Groups, algebras, and the non-linearity of geophysical inverse problems

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SUMMARY

Mathematical methods from the theory of continuous groups are used to determine whether a non-linear inverse problem, in the form of a functional, can be transformed into a linear inverse problem. If such transformations exist they can be constructed from the solutions of a linear system of differential equations. An illustration of the methodology is given by the linearization of the functional relating basement topography to observed surface gravity. The linearized inversion of gravity data for basement topography is applied to observations from Yucca Mountain, Nevada. A 2.0 km step in the basement to the west of Yucca Mountain, corresponding to the Bare Mountain fault, matches the Bouguer gravity anomaly. The resolution and uncertainty associated with the estimates of basement topography indicate that the structure directly beneath the gravity line is well constrained.

Key words: gravity, inverse problem, inversion, numerical techniques.

1 INTRODUCTION

The treatment of linear inverse problems is a well-established part of geophysical inverse theory. There are several effective approaches for constructing estimates of the Earth's properties from observations when the data are linearly related to the model parameters (Parker 1994). Unfortunately, when the relationship between data and parameters becomes non-linear one finds oneself in a very different situation. There are no accepted approaches for the assessment of solutions to non-linear inverse problems. Even though an inverse problem is non-linear, the fundamental observations of Backus & Gilbert (1967, 1968) regarding the determination of a distribution of subsurface properties from a finite set of observations still hold. In particular, if the inverse problem has any solutions then, if the solution set is stable, it will have an infinite number of solutions. A perturbation approach for model assessment has been suggested (Snieder 1991) but this techniques is local, holding only in the neighbourhood of a solution, and computationally intensive.

Regularization or prior information, often in the form of penalty terms, has been suggested as a way to reduce the computational task of finding and assessing solutions. However, regularization is difficult to implement because the degree of regularization or the weighting of the penalty terms will influence the structure of the solution set for a non-linear inverse problem (Vasco 1994). For example, the construction of a trade-off curve is not straightforward in the non-linear case. Even if the degree of regularization has been fixed in some fashion it is a daunting task to attempt to enumerate all solutions to a regularized non-linear inverse problem (Vasco, Peterson & Majer 1996).

A technique that has worked for a number of non-linear inverse problems involves the transformation of the inverse problem to a linear one (Parker 1994). The model assessment can then be conducted for the transformed problem. This is analogous to mathematical analysis in non-linear spaces, where concepts such as derivatives are defined with respect to a transformation to a linear or Euclidean space, the idea of a differential manifold (Helgason 1962; Boothby 1975). Transformations have been successful in treating inverse problems in magnetotellurics (Weidelt 1972; Parker 1980, 1982; Parker & Whaler 1981), seismic traveltimes (Garmany, Orcutt & Parker 1979), seismic reflection (Coen 1981, 1982; Bube & Burridge 1983), and resistivity sounding (Parker 1984).

However, except for the statistical approach in Vasco (1995), to date there has been no systematic transformation methodology for a general non-linear inverse problem. Such a statistical approach involves extensive computation and is only practical for problems involving a few hundred parameters or so.

In this paper I present a general analytical approach based upon the invariance of an inverse problem to transformation groups. Such techniques have been successful in treating non-linear differential equations (Ibragimov 1985; Olver 1986; Bluman & Kumei 1989), and the development and application of these methods has grown dramatically in recent years.
Furthermore, the group methodology now serves as the basis for a geometrical interpretation of non-linear partial differential equations (Hermann 1976; Krasilshchik, Lychagin & Vinogradov 1986; Zharinov 1992). The basic tools of the approach described below are continuous transformation groups (Lie groups) and an associated vector space equipped with a vector product (Lie algebra). Consideration of these particular transformation groups allows one to derive conditions for the existence of a linearizing transformation. Furthermore, these conditions are linear and result in a set of partial differential equations for the transformation parameters. The solution of such partial differential equations has been extensively discussed in recent years and currently several symbolic manipulation packages are available for automatically solving them on a computer (Pirani, Robinson & Shadwick 1979; Kersten 1987; Champagne, Hereman & Winternitz 1991; Reid 1991a, b).

2 METHODOLOGY

In this section I outline the basic concepts utilized in the transformation group approach to treating non-linear equations. Because there are a number of accessible texts in this area (Gilmore 1974; Ibragimov 1985; Olver 1986; Bluman & Kumei 1989; Stephani 1989), it is not my intention to fully describe and illustrate all ideas. I only wish to present techniques that are directly relevant to the problem at hand and that are not generally known by those involved in the inversion of geophysical data.

2.1 Groups, algebras, and transformations

The central structure in the study of transformations of functional and differential equations is the transformation group. Group properties are essential if one is to compose and invert transformations.

Definition: A group is a set \( G \) together with a composition rule, usually called multiplication, such that for any two elements \( g \) and \( h \) of \( G \), the product is also an element of \( G \); \( g \cdot h \in G \). The composition rule is required to be associative:

\[
g \cdot (h \cdot k) = (g \cdot h) \cdot k,
\]

the group \( G \) must contain an identity element \( e \) such that

\[
e \cdot g = g = e \cdot g
\]

and to each element of \( g \in G \) must correspond an inverse \( g^{-1} \) such that

\[
g \cdot g^{-1} = g^{-1} \cdot g = e.
\]

In order to derive useful analytical results the group \( G \) must satisfy some continuity requirements, which brings us to the idea of a Lie group. For a Lie group the collection of elements form a continuous set and the operations of multiplication and inversion are smooth or even analytic maps. Thus, the set of elements of the group \( G \) can be considered as a subset of an \( m \)-dimensional Euclidean space \( \mathbb{R}^m \). A standard example of a group is the set of \( m \times m \) invertible matrices \( M^m \in \mathbb{R}^{m \times m} \), where the composition rule is matrix multiplication which is a continuous (polynomial) function of the matrix coefficients.

For most applications, the power of a Lie group is manifested by its action as a transformation of some space, say \( \mathbb{R}^n \).

For example, the action of a matrix upon a vector representing a point in \( \mathbb{R}^n \) might produce a rotation. This is formalized by the definition of a transformation group.

Definition: A transformation group is a Lie (continuous) group \( G \) and a set \( M \subset \mathbb{R}^n \) along with a smooth map \( \Psi : G \times M \rightarrow M \) which satisfies, for \( g, h \in G, x \in M \).

\[
\Psi(g, \Psi(h, x)) = \Psi(g \cdot h, x),
\]

there is an identity element \( e \) such that

\[
\Psi(e, x) = x,
\]

and an inverse element \( g^{-1} \) such that

\[
\Psi(g^{-1}, \Psi(g, x)) = x.
\]

The map \( \Psi(g, x) \) is also denoted by a multiplication notation:

\[
\Psi(g, x) = g \cdot x.
\]

The subject of Lie transformation groups is a well-developed topic of great mathematical depth (Helgason 1962; Gilmore 1974; Ibragimov 1985). For applications, the most important aspect of the theory is the relationship between Lie groups and a related vector space. This vector space also contains a product between vectors, hence forming an algebra which is known as a Lie Algebra. Consider a one-parameter group of transformations

\[
X = \Psi(\epsilon, x),
\]

parametrized by the scalar \( \epsilon \). The role of the Lie Algebra may be motivated by a Taylor expansion of \( \Psi(\epsilon, x) \) in \( \epsilon \):

\[
\Psi(\epsilon, x) = x + \epsilon \xi(x) + \cdots.
\]

Consider the change in the transformed variable with respect to a change in \( \epsilon \) at \( \epsilon = 0 \) (at the identity transformation):

\[
\frac{\partial \Psi(\epsilon, x)}{\partial \epsilon} \bigg|_{\epsilon=0} = \xi(x).
\]

In the application of Lie group methods to differential equations and functionals, a linear operator derived from \( \xi(x) \).

\[
X_x = \frac{\partial \Psi(\epsilon, x)}{\partial \epsilon} \bigg|_{\epsilon=0} = \xi(x) \frac{\partial}{\partial x},
\]

plays a central role, where the summation convention, summation over repeated indices, has been employed. Some understanding of the importance of this operator can be gained by a re-examination of the Taylor series expansion of \( \Psi(\epsilon, x) \). The Taylor series expansion given in eq. (3) can be shown to be equivalent to a repeated application of the operator \( X_x \) (Bluman & Kumei 1989, p. 41)

\[
\Psi(\epsilon, x) = x + \epsilon X_x x + \frac{\epsilon^2}{2} X_x X_x x + \cdots
\]

and the infinite sum in brackets, known as a Lie series, is often denoted by \( \text{EXP}(X_x) \). Hence the operator \( X_x \) contains all the information concerning a transformation and may form the basis for studying invariance with respect to transformations, as shown in the next section. Because of its utility in the Lie group approach to differential equations and functionals the operator \( X_x \) is formally defined.

