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Finding Global Point Symmetries of Partial Differential Equations

Master's Thesis

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Master of Science in Physics
at University of Groningen under the supervision of
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Abstract

Lie point symmetries are local symmetries of differential equations that map the set of solutions to itself. The underlying theory, which only allows to find continuous symmetries of infinitesimal transformations, is explained and applied to differential equations like the logistic equation, heat equation and filtration equation.

The results are analyzed to check if these Lie point symmetries remain symmetries for non-infinitesimal transformations and possibly form a global symmetry group. It is found that the heat equation contains a local symmetry, which limits the domain of the transformations, restricting the group from being globally defined. However, the symmetry group can be made global when restricting the solution space of the heat equation.

Furthermore, an optimization algorithm is constructed and compared against an analytical method to find discrete point symmetries, and is tested on the spherical Burger's equation, heat equation and the Laplace equation. Using analytical and computational methods, multiple real discrete point transformations were found for the heat equation, with the symmetry group having 4 connected components.

1 Introduction

Sophus Lie's work on Lie groups in the 19th century laid the ground work of continuous symmetries. These symmetries are present in every field of physics today and have transformed the way in which physical systems are treated. Differential equations are among these physical systems, and were a particular focus in Lie's work.

A symmetry of a differential equation is a transformation that maps the set of solutions to the set of solutions. The differential equation is said to be invariant under the symmetry transformation, and the total collection of all such symmetries form a symmetry group of the differential equation. These transformations provide insight about the solutions, and allow to find new solutions from existing solutions.

When Lie worked on his theory of groups, he only considered local groups. It took until the 1920's when Élie Cartan came along, who extended the analysis to global groups [1]. A commonly studied symmetry of differential equations is the continuous Lie point symmetry. Such symmetries transform the independent variables (coordinates) and dependent variables (solutions) locally, such that the original differential equation is still satisfied. This thesis will focus on these symmetries, explain the underlying theory and explore some examples to provide insight about how it works.

The established theory is based on infinitesimal transformations with little understanding what happens to these symmetries when performing transformations beyond this infinitesimal scale. Do these symmetries remain when considering transformations on a larger scale? Are these the only symmetries that can be found? This large step into the non-infinitesimal symmetry transformations will be taken in this thesis, providing a new view of the limits of the theory.

Much work has been done on finding the infinitesimal generators of these local Lie point symmetries with symbolic software, including *Maple*, *REDUCE* and *MATHEMATICA* [2]. This software proves to be useful for quickly finding local symmetries and finding differential equations with specific local symmetries for certain examples.

After the introduction of a continuous Lie point symmetry, Hydon discovered a method to find discrete point symmetries of differential equations ([3], [4]). Even though the continuous Lie point symmetry are only defined locally, their Lie algebra can be used to find discrete point symmetries. Such discrete point symmetries provide insight about the transformations that cannot be found locally, and will aid in the search for what happens beyond the infinitesimal transformations. Furthermore, discrete point symmetries will provide constrains on what types of global Lie groups might be used to describe the symmetry group of a specific PDE.

1.1 Thesis Outline

This thesis is separated into standalone sections, which together form an introduction to the field of symmetry analysis of differential equations with several examples of physical systems and their implications. It is structured into two large chapters, one covering the continuous Lie point symmetries and the other covering the discrete point symmetries.

Continuous Lie point symmetries are covered first, starting with the necessary definitions and theorems in section 2. After the introduction, multiple differential equations are treated to become familiar with the method and to show what these symmetries can do. The logistic equation, heat equation and filtration equation are showcased in light of the theory in section 3, section 4, section 5 respectively.
Afterwards the discrete point symmetries are inspected, starting again with the underlying theory in section 6. The theory is first demonstrated on the spherical Burger's equation in section 7, and is also applied on the heat equation and Laplace equation in section 8 and section 9 respectively.
Lastly, the thesis ends with a conclusion (section 10) on both the methods and directions for future research.

2 Continuous Symmetries Framework

This section covers the important definitions and theorems used throughout this thesis with examples to clarify the underlying theory. Note that the research done in this thesis is a continuation of the work done by Vlad Malai, whose thesis [5] contains much useful information. Together with Olver's extensive textbook [6] they form the main source of the following information and the reader is referred to it for additional information on the topic.

