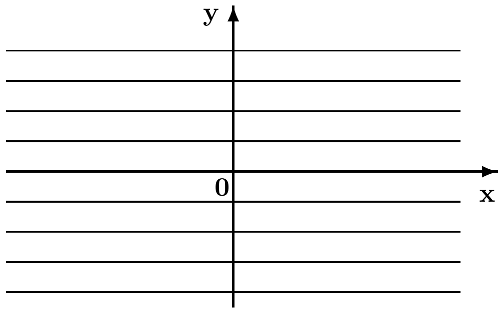

Figure 1: Some solutions of $y' = 0$.

considerable research effort has been directed at understanding the elegant algebraic structure of symmetry groups, but Lie's methods for determining and using symmetries were largely neglected until fairly recently. With the advent of powerful symbolic computation packages, it has become possible to apply Lie's methods to explore the symmetries and conservation laws of a wide range of physical systems.

This article is a straightforward introduction to symmetry methods. Simple examples are used to illustrate each of the major ideas; indeed, §2 is devoted to the simplest of all differential equations. The majority of the article is contained in §3, which deals with the problem of finding symmetries, and §4, which describes various ways of using symmetries. Some extensions of these themes are given in §5, and §6 is a brief description of some newly-developed methods that have not yet been implemented as symbolic packages.

The article concludes with some suggestions for further reading.

2 Symmetries of the simplest differential equation

Some important concepts in symmetry methods can be explained with the aid of the simplest differential equation,

$$y' = 0. \tag{1}$$

The solutions of this ordinary differential equation (ODE) can be represented on the (x, y) plane by the parallel straight lines $y = c$, as shown in Fig. 1. (Here and throughout the paper, arbitrary constants are denoted by c or c_i.)

Roughly speaking, a *point symmetry* of an ODE is a smooth invertible mapping Γ of the (x, y) plane to itself, that maps every solution of the ODE to a solution. Here are some examples of symmetries of (1):

1. reflection in the x-axis, $\Gamma_1 := (x, y) \mapsto (x, -y)$, which maps the solution $y = c$ to the solution $y = -c$;

2. translations in the x-direction, $\Gamma_2 := (x, y) \mapsto (x + \epsilon, y)$, each of which maps each solution to itself;

3. translations in the y-direction, $\Gamma_3 := (x, y) \mapsto (x, y + \epsilon)$, which map the solution $y = c$ to the solution $y = c + \epsilon$.

These are not the only symmetries of the ODE (1) – in fact, there are infinitely many. However, each of the above represents an important aspect of symmetries. First note that Γ_1 maps almost every solution to a different solution; the only exception is $y = 0$, which is mapped to itself. Any solution that is mapped to itself by a symmetry is said to be *invariant*. Translations in the x-direction move points along solution curves, so every solution is invariant. Symmetries that map every solution to itself are called *trivial symmetries*. By contrast, translations in the y-direction map each solution to a different solution.

The translations Γ_2 and Γ_3 each depend on a continuous parameter, ϵ. In each case, $\epsilon = 0$ corresponds to the identity map. These are examples of *Lie point symmetries*. By contrast, Γ_1 does not depend on a continuous parameter; therefore it is said to be a *discrete symmetry*.

The set of all solutions of the ODE can be obtained by finding all solutions in the upper half-plane, and then applying the reflection Γ_1 to each of these solutions. (This yields the set of solutions in the lower half-plane.) A more efficient way to generate all solutions is to find *one* solution and then apply all possible translations Γ_3, allowing ϵ to vary over the real numbers. In this way the dimension of the problem is reduced by one. Instead of having to find a one-parameter family of solutions, we need only find a single solution. This idea is at the heart of symmetry methods for ODE's.

Note that the trivial symmetries Γ_2 do not reduce the number of solutions that we have to find. For this reason, trivial symmetries are of no use to us.

Point symmetries are examples of *point transformations*, which are transformations of the independent and dependent variables. There may also be symmetries that depend additionally on derivatives of the dependent variables. These symmetries are usually less obvious than point symmetries, but they can still be very useful.

3 The linearized symmetry condition

This section describes how to obtain Lie symmetries of a given scalar differential equation. (For brevity, we do not consider systems of differential equations, but everything in the remainder of this paper is applicable to systems as well as scalar equations.) Consider the problem of finding the Lie point symmetries of the ODE

$$y^{(n)} = \omega\left(x, y, y', \ldots, y^{(n-1)}\right). \tag{2}$$

Let us seek conditions under which a smooth invertible mapping

$$\Gamma : (x, y) \mapsto \big(\hat{x}(x, y),\ \hat{y}(x, y)\big)$$

is a symmetry of the ODE. Let $y = f(x)$ be a curve in the (x, y) plane. The image of this curve under the mapping Γ is the parametric curve

$$\hat{y} = \hat{y}(x, f(x)), \qquad \hat{x} = \hat{x}(x, f(x)).$$

In regions in which the second of these equations is invertible, there exists a function $\tilde{f}$ such that $\hat{y} = \tilde{f}(\hat{x})$. It is usual to identify the $(\hat{x}, \hat{y})$ plane with the (x, y) plane; thus the image of the curve $y = f(x)$ is $y = \tilde{f}(x)$.