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The second fundamental theorem of Lie (Gilmore 1974) states that the commutator of any two infinitesimal generators is a linear operator of the form

\[ [X^a, X^b] = C_{ab}^c X^c, \]

where \( C_{ab}^c \) are constants, known as structure constants, which completely describe the structure of the algebra of infinitesimal generators. The formal definition of a Lie algebra is:

**Definition:** The Lie algebra of associated with the group \( G \) is the vector space of infinitesimal generators \( X^a, a = 1, \ldots, r \), with the corresponding product \( [X^a, X^b] \), the commutator.

The properties of the commutator are elaborated in Gilmore (1974), Olver (1986, p. 42), and Bluman & Kumei (1989, p. 81) and will not be repeated here.

### 2.2 Invariance and groups

The development of Lie group and algebra techniques for differential equations and functionals was motivated by the success of Galois' group theory applied to the solution of polynomial equations (Hermann 1976). The crucial observation is that one can replace complicated, non-linear invariance conditions with respect to group transformations by equivalent linear conditions for infinitesimal invariance with respect to the infinitesimal generators of the group. In fact, the theorems for functionals and differential equations build upon invariance theorems for systems of algebraic equations. For this reason, consider a system of \( l \) algebraic equations

\[ F_i(x) = 0, \quad i = 1, \ldots, l, \]

where \( x \in M \subset \mathbb{R}^r \) and the \( F_i(x) \) are smooth real-valued functions of \( x \). An invariance or symmetry group of the system is a group of transformations \( G \) acting on \( M \) such that \( G \) transforms solutions of the system to other solutions. This is formalized in the following definition (Bluman & Kumei 1989, p. 43; Olver 1986, p. 79):

**Definition:** For a group of transformations acting on a set \( M \subset \mathbb{R}^r \) a subset \( \mathcal{M} \subset M \) is called \( G \)-invariant, and \( G \) is called a symmetry group of \( \mathcal{M} \), if whenever \( x \in \mathcal{M} \) and \( g \in G \) then \( \Psi(g, x) = g \cdot x \in \mathcal{M} \).

In order that the complete solution set of a system of equations be \( G \)-invariant the set must form a connected subset of \( M \), invoking the implicit function theorem (Boothby 1975), placing conditions on the Jacobian matrix \( \partial F_i / \partial x_j \). The key theorem relating the symmetry properties to the infinitesimal invariance is (Olver 1986, p. 81; Bluman & Kumei 1989, p. 43):

**Theorem 1:** Let \( G \) be a Lie group of transformations acting on the \( m \)-dimensional set \( M \subset \mathbb{R}^r \). Let \( F : M \to \mathbb{R}^l, l \leq m \), define a system of algebraic equations

\[ F_i(x) = 0, \quad i = 1, \ldots, l \]

and assume that the Jacobian matrix \( \partial F_i / \partial x_j \) is of rank \( l \) at every solution \( x \) of the system. Then \( G \) is a symmetry group of the system if and only if

\[ X_i[F_i(x)] = 0, \quad i = 1, \ldots, l \]

wherever \( F_i(x) = 0, i = 1, \ldots, l \) for every infinitesimal generator \( X_i \) of \( G \).

This theorem follows by applying EXP(\( \varepsilon X_i \)) in eq. (6) to \( F_i(x) \).

**Definition:** The commutator or Lie bracket of infinitesimal generators \( X^a \) and \( X^b \) is given by

\[ [X^a, X^b] = X^a X^b - X^b X^a. \]
2.3 Invariance of functionals

A set of $l$ functionals defined on an open set $\Omega$ with smooth boundary $\partial \Omega$ is a mapping from the space of independent and dependent variables $(x, u(x)) \in X \times U$ to $R^l$:

$$\mathcal{F}_i[u] = \int_{\Omega} \Lambda_i(x, u^{(n)}) \, dx, \quad i = 1, \ldots, l, \quad (17)$$

where the Lagrangian $\Lambda_i(x, u^{(n)})$ denotes some function of $x$ and all derivatives of $u = f(x)$ up to and including order $n$ (see Appendix A).

As with a system of algebraic functions, a system of functionals may be invariant with respect to particular transformation groups (Hermann 1968, Olver 1986, Bluman and Kumei 1989). The formal definition of such a symmetry group is (Olver 1986, p. 257):

**Definition:** A group of transformations $G$ acting on $M \subset \Omega \times U$ is a variational symmetry group of the system of functionals $\mathcal{F}_i[u]$, $i = 1, \ldots, l$, if given a smooth function $u = f(x)$ defined over $\Omega$ and $g \in G$ such that $u = f(\tilde{x}) = g(f(x))$ is a single-valued function defined over the transformed domain $\tilde{\Omega} \subset \Omega$ then

$$\int_{\tilde{\Omega}} \Lambda_i(\tilde{x}, u^{(\tilde{n})}) \, d\tilde{x} = \int_{\Omega} \Lambda_i(x, u^{(n)}) \, dx \quad (18)$$

for $i = 1, \ldots, l$.

Here $u^{(\tilde{n})}(x)$ denotes the prolongation or extension of the transformation to the $n$ derivatives of $f(x)$ which is described in Appendix A. If the Lagrangian $\Lambda_i$ does not depend explicitly on any derivatives of $f(x)$ the prolongation is identically $f(x)$.

Before an infinitesimal criterion for such invariance is given we require the concept of a total derivative (Bluman & Kumei 1989, p. 60; Olver 1986, p. 112). The total derivative of a function $P(x, u^{(n)})$ with respect to $x_i$ is given by

$$D_i P(x, u^{(n)}) = \frac{\partial P}{\partial x_i} + u_{j}^{(n)} \frac{\partial P}{\partial u_j^{(n)}} \quad (19)$$

where $x$ denotes the $g$ components of $u$ if there is more than one dependent variable, $J = (j_1, \ldots, j_k)$ and

$$u_{j}^{(n)} = \frac{\partial (x_j, u_j^{(n)})}{\partial x_i} = \frac{\partial^{k+1} u^{(n)}}{\partial x_i \partial x_{j_1} \cdots \partial x_{j_k}}, \quad (20)$$

which is obtained by differentiating $P(x, u^{(n)})$ with respect to $x_i$ while treating all the $u$s and their derivatives as functions of $x$. The infinitesimal criterion for the invariance of a set of functionals under a group of transformations may now be stated; a proof for a single functional is given by Olver (1986, p. 257):

**Theorem 2:** A group of transformations $G$ acting on $M \subset \Omega \times U$ is a variational symmetry of the above system of functionals if and only if

$$\text{pr}^{(0)} X_{(x, u^{(n)})(\Lambda_i)} = \Lambda_i \text{Div} \xi = 0, \quad i = 1, \ldots, l, \quad (21)$$

for all $(x, u^{(n)}) \in J^{(n)}$ and every infinitesimal generator

$$X_{(x, u^{(n)})} = \xi_1(x, u) \frac{\partial}{\partial x_1} + \phi_1(x, u) \frac{\partial}{\partial u_1^{(n)}} \quad (22)$$

of $G$. Div $\xi$ denotes the total divergence of the $p$-tuple $\xi = (\xi_1, \ldots, \xi_p)$, which is given by Div $\xi = D_1 \xi_1 + D_2 \xi_2 + \cdots + D_p \xi_p$.