2.1 Lie Groups and Algebras

Definition 2.1 (Group, Olver p. 14)**.** A group is a set G together with a group operation $(\cdot)$, called multiplication, such that $\forall g, h \in G$ the product $g \cdot h \in G$ exists. The group operation satisfies the following axioms:
Associativity: If $g, h, k \in G$, then $g \cdot (h \cdot k) = (g \cdot h) \cdot k$.
Identity: There is an element $e \in G$ (identity) with the property $e \cdot g = g \cdot e = g$ for all $g \in G$.
Inverse: $\forall g \in G$, there exist an element g^{-1} (inverse) which satisfies $g \cdot g^{-1} = e = g^{-1} \cdot g$.

An example of a group is the set of integers under addition $(\mathbb{Z}, +)$. A group consists of discrete elements, which limits it applications for physical processes. Lie considered the idea of a group consisting of continuous elements that are in some way connected. The mathematical structure needed to support this idea is a manifold, which is a mathematical space that is locally Euclidean, allowing to use the principles of calculus on a local scale. We distinguish between global and local Lie groups:

Definition 2.2 (Lie Group, Olver p. 15)**.** An r-parameter Lie group, from now on called a global Lie group, is a group G which carries the structure of an r-dimensional smooth manifold such that the group operation

$$m : G \times G \to G, \qquad m(g, h) = g \cdot h, \qquad h, g \in G$$

and the inversion

$$i : G \to G, \qquad i(g) = g^{-1}, \qquad g \in G$$

are smooth maps on this manifold.

The Lie group axioms are those of a regular group, except we know consider the multiplication and inversion to be smooth functions on a manifold. An example of a global Lie group is $SO(3)$, which is the group of rotations in 3d space. Multiplication of these rotations will yield another element in the group. This is different for the definition of a local Lie group.

Definition 2.3 (Local Lie Group, Olver p. 18)**.** An r-parameter local Lie group consist of connected open subsets $V_0 \subseteq V \subseteq \mathbb{R}^r$ containing the origin 0, and smooth maps

$$m : V \times V \to \mathbb{R}^r, \qquad i : V_0 \to V$$

defining the group operation and inversion respectively, with the maps satisfying the following properties.
Associativity: If $x, y, z \in V$, and $m(x, y), m(y, z) \in V$, then $m(x, m(y, z)) = m(m(x, y), z)$.
Identity: For all $x \in V$, $m(0, x) = 0 = m(x, 0)$.
Inverse: For each $x \in V_0$, $m(x, i(x)) = 0 = m(i(x), x)$.
The group axioms are however not necessarily defined everywhere, but always hold near the identity.

The important difference is to note that the multiplication and inverse no longer map from the space of the group G to itself. Multiplying two elements in a subset V of G leads to a new element which can be present outside of V, as can be seen in the following example from Olver.

Example 2.1. Consider the 1-parameter local Lie group $V \subset \mathbb{R}$ with $V = \{x : |x| < 1\}$, where the group multiplication is defined as

$$m(x, y) = \frac{2xy - x - y}{xy - 1} \qquad \forall x, y \in V.$$

Taking $x = y = -\frac{1}{2}$, it indeed follows that $m(-\frac{1}{2}, -\frac{1}{2}) = -2 \notin V$. As the multiplication is only defined within V, there is no way to get back into V using multiplication.
The identity map satisfying the axioms is $i(x) = \frac{x}{2x-1}$. The multiplication is only defined for $|x| < 1$ leading to $|i(x)| < 1$, which is only valid when $V_0 = \{x : |x| < \frac{1}{3}\}$. The space of inverses is thus even smaller than the space where the multiplication is defined.

Note that any global Lie group also satisfies the axioms of a local Lie group, meaning that a global Lie group is just a specific type of local Lie group. For every global Lie group, there exists a local Lie group which is locally isomorphic to the global group around the identity, as stated by the next theorem.