The mapping Γ is a symmetry of the ODE if each solution is mapped to a solution. Therefore $y = \tilde{f}(x)$ satisfies (2) whenever $y = f(x)$ does. Equivalently,

$$\hat{y}^{(n)} = \omega\left(\hat{x}, \hat{y}, \hat{y}', \ldots, \hat{y}^{(n-1)}\right) \qquad \text{when (2) holds.} \tag{3}$$

This equation is called the *symmetry condition* for the ODE (2). In principle, the symmetry condition can be solved by writing out the derivatives of $\hat{y}$ with respect to $\hat{x}$ in full, For instance,

$$\hat{y}' = \frac{\mathrm{d}\hat{y}}{\mathrm{d}\hat{x}} = \frac{\hat{y}_x + y'\hat{y}_y}{\hat{x}_x + y'\hat{x}_y}\,.$$

(The subscripts x and y denote partial derivatives with respect to these variables.) For higher derivatives, the expressions are much messier, and it is hard to solve the symmetry condition for the unknown functions $\hat{x}(x, y)$ and $\hat{y}(x, y)$.

The problem of solving the symmetry condition becomes very much easier if we restrict attention to one-parameter local Lie groups of point symmetries that are near-identity transformations of the plane. These *Lie point symmetries* of a given ODE (2) are symmetries for which

$$\begin{aligned} \hat{x} &= x + \epsilon\xi(x, y) + O(\epsilon^2), \\ \hat{y} &= y + \epsilon\eta(x, y) + O(\epsilon^2). \end{aligned} \tag{4}$$

Here ϵ is a real parameter, and the Lie symmetries are defined for each ϵ sufficiently close to zero. The set of points $(\hat{x}, \hat{y})$ that can be reached from (x, y) by varying ϵ is called the *orbit* through (x, y); Fig. 2 illustrates part of a typical orbit. By substituting (4) into the symmetry condition (3) and expanding the result in powers of ϵ, it is possible to derive a linear partial differential equation (PDE) for $\xi(x, y)$ and $\eta(x, y)$. This PDE is called the *linearized symmetry condition* (LSC).

Perhaps surprisingly, once the LSC has been solved, the Lie point symmetries can be calculated to all orders in ϵ. To do this, define the *infinitesimal generator* of the Lie symmetries to be the first-order partial differential operator

$$X = \xi(x, y)\frac{\partial}{\partial x} + \eta(x, y)\frac{\partial}{\partial y}\,.$$

This operator can be interpreted as the tangent vector field (at $\epsilon = 0$) to the orbits of (4), as illustrated in Fig. 2. Consequently $(\hat{x}, \hat{y})$ are solutions of the initial-value problem

$$\frac{\mathrm{d}\hat{x}}{\mathrm{d}\epsilon} = \xi(\hat{x}, \hat{y}), \qquad \frac{\mathrm{d}\hat{y}}{\mathrm{d}\epsilon} = \eta(\hat{x}, \hat{y}), \qquad (\hat{x}, \hat{y}) = (x, y) \text{ when } \epsilon = 0.$$

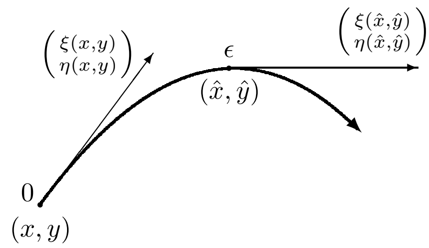

Figure 2: Part of the orbit through (x, y), showing the tangent vectors at $\epsilon = 0$ and at a general value of ϵ.

The solution to this problem can be expressed as a power series, as follows:

$$\hat{x} = e^{\epsilon X} x, \qquad \hat{y} = e^{\epsilon X} y,$$

where

$$e^{\epsilon X} = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!} X^n.$$

Thus, once we know X, it is possible to calculate $(\hat{x}, \hat{y})$; in other words, the orbits can be found.

For nontrivial symmetries, most orbits are curves that are transverse to solution curves, so that points on one solution curve will be mapped onto different solution curves. There are two important exceptions. A point (x, y) on the plane is fixed by the Lie symmetries if and only if the infinitesimal generator is zero there, i.e.

$$\xi(x, y) = \eta(x, y) = 0.$$

Points that satisfy this condition are called *invariant points*; each one is a zero-dimensional orbit.