Here $X_{(x, u^{(n)})}$ denotes the infinitesimal generators associated with the independent and dependent variables. The term $\text{pr}^{(0)} X_{(x, u^{(n)})(\Lambda_i)}$ denotes the prolongation of the infinitesimal generator of $\Lambda_i$ defined in Appendix A. If $\Lambda_i$ does not depend on any derivatives of $u$ then the prolongation is identically $X_{(x, u^{(n)})}$ given in equation (22). The divergence term appears because we are determining the invariance of a functional, an integral over a particular volume.

The criterion of the preceding theorem is difficult to implement in general (Bluman & Kumei 1989, p. 272) due to the divergence term. An alternative approach is to examine the symmetry groups associated with the Euler–Lagrange equations used to find extrema of the functional (Olver 1986, p. 259; Bluman & Kumei 1989, p. 272). The Euler–Lagrange equations associated with the Lagrangian $\Lambda_i(x, u^{(n)})$ are differential equations for which the solution $u = f(x)$ is an extremum of the functional $\mathcal{F}_i[u]$. As in the next paragraph, the criterion for invariance corresponding to the Euler–Lagrange equations is much simpler and hence the symmetry groups are much easier to find. Intuitively, if a function is invariant with respect to a group of transformations (contains a certain symmetry) its set of extrema must also be invariant with respect to the transformations.

The differential equations associated with the Lagrangian $\Lambda_i(x, u^{(n)})$ are

$$E_i(\Lambda_i) = 0, \quad v = 1, \ldots, q, \quad (23)$$

where $E_v$ is the Euler operator defined as

$$E_v = \sum_{J} (-D)_J \frac{\partial}{\partial u_{j}^{(n)}},$$

where $D_J = D_{j_1} D_{j_2} \cdots D_{j_k}$ for a multi-index vector of order $k$ $J = (j_1, j_2, \ldots, j_k)$ (Olver 1986, p. 250; Bluman & Kumei 1980, p. 254). The infinitesimal conditions for a group to be a symmetry group of the Euler–Lagrange equations, a system of partial differential equations, are much simpler than those of the preceding theorem (Olver 1986, p. 106):

**Theorem 3:** Suppose

$$E_v(\Lambda_i) = 0, \quad v = 1, \ldots, q \quad (25)$$

is a system of Euler–Lagrange equations: If $G$ is a group of transformations acting on $X \times U$ and

$$\text{pr}^{(0)} X_{(x, u^{(n)})(E_v(\Lambda_i))} = 0, \quad v = 1, \ldots, q \quad (26)$$

whenever $E_v(\Lambda_i) = 0$ for every infinitesimal generator $X$ of $G$, then $G$ is a symmetry group of the system of Euler–Lagrange equations. Furthermore, if $G$ is a variational symmetry group of the functional which gave rise to the Euler–Lagrange equations, then $G$ is a symmetry group of the associated Euler–Lagrange equations.

The converse does not hold, however: there are symmetry groups of the Euler–Lagrange equations that are not variational symmetry groups of the original functional (Olver 1986, p. 259) just as the set of extrema of a function may contain additional symmetries not found in the underlying function. Therefore, in applying the above theorem the symmetry groups of the Euler–Lagrange equations are found using the infinitesimal criteria and then tested to determine if they truly are symmetry groups of the original functional. In particular, any infinitesimal generators $X_{(x, u^{(n)})}$ satisfying eq. (26) must also satisfy eq. (21).
2.4 Invariance group associated with linearity

The existence of a transformation linearizing a set of functionals is related to the existence of an invariance group associated with superposition (Kumei & Bluman 1982). Specifically, any non-linear equation transformable to a linear equation by a one-to-one mapping must admit an invariance group \( G \) whose generator depends upon an arbitrary solution of some linear equation.

The critical observation concerning the invariance group associated with a linear system of \( l \) functionals

\[
d_i = \mathcal{L}^i [u], \quad i = 1, \ldots, l,
\]

where \( d_i \) are fixed values, is that the system admits an infinite-parameter Lie group of transformations

\[
x' = x, \\
u' = u + \epsilon \alpha(x),
\]

where \( \alpha(x) \) is any function satisfying

\[
\mathcal{L}^i [\alpha] = 0, \quad i = 1, \ldots, l
\]

(Bluman & Kumei 1989, p. 319). That is, \( \alpha(x) \) must be an element of the null space of the set of functionals also known as the annihilator of the problem. The infinitesimal generator associated with this transformation group is

\[
X(x, u) = \alpha(x) \frac{\partial}{\partial u}
\]

(Bluman & Kumei 1990). If criteria associated with the Euler-Lagrange equations (26) are used then \( \alpha(x) \) will satisfy an associated set of partial differential equations as noted in Bluman & Kumei (1990). Furthermore, the resulting set of infinitesimal generators must be substituted into eq. (21) to verify that they are indeed generators for the variational symmetry group. The Lie group in eq. (30) depends on an entire function not on a finite number of parameters. Hence, the Lie group is infinite-dimensional and a test of linearity is the existence of an infinite-dimensional symmetry group. Computer programs are now available to determine whether a Lie group is finite- or infinite-dimensional (Reid 1991a). Such routines, designed for partial differential equations, may be applicable to the analysis of non-linear functionals.

2.5 Mapping a system of non-linear functionals to a system of linear functionals

Consider a given system of functionals fixed at particular values

\[
d_i = \mathcal{F}^i [u], \quad i = 1, \ldots, l,
\]

and a system of linear functionals

\[
d_i = \mathcal{L}^i [w], \quad i = 1, \ldots, l
\]

defined in terms of the independent variables \( z \) and the dependent variables \( w \), but fixed at the same values \( d_i \). We denote the given system of functionals by \( F(x, u) \) and the linear system by \( L(z, w) \). Assume that the system of functionals \( F(x, u) \) is invariant with respect to the transformation group \( G \) with infinitesimal generator

\[
X(x, u) = \xi(x, u) \frac{\partial}{\partial x} + \phi(x, u) \frac{\partial}{\partial u}.
\]

Similarly, the system of linear functionals \( L(z, w) \) is invariant with respect to the transformation group \( G \) whose infinitesimal generators are

\[
Z(z, w) = \zeta(z, w) \frac{\partial}{\partial z} + \phi^w(z, w) \frac{\partial}{\partial w}.
\]

We seek a set of invertible mappings from the system of non-linear functionals \( F(x, u) \) to the system of linear functionals \( L(z, w) \).