Theorem 2.1 (Olver p. 19)**.** Let $V_0 \subseteq V \subseteq \mathbb{R}^r$ be a local Lie group. Then there exists a global Lie group G and a coordinate chart $\chi : U^* \to V^*$, where U^* contains the identity element, such that $V^* \subseteq V_0$, $\chi(e) = 0$ and

$$\chi(g \cdot h) = m(\chi(g), \chi(h)), \qquad\qquad \chi(g^{-1}) = i(\chi(g))$$

for $g, h \in U^*$.
Furthermore, there is a unique connected, simply connected[1] Lie group G^* having the same properties as above. If G is not G^*, then there exists a covering map $\pi : G^* \to G$ which forms a group homomorphism and both groups are locally isomorphic to each other (G^* is called the simply connected covering Lie group of G).

An example of a Lie group and its simply connected covering Lie group are the groups $SO(3)$ and $SU(2)$ respectively. The first is not simply connected, while the latter is. They are locally isomorphic, meaning that there is a mapping from the local structure of $SO(3)$, given by the

[1]Meaning that not all paths from one point to another and back via another path can be contracted to a point, i.e. there are disjoint parts or holes present in space of the group elements.

Lie algebra (see next definition) to the local structure of $SU(2)$.

Although it is reassuring that there exists a local and global Lie group which are locally isomorphic, it does not provide a method to obtain the global Lie group from a local one. It turns out that not every local Lie group is globalizable into a global Lie group, as associativity does not always hold for a local Lie group when taking products of four or more group elements [1]. One possible method to test if a local group is not globalizable is by utilizing its Lie algebra.

By Lie's First Theorem, each local Lie group G has an associated Lie algebra $\mathfrak{g}$, which is a vector space with a specific product. The Lie algebra can be used to create local representations of the group elements of G around the identity. Although at first glance a Lie algebra might not seem that important, the Lie algebra of a group contains almost all information on the local properties of the group and is what makes Lie group theory so powerful. It allows to replace complicated nonlinear group actions by much simpler linear infinitesimal conditions, which will be used later on to simplify calculations.

Definition 2.4 (Lie Algebra, Olver p. 43)**.** A Lie algebra is a vector space $\mathfrak{g}$ together with a bilinear operation

$$[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g},$$

called the Lie bracket for $\mathfrak{g}$, satisfying the following axioms:
Bilinearity: $[c\mathbf{v} + c'\mathbf{v}', \mathbf{w}] = c[\mathbf{v}, \mathbf{w}] + c'[\mathbf{v}', \mathbf{w}]$, $[\mathbf{v}, c\mathbf{w} + c'\mathbf{w}'] = c[\mathbf{v}, \mathbf{w}] + c'[\mathbf{v}, \mathbf{w}']$
Skew-Symmetry: $[\mathbf{v}, \mathbf{w}] = -[\mathbf{w}, \mathbf{v}]$
Jacobi Identity: $[\mathbf{u}, [\mathbf{v}, \mathbf{w}]] + [\mathbf{w}, [\mathbf{u}, \mathbf{v}]] + [\mathbf{v}, [\mathbf{w}, \mathbf{u}]] = 0$
For all $\mathbf{u}, \mathbf{v}, \mathbf{v}', \mathbf{w}, \mathbf{w}' \in \mathfrak{g}$.

Example 2.2. An example of a Lie algebra is $\mathfrak{so}(3)$, which forms the algebra of the Lie group $SO(3)$. Its elements can be represented by matrices that form a basis in the vector space, which in the case of the defining representation, consist of 3 matrices given by [7]

$$J_x = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad J_y = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \qquad J_z = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2.1}$$

These basis vectors are also called *infinitesimal generators*, which will become apparent in the example after the next definition.

To showcase the connection between a Lie group G and its corresponding Lie algebra $\mathfrak{g}$, the following theorem tells about the connecting method called the exponential map.