The other exception occurs when an orbit coincides with a solution curve. As the orbit is determined by the infinitesimal generator, we can write this as a condition on $\xi(x, y)$ and $\eta(x, y)$, as follows. The *characteristic* of the Lie symmetries (4) is the function

$$Q(x, y, y') = \eta(x, y) - \xi(x, y)\, y', \tag{5}$$

which is zero wherever the tangent to a curve $(x, y(x))$ is parallel to the tangent to the orbit. Any curve on which Q vanishes is invariant under the Lie symmetries.

Example 1 The Lie symmetries of the ODE

$$y' = \frac{y^3 + x^2 y - y - x}{xy^2 + x^3 + y - x} \tag{6}$$

include the rotations about the origin,

$$(\hat{x}, \hat{y}) = (x \cos\epsilon - y \sin\epsilon,\ x \sin\epsilon + y \cos\epsilon),$$

which are generated by

$$X = -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\,.$$

Note that the only invariant point is the origin. The characteristic is

$$Q(x, y, y') = x + yy',$$

which vanishes on the circles $x^2 + y^2 = c$. The invariant solutions of the ODE are the common solutions of $Q(x, y, y') = 0$ and the ODE; there is only one such solution, namely

$$x^2 + y^2 = 1.$$

If the Lie symmetries of the ODE (2) are trivial, the characteristic vanishes on every solution. It is possible to factor out the trivial symmetries by insisting that $\hat{x} = x$. The following result enables us to do this without losing any generality.

Theorem 1 *The Lie point symmetries (4) of the ODE (2) are equivalent (up to a trivial symmetry) to the following* dynamical symmetries*:*

$$\begin{aligned} \hat{x} &= x, \\ \hat{y} &= y + \epsilon Q(x, y, y') + O(\epsilon^2), \end{aligned} \tag{7}$$

where $Q(x, y, y') = \eta(x, y) - \xi(x, y)y'$.

Generally speaking, dynamical symmetries are not point symmetries, because $\hat{y}$ depends on y'. However, when (7) is substituted into the symmetry condition, it yields the same LSC as (4). It turns out that (7) is easier to work with than (4); moreover, this formulation is easily extended to other types of symmetry.

To calculate the LSC for the ODE (2), we must calculate the derivatives of $\hat{y}$ with respect to $\hat{x}$. Define the *total derivative* with respect to x, restricted to solutions of the ODE, to be the operator

$$D_x = \frac{\partial}{\partial x} + y'\frac{\partial}{\partial y} + y''\frac{\partial}{\partial y'} + \ldots + \omega\left(x, y, y', \ldots, y^{(n-1)}\right)\frac{\partial}{\partial y^{(n-1)}}\,.$$

Then, letting Q denote $Q(x, y, y')$ (on solutions of the ODE),

$$\frac{\mathrm{d}\hat{y}}{\mathrm{d}\hat{x}} = \frac{\mathrm{d}\hat{y}}{\mathrm{d}x} = D_x\hat{y} = y' + \epsilon D_x Q + O(\epsilon^2).$$

Similarly, on solutions of the ODE,

$$\hat{y}^{(k)} = \frac{\mathrm{d}^k\hat{y}}{\mathrm{d}\hat{x}^k} = y^{(k)} + \epsilon(D_x)^k Q + O(\epsilon^2). \qquad k = 1, 2 \ldots.$$

By substituting these results into the symmetry condition, and looking only at the terms that are first-order in ϵ, we derive the LSC:

$$(D_x)^n Q - \omega_{y^{(n-1)}}(D_x)^{n-1}Q - \omega_{y^{(n-2)}}(D_x)^{n-2}Q - \ldots - \omega_y Q = 0. \qquad (8)$$

If $n \geq 2$ then the LSC depends upon $y', y'', \ldots, y^{(n-1)}$, whereas ξ and η are independent of these variables. Therefore (8) can be split into an overdetermined system of PDEs, as the following simple example shows.

Example 2. Consider the ODE $y'' = 0$. The total derivative operator is

$$D_x = \frac{\partial}{\partial x} + y'\frac{\partial}{\partial y},$$

and therefore the LSC is

$$Q_{xx} + 2y'Q_{xy} + y'^2 Q_{yy} = 0.$$

By substituting (5) into the LSC, and splitting the resulting equation into powers of y', we obtain the overdetermined system

$$\eta_{xx} = 0, \qquad 2\eta_{xy} - \xi_{xx} = 0, \qquad \eta_{yy} - 2\xi_{xy} = 0, \qquad \xi_{yy} = 0.$$

The general solution of this system is

$$\begin{aligned} \xi(x,y) &= c_1x^2 + c_2xy + c_3x + c_4y + c_5, \\ \eta(x,y) &= c_1xy + c_2y^2 + c_6x + c_7y + c_8. \end{aligned}$$