The necessary conditions for the existence of such a mapping, originally presented in Kumei & Bluman (1982), are most clearly given in Bluman & Kumei (1990) for a system of partial differential equations. A reformulation in terms of a system of functionals is:

**Theorem 4**: If there exists an invertible transformation that maps a given system of non-linear functionals \( F(x, u) \) to a system of linear functionals \( L(z, w) \) then the mapping must be a transformation of the form

\[
z_j = \Phi_j (x, u, \xi, \phi), \quad j = 1, \ldots, p
\]

\[
w^v = \Psi^v (x, u, \xi, \phi), \quad v = 1, \ldots, q.
\]

The system \( F(x, u) \) must admit an infinite-parameter Lie group of transformations having the infinitesimal generator

\[
X(x, u) = \xi(x, u) \frac{\partial}{\partial x} + \phi(x, u) \frac{\partial}{\partial u}.
\]

where \( \xi(x, u) \) and \( \phi(x, u) \) are characterized by

\[
\xi(x, u) = \sum_{m=1}^q \alpha_m^\xi (x, u) S^m (x, u),
\]

\[
\phi(x, u) = \sum_{m=1}^q \beta_m^\xi (x, u) S^m (x, u),
\]

where \( \alpha_m^\xi (x, u) \) and \( \beta_m^\xi (x, u) \) are some specific functions of \( (x, u) \) and \( S = (S^1, S^2, \ldots, S^q) \) consists of elements of the null space of the functionals \( L(x, u) \),

\[
\mathcal{L}^i [S] = 0, \quad i = 1, \ldots, l
\]

or solutions to a system of partial differential equations if the Euler-Lagrange approach of theorem 3 is taken.

The proof is presented in the Appendix. Equation (37) implies that elements of the null space determine the nature of the transformations. Sufficient conditions are also given in Bluman & Kumei (1990). In terms of a system of functionals, the theorem for sufficiency is:

**Theorem 5**: Let a given system of functionals \( F(x, u) \) admit an infinitesimal generator

\[
X_{(x,u)} = \xi_{(x,u)} \frac{\partial}{\partial x} + \phi_{(x,u)} \frac{\partial}{\partial u}
\]

whose coefficients are of the form

\[
\xi_{(x,u)} = \sum_{m=1}^q \alpha_m^{\xi_{(x,u)}} S^m (x, u),
\]

\[
\phi_{(x,u)} = \sum_{m=1}^q \beta_m^{\xi_{(x,u)}} S^m (x, u),
\]

where the components of \( S \) are elements of the null space of the system of functionals \( L(z, w) \) or solutions to a system of
homogeneous partial differential equations if the Euler–Lagrange approach is taken. If the linear homogeneous system of q first-order partial differential equations for the scalar \( \Phi \),

\[
\frac{\partial \Phi}{\partial x_m} + \beta_m \frac{\partial \Phi}{\partial u} = 0, \quad m = 1, \ldots, q,
\]

has \( p \) functionally independent solutions \( P_n(x, u) \) for \( n = 1, \ldots, p \), and the linear system of \( q^2 \) first-order partial differential equations

\[
\frac{\partial^m \Psi^p}{\partial x_j^{p}} + \beta^m \frac{\partial \Psi^p}{\partial u} = \delta^{mp},
\]

where \( \delta^{mp} \) is the Kronecker delta and \( m = 1, \ldots, q \) has a solution \( \Psi = (\Psi^1(x, u), \ldots, \Psi^q(x, u)) \), then the invertible mapping given by

\[
z = \Phi(x, u) = P_j(x, u), \quad j = 1, \ldots, p
\]

transform \( F(x, u) \) to the system of linear functionals \( L(z, \omega) \).

A proof is given in the Appendix.

Note that the transformations may be non-unique: any set of \( p \) annihilators of the \( J \) functionals can serve as the basis of the transformation.

3 ILLUSTRATION

3.1 Inversion of gravity data

In this section the problem of inferring the depth to basement from regional gravity observations is considered. The 2-D problem will be analysed using the group techniques described above. The result is a linear relation between the gravity at a point on the surface and the boundary geometry. An alternative approach, based upon transformations in the complex plane, has been used recently to map the boundary inverse problem into a Fredholm integral equation of the first kind (Aparicio & Pidcock 1996).

The integral relating the depth to the basement \( h(x) \), as a function of distance along the surface of the earth \( x \), is given by (Parker 1994, p. 295)

\[
d(x) = \int_{0}^{x} G \Delta \rho \ln \left( \frac{(x_1 - x)^2 + h^2(x)}{(x_1 - x)^2} \right) dx.
\]

The gravitational constant is denoted by \( G \) and the constant density contrast between the basement rocks and the overlying material is \( \Delta \rho \). In order to simplify the analysis, the data \( d \) are normalized by \( G \Delta \rho \), and the problem is written

\[
do = \int_{0}^{x} \ln \left( 1 + \frac{h^2(x)}{(x_1 - x)^2} \right) dx.
\]

As a further simplification the functional can be written in terms of a new function of \( x \): \( u(x) = h(x)/(x_1 - x) \):

\[
\frac{du}{\Delta \rho} = \int_{0}^{x} \ln \left[ 1 + u^2(x) \right] dx.
\]

One source of symmetry arises because the Lagrangian does not explicitly depend on \( x \). Hence, the translational group is a variational symmetry of the functional (Olver 1986, p. 257).

The Euler–Lagrange approach can be used to search for a group transformation to linearize the functional. The Lagrangian is

\[
\Lambda(x, u) = \ln (1 + u^2(x)),
\]

and the Euler–Lagrange equation is

\[
E(\Lambda) = \sum_{j=0}^{\infty} ( - D_j ) \frac{\partial \Lambda}{\partial u_j} = 0.
\]

or

\[
\frac{\partial \Lambda}{\partial u} - D_x \frac{\partial \Lambda}{\partial u_x} = 0.
\]

Now,

\[
\frac{\partial \Lambda}{\partial u} = 2\phi(x,u) \frac{\partial}{\partial x} + \phi(x,u) \frac{\partial}{\partial u}.
\]

\( F(x, u) \) does not explicitly depend on \( x \), so \( \partial F(x, u)/\partial x = 0 \), and

\[
\frac{\partial F(x, u)}{\partial u} = \frac{2}{1 + u^2(x)} \frac{4u^2(x)}{(1 + u^2(x))^2}.
\]

When \( F(x, u) = 0 \) the second term vanishes and

\[
\frac{\partial F(x, u)}{\partial u} = \frac{2}{1 + u^2(x)},
\]

resulting in

\[
X(x, u) \frac{\partial \Lambda(x, u)}{\partial x} = \frac{2\phi(x,u)}{1 + u^2(x)} = 0,
\]

which implies that \( \phi(x, u) = 0 \). Therefore, the infinitesimal generator of the invariance group must be of the form

\[
X(x, u) = \chi(x, u) \frac{\partial}{\partial x} + \phi(x,u) \frac{\partial}{\partial u}.
\]

In order for \( X(x, u) \) to be the infinitesimal generator of an invariance group of the functional it must also satisfy the condition in Theorem 2 given by eq. (21):

\[
\frac{\partial \chi(x, u)}{\partial x} + \Lambda(x, u) \left( \frac{\partial \xi(x, u)}{\partial x} + u_x \frac{\partial \xi(x, u)}{\partial u} \right) = 0
\]

in terms of the gravity functional

\[
\ln (1 + u^2(x)) \frac{\partial \xi(x, u)}{\partial x} + u_x \ln (1 + u^2(x)) \frac{\partial \xi(x, u)}{\partial u} = 0.
\]

This is a linear, homogeneous, first-order partial differential equation for the coefficient \( \xi(x, u) \) of the infinitesimal generator. Note that the coefficients of the equation depend on the unknown function \( u(x) \) and its derivative with respect to \( x \). Therefore, the gravity functional satisfies the necessary condition that it admit an infinite-parameter group of transformations stated in Theorem 4.