Definition 2.5 (Exponential Map, Olver p. 45)**.** Let $\mathbf{v} \neq 0$ be a right-invariant vector field on a Lie group G with Lie algebra $\mathfrak{g}$. There exists a mapping from the Lie algebra to a Lie group, called the exponential map.

$$\exp : \mathfrak{g} \to G$$

This mapping generates a flow by $\mathbf{v}$ through the identity, namely

$$g_\epsilon = \exp(\epsilon\mathbf{v})e = \exp(\epsilon\mathbf{v}),$$

which is defined for all $\epsilon \in \mathbb{R}$ and forms a one-parameter subgroup of G, with

$$g_{\epsilon+\delta} = g_\epsilon \cdot g_\delta, \qquad g_0 = e, \qquad g_\epsilon^{-1} = g_{-\epsilon}.$$

Example 2.3. Take the infinitesimal generator J_z from the Lie algebra $\mathfrak{so}(3)$ from the previous example, and apply the definition of the exponential map. We find a matrix

$$e^{\theta J_z} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.2}$$

which creates rotations around the z axis when multiplied by a vector of coordinates. The mapping forms a 1-parameter Lie subgroup of $SO(3)$ with parameter θ. These rotations form a subset of the elements present in $SO(3)$ for all θ. Furthermore, exponentiating J_x and J_y leads to two additional subgroups of rotations in the y and z axis respectively. Each rotation in 3D space can be seen as 3 separate rotations in each orthogonal direction, and therefore all elements of $SO(3)$ can be created from the three 1-parameter subgroups described above.

Proposition 2.1 (Olver, p. 20)**.** Let G be a connected global Lie group and $U \subset G$ a neighborhood of the identity. Let $U^k = \{g_1 \cdot g_2 \cdot ... \cdot g_k : g_i \in U\}$ be the set of k products of elements of U. Then

$$G = \bigcup_{k=1}^{\infty} U^k. \tag{2.3}$$

This means that each element g of G can be written as a product of elements in U.

Using the proposition above, we see that all the group elements can be found by taking the product of a finite but arbitrarily large amount of group elements. Elements around the identity can be found using the exponential map, and therefore all group elements can be generated using the infinitesimal generators $\mathbf{v_i}$ and taking products of exponential maps, written as

$$g = \exp(\epsilon_1 \mathbf{v_1}) \exp(\epsilon_2 \mathbf{v_2}) ... \exp(\epsilon_k \mathbf{v_k}). \tag{2.4}$$

Finding the group elements this way tends to be easier then finding the most general group element expression. The following sections explain what a symmetry group of differential equations is and how to derive the symmetry group of a given PDE using the infinitesimal generators.

2.2 Symmetry Groups of PDEs

For any PDE, there are p independent variables $x = (x^1, ..., x^p)$ and 1 dependent variable u. The solutions of the PDE will be of the form $u = f(x)$. The space of all possible values for the independent and dependent variables are defined as X and U respectively. The space can be further restricted, for example by only considering a certain domain, given by a manifold $M \subseteq X \times U$. Before the definition of a symmetry group is covered, the notion of a local group of transformations must be defined.

Definition 2.6 (Local Group of Transformations, Olver p. 21)**.** Let M be a smooth manifold. A *local group of transformations*[2] acting on M is given by a local Lie group G, an open subset $\mathscr{U}$ with

$$\{e\} \times M \subseteq \mathscr{U} \subseteq G \times M,$$

where the group action of G is defined, and a smooth map $\Psi : \mathscr{U} \to M$ with the following properties:
(a) If $(h, x) \in \mathscr{U}$, $(g, \Psi(h, x)) \in \mathscr{U}$ and $((g \cdot h), x) \in \mathscr{U}$, then

$$\Psi(g, \Psi(h, x)) = \Psi((g \cdot h), x).$$

(b) For all $x \in M$,

$$\Psi(e, x) = x.$$

(c) If $(g, x) \in \mathscr{U}$, then $(g^{-1}, \Psi(g, x)) \in \mathscr{U}$ and

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

For any element g in G, there is an open submanifold $M_g = \{x \in M : (g, x) \in \mathscr{U}\}$ of M where the transformation created by g is defined. In certain cases the only group element which acts on the total space is the identity element e, in other cases the transformations given by a group element g is defined over all of M. A *global group of transformations* is when $\mathscr{U} = G \times M$, and thus for all elements $g \in G$ the transformation $\Psi(g, x)$ is defined for all $x \in M$.