Therefore every infinitesimal generator of Lie point symmetries of $y'' = 0$ is a linear combination of

$$X_1 = x^2\frac{\partial}{\partial x} + xy\frac{\partial}{\partial y}, \qquad X_2 = xy\frac{\partial}{\partial x} + y^2\frac{\partial}{\partial y}, \qquad X_3 = x\frac{\partial}{\partial x}, \qquad X_4 = y\frac{\partial}{\partial x},$$

$$X_5 = \frac{\partial}{\partial x}, \qquad X_6 = x\frac{\partial}{\partial y}, \qquad X_7 = y\frac{\partial}{\partial y}, \qquad X_8 = \frac{\partial}{\partial y}.$$

The process used above can also be applied to more complicated ODEs. The basic step of splitting the LSC into an overdetermined system is easily accomplished with the aid of computer algebra. Hereman [1] reviews a wide variety of packages for doing this. Some packages also use various heuristics to try to solve the overdetermined system. A nicer approach uses differential algebra to simplify the overdetermined system first [2]. Within the computer algebra system Maple [3], for example, this can be done by using the package `rifsimp`, which reduces the system to a simple 'involutive' form [4].

Example 3. In this example, we use Maple to find the Lie point symmetries of the nonlinear ODE

$$y'' = y'/y^2.$$

The symmetries can be found very quickly with a few lines of Maple code, which are listed in the Appendix. It is instructive to follow the solution process in some detail. The LSC is

$$(D_x)^2 Q - \frac{1}{y^2} D_x Q + \frac{2y'}{y^3} Q = 0,$$

where

$$D_x = \frac{\partial}{\partial x} + y' \frac{\partial}{\partial y} + \frac{y'}{y^2} \frac{\partial}{\partial y'} \, .$$

As before, the LSC is split into a system of PDEs by equating terms that have the same dependence on y'. The overdetermined system that results from this process is

$$\begin{aligned} y^3 \eta_{xx} - y\eta_x &= 0, \\ 2y^3 \eta_{xy} - y^3 \xi_{xx} - y\xi_x + 2\eta &= 0, \\ y^3 \eta_{yy} - 2y^3 \xi_{xy} - 2y\xi_y &= 0, \\ y^3 \xi_{yy} &= 0. \end{aligned}$$

This rather untidy system is reduced by `rifsimp` to the equivalent form

$$\eta_x = 0, \qquad \xi_x = 2\eta/y, \qquad \eta_y = \eta/y, \qquad \xi_y = 0,$$

which is easily solved:

$$\xi = 2c_1 x + c_2, \qquad \eta = c_1 y.$$

Therefore the symmetry generators are linear combinations of

$$X_1 = 2x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} \, , \qquad X_2 = \frac{\partial}{\partial x} \, .$$

The Maple code listed in the Appendix is adapted from the documentation for `rifsimp`. It is short and simple, and is easily changed to determine symmetries of other ODEs. Newcomers to symmetry methods who have access to Maple may wish to experiment by trying to find symmetries of various ODEs of order two or more. Readers with other computer algebra systems should consult their documentation for help on finding symmetries. Hereman's review [1] covers most of the add-on packages that are available.

So far we have focused on ODEs. However, the same approach can be used to find Lie symmetries of PDEs. For simplicity, we shall restrict attention to PDEs with one dependent variable, u, and two independent variables, x and t. Then the infinitesimal generator of Lie point symmetries is of the form

$$X = \xi(x,t,u)\frac{\partial}{\partial x} + \tau(x,t,u)\frac{\partial}{\partial t} + \eta(x,t,u)\frac{\partial}{\partial u} \, .$$

The characteristic is

$$Q = \eta(x,t,u) - \xi(x,t,u)u_x - \tau(x,t,u)u_t. \tag{9}$$

Once again, invariant solutions satisfy the condition $Q = 0$, and trivial symmetries may be factored out by looking for symmetries of the form

$$\begin{aligned}
\hat{x} &= x, \\
\hat{t} &= t, \\
\hat{u} &= u + \epsilon Q + O(\epsilon^2)
\end{aligned}$$

As before, the symmetry condition requires that the PDE must hold in the transformed variables whenever it holds in the original variables. The LSC is obtained by retaining only the first-order terms.