Consider the variational symmetry condition provided by Theorem 2, which precedes eq. (57). The equation can be integrated and simplified because the Lagrangian does not depend explicitly on \( x \). The use of integration by parts and the
divergence theorem produces
\[
\int_{\Omega} \Lambda(x, u) \zeta(x, u) dx - \int_{\Omega} \zeta(x, u) \text{div} \Lambda(x, u) dx = 0,
\]
where \( \Omega \) denotes the volume of integration and \( \partial \Omega \) the boundary of the integration volume. Because the Lagrangian is assumed to vanish at the boundary, the ends are assumed fixed at a known depth which is taken to be 0, the first term vanishes and we have
\[
- \int_{\Omega} \zeta(x, u) \text{div} \Lambda(x, u) dx = 0.
\]

Thus, the necessary conditions of eq. (37) are satisfied, and \( \zeta(x, u) \) can be written as a combination of functions which lie in the null space of a linear functional. From the form of the infinitesimal generator \( X_{x,u} \) and theorems 4 and 5 it is deduced that \( \beta_1 = 1 \) and \( \beta_2 = 0 \) resulting in a partial differential equation for the transformation \( z = \Phi(x, u) \), eq. (41),
\[
\frac{\partial \Phi(x, u)}{\partial x} = 0,
\]
implying that \( \Phi(x, u) \) is a function of \( u \) only. In addition, eq. (42) for the transformation \( w = \Psi(x, u) \) is
\[
\frac{\partial \Psi(x, u)}{\partial x} = 1,
\]
constraining that transformation to have the functional form
\[
w = \Psi(x, u) = x + f(u),
\]
where \( f(u) \) is an arbitrary function of \( u \) only. Here, the simplest transformations
\[
z = \Phi(u) = u \quad (61)
\]
and
\[
w(z) = \Psi(x, u) = x \quad (62)
\]
will be considered. This is an interchange of the dependent and independent variables as in the hodograph transformation of fluid dynamics (Seshadri & Na 1985).

The gravity functional can now be rewritten in the new variables. First, note that \( dx = w'(z) dz \), and the functional now has the form
\[
\frac{d}{G \Delta \rho} = \int \ln(1 + z^2) w'(z) dz,
\]
which can be integrated by parts:
\[
\frac{d}{G \Delta \rho} = \int \frac{2z}{1 + z^2} \frac{dx}{dz} + \ln(1 + z^2) w'(z) dz.
\]
It is assumed that the boundaries are fixed at the end points of the model because it is assumed that the depth is known there, that is
\[
z = \Phi(x) = 0 \quad (65)
\]
and hence the last term on the right vanishes and
\[
d = \int_0^b \frac{2z}{1 + z^2} w(z) dz,
\]
a linear functional for the \( x \) position of the interface as a function of the tangent of the angle between the surface and a line connecting the station with that point on the interface. This integral implies that we can calculate the gravity anomaly at a point on the surface by integrating a curve of boundary \( x \) position as a function of angle, weighting each value of \( w(z) \) by the kernel \( K(z) = 2\pi/(1 + z^2) \).

There are a few things to note at this point. First, for an undulating boundary there may be discontinuities in \( w(z) \), that is for small changes in the angle the \( x \) position of the boundary may change abruptly. This is much like the situation in travel-time inversion using the tau method (Bessonova et al. 1974, 1976; Garmy et al. 1979). These discontinuities are also the source of non-uniqueness for the inverse problem, somewhat akin to low-velocity zones in traveltime inversion. That is, on the side of a strong boundary undulation distant from the station the boundary can have various configurations and still generate an identical gravity anomaly at the station. For a suite of stations this non-uniqueness is reduced; the extreme case is a continuous distribution of stations between 0 and \( \alpha \) in which case the boundary is uniquely determined (Smith 1961). As a related note, we see that the kernel \( K(z) \) vanishes at an angle of 90° and at 0° and 180°. This is due to the fact that the \( x \) value directly below the station is fixed, as are the \( x \) values at the boundaries of the model.

Because the independent variable \( z \) is the tangent of the angle between the Earth’s surface and a line connecting the station to a particular point on the interface, there is a singularity directly beneath the station. That is, \( z \) goes to infinity as the angle approaches 90° and negative infinity as the angle approaches 90° from the other side. This coordinate singularity can be removed by changing coordinate systems from \( z = \tan(\alpha) \) to \( q = \cos \alpha \). That is,
\[
\frac{1 - q^2}{q} = \tan \alpha \quad (67)
\]
and the integral in eq. (66) becomes
\[
d = \int_1^{-1} \frac{2G \Delta \rho}{q} w(q) dq,
\]
which has smooth coordinates over the interval of integration but the kernel contains a singularity at \( q = 0 \). The integration requires special care but can be accomplished using a Taylor series expansion of \( w(q) \).

In Fig. 1 an idealized basin model is presented in order to illustrate the transformed linear approach. A station is denoted by the inverted triangle and the angle \( \alpha \), the angular span between the surface and a line connecting the station and the point of the boundary at location \( x \), is shown. Using a model such as that in Fig. 1, for each station a curve of the position of the sediment–basement interface, \( w(q) \), as a function of \( q = \cos \alpha \) is generated. In Fig. 2, three such curves are shown for stations 5, 15, and 25 at \( x = 0.49 \), 1.40, and 2.42 km respectively. It is then a straightforward matter to evaluate the integral in eq. (68) numerically, accounting for the singularity at \( q = 0 \). In Fig. 3, the Bouguer gravity anomalies for 29 stations are shown along with anomalies calculated using the summation technique of Talwani, Worzel & Ladisman (1959).

In order to calculate the solution of the inverse problem efficiently, the sediment–basement interface will be represented by a finite number of parameters. Note that this is not essential: a continuous approach, such as that suggested by Backus & Gilbert (1967) could be adopted. The solution is parametrized,
Figure 1. Basement structure used to generate a set of synthetic gravity data. The model is a syncline containing low-density sediments relative to homogeneous basement. The dashed line connecting the station location to a point \( w(q) \) on the basement is at an angle \( \alpha \) to the surface.

i.e. \( w(q) \) is represented by a sum of \( N \) basis functions,

\[
w(q) = \sum_{j=1}^{N} a_j W_j(q),
\]

where \( W_j(q) \) are a set of orthogonal basis functions, for example constant rectangular boxcar functions. This representation is substituted into the above integral:

\[
d_i = \int_{q_i}^{q_f} \frac{2G\rho}{q} \sum_{j=1}^{N} a_j W_j(q) dq.
\]

Interchanging the integration and summation results in a linear system of equations,

\[
d = Qa,
\]

where the components of the \( M \times N \) matrix \( Q \) are given by

\[
Q_i = \int_{q_i}^{q_f} \frac{2G\rho}{q} W_i(q) dq.
\]

The station location enters into the calculation as a scaling of the independent variable \( q \). For a particular station, the cosine of the angle \( \alpha \) will be different from the angle with respect to the reference point, the angle from the designated origin. This induces a variable scaling of the \( q \)-axis from the reference axis, which can be designated \( q' = q'(q) \), with the corresponding inverse transformation \( q = q(q') \). For example, if rectangular boxcar functions are used as a basis set \( W_j(q) \), the width of each boxcar is scaled differently for the integration associated with each station.

In the simple 29-station example presented above, the sediment–basement interface is described by nine rectangular constant basis functions. A generalized inverse (Menke 1984) was used to solve the linear inverse problem. The generalized inverse was constructed using a singular value decomposition with a singular value cut-off in which all singular values less than \((1/100)\)th of the maximum value are set to zero. The resulting interface estimate is shown in Fig. 4 as a plot of boundary depth versus distance. Even with this crude 9-coefficient parametrization, the relatively steep valley wall on the right-hand-side of the syncline is recovered.

4 APPLICATION

4.1 Yucca Mountain gravity survey

In this section, the linearization developed for the gravity function will be used to invert a set of gravity data from Yucca Mountain.
Figure 4. Generalized inversion of the data in Fig. 3 for a basin interface parametrized by nine segments. Note the steep basin boundary on the right-handside which agrees with the model in Fig. 1.