Example 2.4. Consider a 1-parameter local Lie group G with a Lie algebra $\mathfrak{g}$. Suppose the algebra contains one infinitesimal generator $\mathbf{v} = x^2 \partial_x$, such that each element of G can be expressed as $g_\epsilon = \exp(\epsilon \mathbf{v})$. Let manifold $M = \mathbb{R}$ represent the coordinate space of x, then letting the element g_ϵ act on x yields

$$\begin{aligned}
\Psi(g_\epsilon, x) &= \Psi(\exp(\epsilon \mathbf{v}), x) \\
&= \left(1 + \epsilon \mathbf{v} + \frac{\epsilon^2}{2!}\mathbf{v}^2 + ...\right) x \\
&= \left(x + \epsilon x^2 \partial_x(x) + \frac{\epsilon^2}{2!} x^2 \partial_x(x^2 \partial_x(x)) + ...\right) \\
&= \left(x + \epsilon x^2 + \epsilon^2 x^3 + ...\right) \\
&= \frac{x}{1 - \epsilon x} \qquad \text{for } |\epsilon x| < 1
\end{aligned} \tag{2.5}$$

By letting the local group act on the manifold M, the space has been reduced further such that $\mathscr{U} \subseteq G \times M$ is only defined when $|\epsilon x| < 1$, even if the group element itself may be defined for all ϵ. All the conditions of Ψ are met with $g_\epsilon \in G$, and thus G forms a local group of transformations when acting on M on the domain shown in Figure 1.

[2] All local groups of transformations G acting on M are assumed to be *connected*, which is defined as (Olver, p. 22): (a) G is a connected local Lie group, M is a connected manifold. (b) $\mathscr{U} \subseteq G \times M$ is a connected open set. (c) For each $x \in M$, local group G_x is connected.

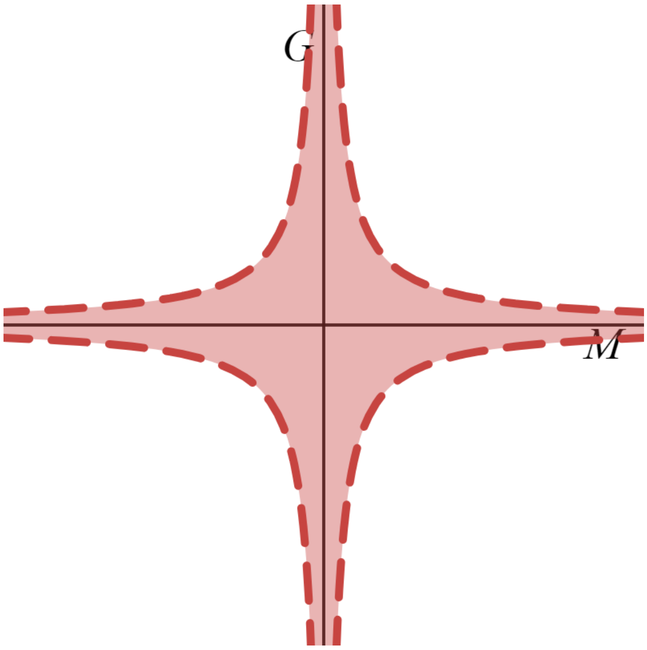


Figure 1: Domain $\mathscr{U}$ of the local group of transformations.

From now on, the mapping $\Psi(g,x)$ will be replaced with $g \cdot x$ for short-hand notation. If we consider the local group of transformations G to be acting on $M \subseteq X \times U$, the transformed coordinates will be denoted as

$$(\tilde{x}, \tilde{u}) \equiv g \cdot (x, u). \tag{2.6}$$

Lie himself addressed the idea of a continuous Lie point symmetry of a given PDE. He considered local groups of point transformations[3] on the space of independent and dependent variables of the PDE, in a continuous manner. Point transformations transform every point in some space, just like the local group of transformations from Definition 2.6. When such a local group of transformations is applied to the space of a PDE, and it maps the set of solutions to itself, then a continuous Lie point symmetry group is obtained.