Example 4. The symmetry condition for the heat equation, $u_t = u_{xx}$, is

$$\hat{u}_{\hat{t}} = \hat{u}_{\hat{x}\hat{x}} \qquad \text{when} \quad u_t = u_{xx}.$$

Therefore the LSC is

$$D_t Q = (D_x)^2 Q \qquad \text{when} \quad u_t = u_{xx},$$

where

$$\begin{aligned}
D_x &= \frac{\partial}{\partial x} + u_x \frac{\partial}{\partial u} + u_{xx} \frac{\partial}{\partial u_x} + u_{xt} \frac{\partial}{\partial u_t} + \dots, \\
D_t &= \frac{\partial}{\partial t} + u_t \frac{\partial}{\partial u} + u_{xt} \frac{\partial}{\partial u_x} + u_{tt} \frac{\partial}{\partial u_t} + \dots,
\end{aligned}$$

are the total derivatives with respect to x and t respectively. After replacing u_{xx} by u_t wherever it occurs, one can split the LSC into an overdetermined system by equating powers of u_{xt}, u_{tt}, u_x and u_t. This system can be solved by hand, but it is easier to use computer algebra. The infinitesimal generator is a linear combination of

$$X_1 = \frac{\partial}{\partial x}, \qquad X_2 = \frac{\partial}{\partial t}, \qquad X_3 = u\frac{\partial}{\partial u}, \qquad X_4 = x\frac{\partial}{\partial x} + 2t\frac{\partial}{\partial t},$$

$$X_5 = 2t\frac{\partial}{\partial x} - xu\frac{\partial}{\partial u}, \qquad X_6 = 4xt\frac{\partial}{\partial x} + 4t^2\frac{\partial}{\partial t} - (x^2 + 2t)u\frac{\partial}{\partial u},$$

$$\left\{ X_U = U(x,t)\frac{\partial}{\partial u} \;:\; U_t = U_{xx} \right\}. \tag{10}$$

Note that there is an infinite family of infinitesimal generators, which depend upon solutions of the heat equation. The effect of these symmetries is to add an arbitrary multiple of one solution to the original solution:

$$\hat{u} = u + \epsilon\, U(x,t), \tag{11}$$

where $U_t = U_{xx}$. This corresponds to the principle of linear superposition. Similarly, every PDE that is linear (or linearizable by a point transformation) has an infinite family of Lie point symmetries.

Example 5. The LSC for the Thomas equation, $u_{xt} = u_x u_t - 1$, is

$$D_x D_t Q = u_t D_x Q + u_x D_t Q \qquad \text{when} \quad u_{xt} = u_x u_t - 1.$$

Once again, there is an infinite family of Lie point symmetry generators, spanned by

$$X_1 = \frac{\partial}{\partial x}, \qquad X_2 = \frac{\partial}{\partial t}, \qquad X_3 = \frac{\partial}{\partial u}, \qquad X_4 = x\frac{\partial}{\partial x} - t\frac{\partial}{\partial t},$$
$$\left\{ X_V = V(x,t)\, e^u \frac{\partial}{\partial u} \; : V_{xt} = V \right\}. \tag{12}$$

This suggests that the Thomas equation is linearizable to $v_{xt} = v$ by a point transformation. The required transformation is obtained by looking for variables in which X_V generates linear superpositions. In this case $v = -\exp\{-u\}$ will do, for then

$$e^u \frac{\partial}{\partial u} = \frac{\partial}{\partial v}.$$

4 Some uses of Lie point symmetries

4.1 Reduction of order

For ODEs, a one-parameter local Lie group of symmetries can be used to reduce the order of the ODE by one. In particular, first-order ODEs can be solved completely. This is done by introducing a new set of coordinates that are suited to the symmetries. In terms of these new *canonical coordinates*, nontrivial symmetries become translations between solutions (similar to Γ_3 in §2).

Let (r, s) be a pair of canonical coordinates, where s is the direction of translation. Then the Lie symmetries are

$$(\hat{r}, \hat{s}) = (r, s + \epsilon),$$

and so a first-order ODE $y' = \omega(x, y)$ that admits such symmetries may be rewritten in the form

$$\dot{s} \equiv \frac{\mathrm{d}s}{\mathrm{d}r} = \Omega(r). \tag{13}$$

Note that Ω is independent of s, because s varies with ϵ, whereas r and $\dot{s}$ are invariant. The transformed equation (13) is easy to solve:

$$s + c = \int \Omega(r)\, \mathrm{d}r.$$

The effect of the symmetry group is clear: each symmetry changes the arbitrary constant of integration.

Canonical coordinates can be constructed systematically from the infinitesimal generator X. This represents the tangent vector field, which is independent of the coordinate system that is used. In canonical coordinates,

$$X = \frac{\partial}{\partial s}.$$

Therefore

$$\begin{aligned}\xi(x,y)\frac{\partial r}{\partial x}+\eta(x,y)\frac{\partial r}{\partial y} &= Xr = 0,\\ \xi(x,y)\frac{\partial s}{\partial x}+\eta(x,y)\frac{\partial s}{\partial y} &= Xs = 1.\end{aligned} \tag{14}$$

This system of first-order linear PDEs can be solved by the method of characteristics, which is a simple task for most symmetries of mathematical models of physical systems. Thus, it is usually easy to obtain canonical coordinates; any nondegenerate solution (r, s) of (14) will do. Canonical coordinates cannot be defined at an invariant point; as X is zero there, the second equation of (14) cannot be satisfied. Therefore it is usually necessary to use several sets of canonical coordinates to cover all regions of the plane.