Figure 5. Bouguer gravity data gathered at Yucca Mountain, Nevada (solid squares). Estimated error bars of 0.3 mgal are associated with each observation.

Yucca Mountain lies within the basin and range tectonic province of North America. The region is extensively cut by steeply dipping extensional faults trending roughly north-south. This regional structure is cross-cut by numerous north-west trending sub-faults. The faulting has formed basins which are filled with heterogeneous collections of volcanic tuffs and flows. At several locations there are calderas and other volcanic structures, further complicating the distribution of seismic reflection data in constraining the variations in depth to regions. However, in some cases, due to poor penetration of the seismic energy, gravity data have become the primary source of information on large-scale depth variations of the basement. In this section, a single regional gravity line will be analysed, Regional Line-2, with the purpose of calculating the resolution and uncertainty associated with estimates of basement-depth variation.

4.2 Gravity data collection and reduction

The gravity data were gathered using two LaCoste and Romberg Model G gravity meters obtained from the University of California at Berkeley. The meters were calibrated for the Yucca Mountain region on the basis of four different runs on the Charleston Peak gravity calibration loop (Ponce & Oliver 1981). All gravity measurements are tied to the absolute gravity station MERCA, located at the US Geological Survey Core Library building in Mercury, Nevada (Zumberge et al. 1988), and each day of gravity measurements began and ended at this station. The two gravity meters operated in a leap-frog fashion, and at least every tenth station was occupied by both instruments. This redundancy of over 10 per cent of the readings helped identify possible errors associated with meter operation.

The solid earth tides were removed using a predictive algorithm. Instrument drift was estimated assuming a linear drift each day for each gravity meter. The drift rate was calculated using a least-squares procedure, based upon data from stations that were occupied more than once during the day. All measurements were referenced to the common base station MERCA. Terrain corrections were performed using topography data from orthophotos and from digital elevation data. The gravity associated with topographic relief was calculated by integrating the 3-D topographic features in a spherical coordinate system (Johnson & Litieiser 1972). Implicit in this correction is a curvature correction which accounts for the fact that the mass of the Bouguer correction is distributed as a spherical shell rather than a flat slab.

The gravity meters themselves can be read to a precision of about 0.01 mgal, but other effects introduce additional uncertainty. Errors are contributed by instrument drift, tides, topography, station mislocation, and station elevation. One check on several of these errors is to compare cross-over estimates for intersecting surveys. As an estimate of the error associated with the observations, gravity values at some 20 crossing points were examined. Of the 20 intersections, 10 crossed such that the elevation differences between the respective lines were less than 0.5 m. The difference in linear interpolated gravity values at the crossing point was generally less than 0.1 mgal. This value will serve as a rough estimate of the overall error associated with the gravity anomalies. All Bouguer gravity anomalies, a total of 192 values, and error bars of 3 standard errors (0.3 mgal) for line 2 are shown in Fig. 5.

4.3 Geological and density structure

Yucca Mountain lies within the basin and range tectonic province of North America. The region is extensively cut by steeply dipping extensional faults trending roughly north-south. This regional structure is cross-cut by numerous north-west trending sub-faults. The faulting has formed basins which are filled with heterogeneous collections of volcanic tuffs and flows. At several locations there are calderas and other volcanic structures, further complicating the distribution of
material properties in the subsurface. The volcanics, primarily of Tertiary age, overlie a Palaeozoic basement cut by normal faults. Regional line-2 (Fig. 5) crosses one such normal fault, the Bare Mountain fault, at about 3.0 km along the survey. About 2.0 km along the profile, Palaeozoic basement outcrops at the surface at Bare Mountain. Near the end of the profile the survey crosses Yucca Mountain, the site of the proposed repository.

Inference of basement topography based upon gravity measurements depends critically on the density contrast across the sediment–basement interface. Rarely is the density contrast a simple density jump at the interface between two homogeneous materials. Rather, both the sediments and the basement rocks contain density variations which influence the surface gravity. This is also true at Yucca Mountain, where the basin fill consists of alluvium, non-welded, partially welded, and welded tuffs and the basement is composed of various metamorphic rocks. Therefore, the basement depth estimates presented in this section are only effective basement depths of a hypothetical simple interface.

Previous gravity studies at Yucca Mountain and the Nevada test site contain considerable information on the densities of the various rock types found at the site (Healey 1968; Snyder & Carr 1984; Ferguson et al. 1988; Reamer & Ferguson 1989). The near-surface alluvium appears to have densities between 1.49 and 2.34 g cm\(^{-3}\). The partially welded and welded tuffs range in density from 1.85 to 2.5 g cm\(^{-3}\), with an average value of 2.14 g cm\(^{-3}\). Surface samples of the older basement rocks gave a range of 2.60 to 2.82 g cm\(^{-3}\) and borehole samples of the Palaeozoic limestone produced density estimates of 2.75 g cm\(^{-3}\). The simplified density model used in this analysis assumes that the basin fill has a density of 2.1 g cm\(^{-3}\) and the basement rocks have an associated density of 2.77 g cm\(^{-3}\).

### 4.4 Gravity data inversion and assessment

The inversion of the gravity data, shown in Fig. 5, utilized the techniques described in the previous section. First, the basement model was parametrized in the model parameter space of boundary position as a function of angle from a reference point, as in eq. (69). For this inversion, the fill-basement interface 0 ≤ x ≤ 40 km was subdivided into 99 equal-distance (approximately 0.4 km) increments. The reference point was located at position 0.14 km along the line, to the left of the first station. The angular increments were defined by the boundaries of the intervals and this reference point. The integral in eq. (72) was evaluated numerically in order to compute the coefficients for the matrix \(Q\) in eq. (71).

Rather than solve the often-singular matrix equation (71) directly, a regularization approach was adopted. Perhaps the simplest way to view the approach is as a penalized least-squares technique in which the sum of the squares of the residuals,

\[
(d - Qa)(d - Qa)^T,
\]

is minimized in conjunction with a term that penalizes deviations from an initial model of basement topography, \(a_0\). Minimization of the linear combination of the sum of the squares of the residuals and the penalty term weighted by a factor \(\tau\),

\[
(d - Qa)(d - Qa)^T + \tau(a - a_0)(a - a_0)^T,
\]

results in a matrix equation for \(a\) (Menke 1984; Parker 1994). A stable algorithm for the solution of the matrix equation was implemented using singular value decomposition (Menke 1984; Parker 1994). Note that the solution itself is parametrized by the weighting parameter \(\tau\), which controls the trade-off between fitting the data and obtaining a model similar to the initial model \(a_0\). Estimation of a satisfactory value of \(\tau\) is based upon the construction of a trade-off curve (Menke 1984; Parker 1994), a plot of root-mean-square (RMS) misfit versus the root-mean-square size of the model. The trade-off curve, shown in Fig. 6, is constructed by repeatedly minimizing eq. (74) over a range of \(\tau\). Three values of \(\tau\) are shown in Fig. 6, two values at the extreme ends of the trade-off curve and one at the bend or knee of the curve. At the sharp bend in the trade-off curve, the misfit increases dramatically for small decreases in the model norm as \(\tau\) is increased. As \(\tau\) is decreased, the model size or norm increases significantly for small decreases in RMS misfit. Therefore, as is common practice (Menke 1984), the value of \(\tau\) at the knee of the curve (30 000) will be used in the inversion and model assessment. The construction of a trade-off curve for the transformed problem is one advantage of the linearization. Determining trade-off curves for nonlinear problems is very difficult due to the appearance and disappearance of solutions, i.e. the branching of solutions, as the trade-off parameter is varied (Vasco 1994).