Example 1 (cont.) Recall that the ODE

$$y' = \frac{y^3 + x^2y - y - x}{xy^2 + x^3 + y - x} \tag{15}$$

has Lie symmetries generated by

$$X = -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\,.$$

In the region $x > 0$, the equations (14) for canonical coordinates have a well-known solution, namely the polar coordinates

$$r = \sqrt{x^2+y^2}, \qquad s = \tan^{-1}\{y/x\}.$$

In these coordinates, (15) is transformed to

$$\dot{s} = \frac{1}{r(1-r^2)}\,,$$

which is undefined at the invariant point $r = 0$ and on the invariant solution $r = 1$. The general solution of the transformed ODE is

$$s + c = \frac{1}{2}\ln\left|\frac{r^2}{1-r^2}\right|\,,$$

which can easily be rewritten in terms of x and y to yield the general solution of (15) in the region $x > 0$. The remainder of the plane can be treated similarly.

For a second-order ODE, the introduction of canonical coordinates enables the ODE to be written in the form

$$\ddot{s} = \Omega(r, \dot{s}),$$

which is equivalent to a first-order ODE for $v = \dot{s}$. If the solution of this 'reduced' ODE is $v = f(r, c_1)$ then

$$s + c_2 = \int f(r, c_1)\,\mathrm{d}r.$$

Of course, there is no guarantee that the solution of the reduced ODE can be found, unless a one-parameter Lie group of its symmetries is known. However, if there are at least two independent infinitesimal generators for the original ODE, it is almost always possible to arrange the reduction so that the reduced ODE inherits some Lie symmetries, as follows. Calculate the *commutator* of each pair of infinitesimal generators, which is the first-order partial differential operator

$$[X_1, X_2] = X_1 X_2 - X_2 X_1.$$

It can be shown that each commutator is an infinitesimal symmetry generator, and therefore the set of all infinitesimal generators is a *Lie algebra*. If one can find a pair of generators X_i, X_j whose commutator is a multiple of X_i, write the ODE in terms of the canonical coordinates obtained from X_i; the reduced ODE is then guaranteed to inherit the symmetries generated by X_j, which can be used to solve it.

Example 3 (cont.) Earlier, we found that the Lie point symmetry generators of the second-order ODE

$$y'' = \frac{y'}{y^2}$$

are linear combinations of

$$X_1 = 2x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}, \qquad X_2 = \frac{\partial}{\partial x}.$$

The commutator of X_1 with X_2 is

$$[X_1, X_2] = -2\frac{\partial}{\partial x} = -2X_2.$$

Therefore, according to the above recipe, we should use canonical coordinates determined by X_2 to reduce the ODE. The simplest choice of such coordinates is $(r, s) = (y, x)$. Therefore $\dot{s} = 1/y'$, and

$$\ddot{s} = -\frac{y''}{(y')^3} = -\frac{1}{y^2(y')^2} = -\frac{(\dot{s})^2}{r^2}.$$

Let $v = \dot{s}$; then the reduced ODE is

$$\dot{v} = -\frac{v^2}{r^2}.$$

It is worth noting that, in terms of these canonical coordinates, the symmetries generated by X_1 are

$$(\hat{r}, \hat{s}) = (e^{\epsilon} r, e^{2\epsilon} s)$$

Therefore

$$\hat{v} = \frac{\mathrm{d}\hat{s}}{\mathrm{d}\hat{r}} = e^{\epsilon}\frac{\mathrm{d}s}{\mathrm{d}r} = e^{\epsilon}v,$$

and so the infinitesimal generator for these symmetries on the (r,v) plane is

$$\tilde{X}_1 = r\frac{\partial}{\partial r} + v\frac{\partial}{\partial v}\,.$$

As promised, these are symmetries of the reduced ODE. This ODE happens to be separable, so it can be solved without using canonical coordinates for $\tilde{X}_1$, but the recipe ensures that such coordinates are available. At this stage, the solution is easy to complete, and is left as an exercise.

Suppose that we had reduced the original ODE using the 'wrong' generator X_1. Then, in terms of the canonical coordinates $(r,s) = (y/\sqrt{x},\ \ln(x)/2)$, the original ODE becomes

$$\ddot{s} = -(2/r + r)(\dot{s})^3 - 2(\dot{s})^2/r^2.$$

The reduced ODE does not inherit the symmetries generated by X_2, and it appears to be intractable.

For simplicity, we have restricted attention to first- and second-order ODEs. However, the same ideas are equally applicable to higher-order ODEs. The structure of the Lie algebra determines whether or not there exists a pair of generators such that $[X_i, X_j]$ is a multiple of X_j. More generally, the Lie algebra determines whether or not an ODE can be integrated step-by-step. For further details, consult [5, 6].

4.2 Invariant solutions

Most PDEs do not have a 'general solution,' but symmetries can be used to find families of invariant solutions. Just as for invariant solutions of ODEs, we seek solutions of the differential equation that also satisfy $Q = 0$. Invariant solutions commonly include travelling waves and similarity solutions (which can be found almost by inspection), but they also include solutions that are not obvious. It is possible to classify *all* invariant solutions, using the structure of the Lie algebra. In the following, attention is restricted to a few examples, in order to convey the basic method.

Given an infinitesimal generator,

$$X = \xi(x,t,u)\frac{\partial}{\partial x} + \tau(x,t,u)\frac{\partial}{\partial t} + \eta(x,t,u)\frac{\partial}{\partial u}\,,$$

the solutions of $Q = 0$ are first integrals of the characteristic equations

$$\frac{\mathrm{d}x}{\xi} = \frac{\mathrm{d}t}{\tau} = \frac{\mathrm{d}u}{\eta}\,.$$

All such first integrals are invariant under the symmetries generated by X. If r and v are functionally independent first integrals, and if v depends nontrivially on u, then we can substitute first integrals of the form $v = F(r)$ into the original PDE. In general, the PDE will reduce to an ODE for F. The solution of this ODE yields a family of invariant solutions to the original PDE. If r depends on u, it is also necessary to seek solutions of the form $r = c$, because such solutions cannot be written in the form $v = F(r)$.

Example 4 (cont.) We shall first seek invariant solutions of the heat equation, $u_t = u_{xx}$, under the symmetries generated by

$$X_5 = 2t\frac{\partial}{\partial x} - xu\frac{\partial}{\partial u}\,.$$

The characteristic equations are

$$\frac{\mathrm{d}x}{2t} = \frac{\mathrm{d}t}{0} = \frac{\mathrm{d}u}{-xu}\,,$$

which have two functionally independent first integrals:

$$r = t, \qquad v = u\,\exp\left\{\frac{x^2}{4t}\right\}.$$

Therefore, we substitute

$$u = \exp\left\{-\frac{x^2}{4t}\right\}F(t)$$

into the heat equation, which yields the reduced ODE

$$F'(t) = -\frac{1}{2t}F(t).$$

The general solution of this ODE is $F(t) = c/\sqrt{t}$; hence the invariant solutions under the symmetries generated by X_5 are the Gaussian profiles

$$u = \frac{c}{\sqrt{t}}\,\exp\left\{-\frac{x^2}{4t}\right\}.$$

Applying the same procedure for the symmetries generated by

$$X_6 = 4xt\frac{\partial}{\partial x} + 4t^2\frac{\partial}{\partial t} - (x^2 + 2t)u\frac{\partial}{\partial u}$$

yields the invariants

$$r = \frac{x}{t}\,, \qquad v = u\sqrt{t}\,\exp\left\{\frac{x^2}{4t}\right\}.$$

The ODE that is obtained by substituting

$$u = \frac{1}{\sqrt{t}}\,\exp\left\{-\frac{x^2}{4t}\right\}F\left(\frac{x}{t}\right)$$

into the heat equation is $F'' = 0$, whose solution is $F(r) = c_1 r + c_2$. Therefore invariant solutions of the symmetries generated by X_6 are a linear superposition of

$$u = \frac{x}{t^{3/2}} \exp\left\{-\frac{x^2}{4t}\right\}$$

and the solutions obtained from X_5.

The heat equation has several large families of invariant functions, which have been classified [6]. The same is true of many important physical systems [7, 8].

4.3 Some other uses

The methods that have been described up to this point are very powerful, and can be applied to almost any differential equation. They are based on the simple idea of a one-parameter Lie group. However, there are also many ways of using symmetries that use information about *all* of the Lie point symmetries. Here are two examples; they are not discussed in detail, but the interested reader is referred to the literature.

- Provided that the number of linearly independent symmetry generators exceeds the order of the ODE, it is possible to construct the first integrals of the ODE directly from the symmetries; there is no need to consider the structure of the Lie algebra [5].

- Lie symmetries can be used to construct the discrete symmetries of a given differential equation [9, 10]. It is very hard to construct discrete symmetries directly from the symmetry condition; I know of only one substantial example in which this has been achieved [11]. However, it is possible to find discrete symmetries indirectly by looking at their action on the Lie algebra. Such actions have been classified for almost all Lie algebras of symmetries of ODEs [12]. Discrete symmetries have many uses; most notably, they affect the stability of nonlinear dynamical systems [13].