Before the solution is discussed, let us consider the resolution of the basement topography estimates. In particular, consider the formal resolution matrix associated with the solution to the inverse problem. Briefly, the resolution matrix \(R\) relates the estimate of \(a\) denoted by \(\hat{a}\) to a hypothetical ‘true’ coefficient vector \(a_t\):

\[\hat{a} = Ra_t\]

(Menke 1984; Parker 1994). The elements of the \(i\)th row of the resolution matrix represent averaging coefficients measuring the contribution of adjacent boundary coefficients to the estimate of \(i\)th boundary coefficient \(\hat{a}_i\). The diagonal elements of the resolution matrix vary between 0 and 1 and provide a rough

\[\text{Figure 6. Trade-off curve portraying the variation in RMS misfit and RMS model norm as the weighting parameter, }\tau, \text{ in eq. (74), is varied. Three values of }\tau \text{ are shown for reference; two values at the extreme ends of the trade-off curve and a point at the sharp bend in the curve.}\]

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Figure 7. Graphical depiction of the resolution matrix for the Yucca Mountain gravity inversion. Each curve represents a row of the resolution matrix, indicating the contribution of adjacent basement coefficients to an estimate at a particular horizontal distance.

Figure 8. Basement topography estimates and associated uncertainties for the Yucca Mountain gravity inverse problem. The solid squares are located at the centre point of each horizontal increment of the basement interface model.

5 DISCUSSION AND CONCLUSIONS

Group methods represent one of the most general analytical tools for analysing non-linear equations. Approaches based upon transformation groups unify several techniques for solving differential equations, including: the Laplace transform, integrating factors, similarity methods, the method of undetermined coefficients, and the variation of parameters (Bluman & Kumei 1989). Modern group analysis techniques
have been applied to numerous problems and are the subject of extensive research (Ibragimov, Torrisi & Valenti 1993). As shown in this paper, using group techniques it is possible to determine if an inverse problem, in the form of a functional, can be linearized. From the analytical form of the functional representing the inverse problem, a set of linear partial differential equations, the defining equations, can be derived. The solutions to the defining equations provide the generators from which a transformation group can be constructed. The methods presented in this paper are well suited for computation, and numerical algorithms and several symbolic manipulation programs exist for treating the determining equations (Schwarz 1985, 1988; Kersten 1987; Champagne et al. 1991) or for determining if a system of equations can be linearized without explicitly solving the determining equations (Reid 1991a,b).

Group invariance and symmetry have other applications to inverse problems. In a general sense, a symmetry group of a system of non-linear equations is a group that transforms solutions of the system to other solutions. Therefore, the symmetry groups associated with an inverse problem can be used to construct new solutions from a particular solution. Thus, it is possible to explore the range of solutions satisfying a given data set using transformation groups. In addition, Lie group techniques may be used to map differential equations with variable coefficients to equations with constant coefficients (Bluman 1983; Bluman & Kumei 1989). Such mappings could prove useful in treating inverse problems formulated in terms of differential equations containing unknown coefficients.

It should be noted that the perturbation expansions used by Snieder (1991) to study non-linear inverse problems can be interpreted as transformations parametrized by the expansion coefficient c. However, as noted by Steinberg (1986), Lie transformations are not power-series expansions but rather factored-product expansions. There are several advantages in using such expansions, particularly in constructing inverses of the transformations, in composing transformations, and in implementations using a computer symbolic manipulator (Steinberg 1986).

There are more general notions of symmetry groups than that treated here, transformations which are functions of only the independent and dependent variables. In particular, the group of transformations might also be functions of the first derivative of the dependent variable, the so-called contact transformations (Olver 1986; Bluman & Kumei 1989; Stephani 1989). An even more general approach makes the transformations functions of an arbitrary number of derivatives of the dependent variable, the Lie–Backlund or generalized symmetry groups (Noether 1971; Olver 1986; Bluman & Kumei 1989; Stephani 1989). Such symmetry groups are intimately related to linearizing a system through a change of variables or some form of inverse scattering method (Wahlquist & Estabrook 1975; Lamb 1980; Rogers & Shadwick 1982). Such generalizations can significantly expand the range of application of group methods. Finally, there are non-local transformation groups such as the multi-point symmetries utilized by Klein (1979) and the potential symmetries described in Bluman (1993) which may also be useful in linearizing inverse problems.

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space dimensions in the problem. Specifically, there is an underlying space of independent variables $x$, such as spatial coordinates and time, and a space of dependent variables $u$, such as material properties. Jointly, the independent and dependent variables form a product space $X \times U$, the basic space. For functionals and differential equations which may contain derivatives with respect to the independent variables it is necessary to prolong the basis space $X \times U$ to a higher-dimensional space. The prolonged space, or 'prolongation' as it is called in the mathematical literature, is related to the idea of the 'jet space' of a function. The concept is an abstraction of the Taylor series expansion of a function, in which the coefficients of the Taylor expansion can be considered to be coordinates in function space. If the Taylor series expansion of a function of $p$ variables, $f(x_1, \ldots, x_p)$, is truncated to some order $n$ there will be a $K$-dimensional space of series coefficients. It can be shown that, for any given order $l \leq n$, there are

$$K_l^p = \binom{p+l-1}{l}$$

(A1)

Taylor series coefficients

$$\delta_j f(x) = \frac{\partial f(x)}{\partial x_j} + \frac{\partial^2 f(x)}{\partial x_j \partial x_j} + \cdots + \frac{\partial^p f(x)}{\partial x_j \cdots \partial x_j}$$

(A2)

where $K_l^p$ denotes the number of combinations of $p+l-1$ unordered objects taken $l$ at a time. The symbol $J$ denotes a multi-index, essentially an ordered $l$-vector of integers $J = (j_1, j_2, \ldots, j_l)$ denoting which partial derivative is being computed. If $f(x)$ is a vector-valued function with $q$ components then there are $qK_l^p$ values for a given order $l$. Let $U_l \in R^{qK_l^p}$ represent the subspace of coefficients associated with derivatives of order $l$, then the jet space $J^p$ is composed of the product space $X \times U_0 \times U_1 \times \cdots \times U_n$. The dimension of this space is

$$K = \dim J^p = q + K_1^p + \cdots + qK_n^p$$

(A3)

and the coordinates represent all the derivatives of the functions $u = f(x)$ of all orders from 0 to $n$:

$$(x_1, \ldots, x_p, u, \ldots, u^p, \partial x_1, u, \ldots, \partial x_p, u, \ldots, \partial x_1 \partial x_1, u, \ldots, \partial x_p \partial x_p, u^p).$$

The prolongation of a function, $u = f(x)$, $f : X \to U$, denoted $u^p = \text{pr}^p f(x)$, is a mapping from $X$ to the space $U^p = U_0 \times U_1 \cdots \times U_n$. The quantity $\text{pr}^p f(x)$ is a vector whose entries represent the values of $f$ and all its derivatives up to order $n$ at the point $x$.

An infinitesimal generator in the space $X \times U$ is of the form (Olver 1986, p. 113)

$$X_{(x,u)} = \xi(x,u) \frac{\partial}{\partial x} + \phi(x,u) \frac{\partial}{\partial u^q}$$

(A4)

for $i = 1, \ldots, p$ and $z = 1, \ldots, q$. I reiterate that the summation convention is invoked for all repeated indices. The prolongation of $X_{(x,u)}$ is an extended vector field defined over the jet space $J^p$. The prolongation of the vector field $X_{(x,u)}$ has the form

$$\text{pr}^p X_{(x,u)} = \xi(x,u) \frac{\partial}{\partial x} + \phi(x,u) \frac{\partial}{\partial u^q}$$

(A5)

for $i = 1, \ldots, p$, $x = 1, \ldots, q$, and $J$ ranging over all multi-indices of orders $0 \leq |J| \leq n$. The notation $|J|$ denotes the dimension, the number of components contained in the multi-index vector $J = (j_1, j_2, \ldots, j_l)$. Note that for quantities that do not depend on the derivatives of $u$ the prolongation of $X_{(x,u)}$ is identically $X_{(x,u)}$.