5 Higher symmetries

To find Lie point symmetries, one must split the LSC into an overdetermined system of PDEs. For ODEs of order $n \geq 3$, there is no need for Q to be linear in y'; the LSC can be split by equating powers of y''. More generally, Q may depend on any of the variables $x, y, y', \ldots, y^{(n-1)}$, provided that the form of Q enables the LSC to be split in a way that enables any unknown functions to be determined. All such symmetries are collectively known as dynamical symmetries; as in Theorem 1, the independent variables are fixed.

A similar idea can be extended to PDEs; here Q may depend upon arbitrarily many derivatives of the dependent variable. Such symmetries are called *generalized* or *Lie-Bäcklund* symmetries. For PDEs that come from a variational formulation, Noether's Theorem enables *conservation laws* to be derived from symmetries that leave the variational problem unchanged; typically, these are generalized symmetries. The nontrivial conservation laws of a PDE for $u(x, t)$ are expressions of the form

$$D_t(F) + D_x(G) = 0,$$

that hold on solutions of the PDE, but do not hold identically. Integrable systems (such as the Korteweg–de Vries equation) are partly characterized by the existence of an infinite number of conservation laws.

Even if a PDE does not have a known variational formulation, its conservation laws can be found systematically by a direct method that is analogous to the search for symmetries [6]. There are several different ways of implementing this approach with computer algebra [14, 15].

6 Some recent developments

This section highlights two new areas of symmetries research that promise to be widely applicable, for which computer algebra will be needed.

6.1 Symmetries of initial-value problems

So far, we have not referred to initial conditions or boundary conditions, but such conditions are usually stated in the formulation of a physical problem. Surprisingly, it is not generally true that the symmetries of an initial-value problem are also symmetries of the unconstrained differential equation. For example, the set of solutions of $y''' = 0$ subject to the initial condition $y''(0) = 0$ is the same as the set of solutions of $y'' = 0$. However, $y'' = 0$ has symmetries generated by

$$X = y \frac{\partial}{\partial x},$$

whereas $y''' = 0$ has no such symmetries. It has been shown that (subject to technical conditions) the Lie point symmetries of ODEs with specified initial conditions can be constructed with the aid of Taylor series [16]. Whilst this is far more computationally intensive than the methods described in §3, it is a way of solving some problems that cannot be solved by the standard approach.

6.2 Difference equations

Within the numerical analysis community, there is a rapidly-growing interest in *geometric integration*, which describes the transfer of geometric structures from a given differential equation to its numerical approximation. Such structures include symmetries, conservation laws, and symplectic structures [17].

The geometric structure of difference equations is also important for integrable systems, as there are large classes of discrete integrable systems. At present, far more is known about continuous integrable systems than about their discrete counterparts.

The problem of finding local symmetries of difference equations can be tackled in much the same way as for differential equations, but the LSC is a functional equation, rather than a PDE. Nevertheless, a technique for obtaining the solutions of the LSC has recently been developed [18]; this technique has also been used to determine conservation laws of partial difference equations [19]. At present, the calculations cannot usually be done entirely by hand or by computer algebra (due to weaknesses in routines for solving differential equations). It remains to be seen whether it is possible to develop a computational package that will do this type of calculation reliably.

7 Conclusions and further reading

This article has shown something of the power and scope of symmetry methods. Of necessity, it has only touched the surface of what is possible; indeed, current research on symmetries suggests that there are simple, widely-applicable methods still to be discovered.

For readers who would like a fuller introduction, I recommend the texts by Stephani [20] and Hydon [5]. The outstanding advanced text by Olver [6] is essential reading for anyone who is interested in research into symmetry methods. Ovsiannikov [21] and Bluman & Kumei [22] each include a number of useful results that do not appear in other texts.

The Lie symmetries and conservation laws of many physically-important systems have been classified; the first two volumes of a handbook of symmetry analysis edited by Ibragimov [7, 8] are excellent sources for such classifications.

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Appendix

Here is the Maple code that was used to obtain the Lie point symmetries of the ODE $y'' = y'/y^2$. For brevity, the output is omitted here, as it has been included in §3 of the main text. For more information, refer to the Maple documentation for the commands `rifsimp` and `odepde`.

```
> restart:
> with(DEtools):

First define the ODE whose symmetries are to be found.
> ODE:=diff(y(x),x,x)-diff(y(x),x)/y(x)^2;
```

```
The DEtools command "odepde" creates the LSC, whose numerator is
split into an overdetermined system by "coeffs."
> overdetsys:={coeffs(numer(odepde(ODE,[xi,eta](x,y),y(x))),_y1)};

The above system of determining equations is greatly simplified
by "rifsimp."
> simplesys:=rifsimp(overdetsys);

The simplified system is easily solved by hand;
however, "pdsolve" will also do the job.
> pdsolve(simplesys['Solved']);
```

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