**APPENDIX B**

**Proofs of necessary and sufficient conditions**

Here, proofs describing necessary and sufficient conditions for the existence of a mapping from a set of non-linear functionals to a set of linear functionals are outlined. The proofs are variations of those presented in Bluman & Kumei (1990) pertaining to differential equations. For a given system of functionals, denoted by $F(x, u)$ with $p$ independent variables $x = (x_1, \ldots, x_p)$ and $q$ dependent variables $u = (u^1, \ldots, u^q)$ let $G_z$ denote a one-parameter group of transformations for which the functionals are invariant, given by

$$x_i' = x_i + \epsilon x_i'(x, u) + \cdots, \quad i = 1, \ldots, p$$

(B1)

and

$$u^v' = u^v + \epsilon u^v'(x, u) + \cdots, \quad v = 1, \ldots, q.$$  

The corresponding infinitesimal generator to $G_z$ is given by $X_{(x,u)}$:

$$X_{(x,u)} = \xi u + \phi^u \frac{\partial}{\partial u^q}. $$

(B2)

Similarly, consider a system of linear functionals, denoted by $L(z, w)$ with $p$ independent variables $z = (z_1, \ldots, z_p)$ and $q$ dependent variables $w = (w^1, \ldots, w^q)$. Let $G_z$ denote a one-parameter group of transformations given by

$$z_i' = z_i + \epsilon z_i'(z, w) + \cdots, \quad i = 1, \ldots, p$$

(B3)

and

$$w^v' = w^v + \epsilon w^v(z, w) + \cdots, \quad v = 1, \ldots, q.$$  

The infinitesimal generator associated with this group $G_z$ is given by

$$Z_{(z,w)} = \xi z + \phi^z \frac{\partial}{\partial z^p}. $$

(B4)

Consider a mapping $\mu$ which transforms any solution $u = U(x)$ of the system of functionals $F(x, u)$ to a solution $w = W(z)$ of a system of linear functionals $L(z, w)$. The mapping $\mu$ is of the form

$$z_j = \Phi_j (x, u), \quad j = 1, \ldots, p$$

(B5)

$$w^v = \Psi^v (x, u), \quad v = 1, \ldots, q.$$  

Bluman & Kumei (1990) show that in order for the compositions $\mu g_\alpha (z)$ and $g_\alpha (x) \mu$, for $g_\alpha (z) \in G_z$ and $g_\alpha (x) \in G_x$, to produce the same result in $(x, u)$ space the infinitesimal generators must satisfy

$$\eta(x,u) \Phi = Z_{(z,w)} z$$

(B6)

and

$$\eta(x,u) \Psi = Z_{(z,w)} w.$$  

These equations are necessary conditions that the mapping $\mu$ must satisfy in terms of the symmetries of $F(x, u)$ and $L(z, w)$. First, a theorem relating the Lie algebras of $F(x, u)$ and $L(z, w)$ will be stated without proof. A proof is discussed in Bluman & Kumei (1990) for differential equations, and similar arguments hold for symmetries of functionals.
Theorem 7: Suppose $F(x, u)$ is invariant with respect to the group $G$, with associated Lie algebra $\mathcal{G}$, which is spanned by the infinitesimal generators $X_1, X_2, \ldots$. Let $\mu$ be an invertible mapping from $F(x, u)$ to $L(z, w)$. Then the corresponding Lie algebra $\mathcal{G}$ spanned by $Z_1, Z_2, \ldots$ is isomorphic to $\mathcal{G}$, that is there exists a one-to-one and onto map between the Lie algebras.

Now a proof of the necessary conditions for the existence of an invertible transformation can be given:

**Proof (Theorem 4, Necessary conditions):** If a mapping $\mu$ of the form

$$
\begin{align*}
z_j &= \Phi_j(x, u), & j = 1, \ldots, p \\
w^v &= \Psi^v(x, u), & v = 1, \ldots, q
\end{align*}
$$

exists, then the resulting system of linear functionals $L(z, w)$ is represented by a linear mapping from $w(z)$ to the real line where the kernel of the functional only depends on the independent variables $z$:

$$
d_i = \mathcal{L}_i(z)[w], & i = 1, \ldots, l.
$$

As noted previously, such a system admits a symmetry with the associated infinitesimal generator

$$
Z_{(z, w)} = f'(z) \frac{\partial}{\partial w^v},
$$

where $f(z) = (f^1(z), f^2(z), \ldots, f^q(z))$ is an arbitrary annihilator of the system of functionals

$$
\mathcal{L}_i(z)[f] = 0, & i = 1, \ldots, l
$$

or the solution of the associated partial differential equations. Corresponding to the generator $Z_{(z, w)}$ there is an infinitesimal generator

$$
X_{(z, w)} = \xi_i(x, u) \frac{\partial}{\partial x_j} + \phi^v(x, u) \frac{\partial}{\partial w^v},
$$

admitted by $F(x, u)$ such that the components of the mapping $\mu, \Phi_i, \Psi^v$, and the coefficients $\xi_i(x, u), \phi^v(x, u)$ of $X_{(z, w)}$ satisfy the mapping equations (B6):

$$
\begin{align*}
\xi_i(x, u) \frac{\partial \Phi_j}{\partial x_i} + \phi^v(x, u) \frac{\partial \Phi_j}{\partial w^v} &= 0, & i = 1, \ldots, p \\
\xi_i(x, u) \frac{\partial \Psi^v}{\partial x_i} + \phi^v(x, u) \frac{\partial \Psi^v}{\partial w^v} &= f^v(\Phi), & v = 1, \ldots, q.
\end{align*}
$$

Because the mapping $\mu$ is invertible the Jacobian is non-zero and we can solve these equations for $\xi_i(x, u)$ and $\phi^v(x, u)$. They are both linear and homogeneous in $f$:

$$
\begin{align*}
\xi_i(x, u) &= \sum_{m=1}^{q} x_i^m(x, u) f^m(\Phi(x, x, u)), \\
\phi^v(x, u) &= \sum_{m=1}^{q} \beta^v_m(x, u) f^m(\Phi(x, x, u)),
\end{align*}
$$

where $x_i^m(x, u)$ and $\beta^v_m(x, u)$ are specific functions of $(x, u)$. Set $x' = \Phi(x, u)$, then $F = (f^1(x'), \ldots, f^q(x'))$ satisfies

$$
\mathcal{L}_i(x')[f'] = 0, & i = 1, \ldots, l.
$$

**Proof (Theorem 5, Sufficient conditions):** The mapping $\mu$ defined by

$$
\begin{align*}
\zeta_j(x, u) &= \Phi_j(x, u), & j = 1, \ldots, p \\
w^v &= \Psi^v(x, u), & v = 1, \ldots, q
\end{align*}
$$

are invertible by construction. Let $f'(z) = F'(x, u), v = 1, \ldots, q$. Then $\mu$ transforms $X_{(x, u)}$ admitted by $F(x, u)$ to $Z_{(z, w)}$, which is of the form

$$
Z_{(z, w)} = f'(z) \frac{\partial}{\partial w^v},
$$

for any $f(z) = (f^1(z), \ldots, f^q(z))$ satisfying $\mathcal{L}_i(z)[f'] = 0, i = 1, \ldots, l$, or the associated Euler–Lagrange equations. Since the mapping $\mu$ is invertible it follows that the system of functionals admitting $Z_{(z, w)}$ must be of the form

$$
\mathcal{L}_i(z)[w] = d_i, & i = 1, \ldots, l.
$$