Definition 2.7 (Symmetry Group, Olver p. 93)**.** A *symmetry group* G_s of a PDE is a local group of transformations G, acting on the space of dependent and independent variables $M \subseteq X \times U$, with the property that if $u = f(x)$ is a solution of the PDE, then $u = g \cdot f(x)$ is also a solution of the PDE if $g \cdot f$ is defined for $g \in G$. A solution is a smooth function $f(x)$ that satisfies the PDE, defined on some subdomain $\Omega \subseteq X$.

Finding the symmetry groups of a PDE is an important goal during the thesis. Each symmetry group can be used to find new solutions of a PDE using a symmetry transformation. So far, only the transformations created by g of the (in)dependent variables have been discussed, not yet how these transformations change a solution $u = f(x)$. Let g be an element from the symmetry group G_s, acting on $M \subseteq X \times U$. The most general transformation is given by $(\tilde{x}, \tilde{u}) = (\Xi_g(x,u), \Phi_g(x,u))$, which has a complicated structure to convert to new solutions

[3]Note that the transformation from a local symmetry, often seen in e.g. quantum mechanics, is different from a local group of transformations, as the latter does not have to be globally defined for all x.

due to the possible nonlinear transformations of u. Fortunately, most variable transformations found in practice and all transformations covered in this thesis will be of the form

$$(\tilde{x}, \tilde{u}) = g \cdot (x, u) = (\Xi_g(x), \Phi_g(x)u) \tag{2.7}$$

If a differential equation is given by some differential operator $D(x)$ acting on u, i.e. $D(x)u = 0$, then applying an element from a local group of transformations changes it into $D(\tilde{x})\tilde{u}$. This can be written in the previous (in)dependent variables as

$$D(\Xi_g(x))\Phi_g(x)u = 0. \tag{2.8}$$

If we consider solutions $u = f(x)$ and substitute $x = \Xi_g^{-1}(x)$, the equation can be rewritten into

$$D(x)\Phi_g(\Xi_g^{-1}(x))f(\Xi_g^{-1}(x)) = 0. \tag{2.9}$$

Now that the differential operator is expressed in its original independent variables again, we know that if $f(x)$ was a solution of $D(x)f(x) = 0$, so is

$$\tilde{f}(x) = \Phi_g(\Xi_g^{-1}(x))f(\Xi_g^{-1}(x)), \tag{2.10}$$

if g is a group element of the symmetry group G_s of the PDE expressed by $D(x)u = 0$. Hence the formula above can be used to find new solutions if the transformations caused by an element of the symmetry group is known, or alternatively to check if a transformation belongs to the symmetry group of the PDE.

Example 2.5. Suppose a PDE is defined on manifold $M = X \times U$ which only has polynomial solutions. To find out if a local group of transformations G acting on M is a symmetry group of the PDE, Equation 2.10 can be used. Consider two transformation groups which change the variables as follows

$$\begin{aligned} G_1 &: (x, u) \to (x + \epsilon, u) \\ G_2 &: (x, u) \to (x^\epsilon, u). \end{aligned} \tag{2.11}$$

The inverse of the first operation is given by $\Xi^{-1}(x) = 1 - \epsilon$, and the second one is given by $\Xi^{-1}(x) = x^{1/\epsilon}$. Let $u = f(x)$ be a polynomial solution to the PDE, giving the new transformed solutions to be found by applying Equation 2.10 as

$$\begin{aligned} \tilde{f}_1(x) &= f(x - \epsilon) \\ \tilde{f}_2(x) &= f(x^{1/\epsilon}). \end{aligned} \tag{2.12}$$

The first transformed solution changes any polynomial into another polynomial, the second does not in general. Therefore the group of transformations G_1 is a symmetry group of this specific PDE, and the second one is not.

There are three distinct notions of groups that should not be confused when calculating the symmetry groups of a PDE. The foundational structure is always a local Lie group G. If an element g of G is applied to a specific space of variables (x, u) on a manifold M, we obtain a local group of transformations of those variables. Lastly, any PDE has its own set of solutions, which determine if the local group of transformations is a symmetry group (G_s) or not. Continuous Lie point symmetry groups and symmetry groups are used interchangeably throughout the thesis, but both refer to the group from Definition 2.7.

2.3 Prolongation

To find the Lie point symmetries of a specific PDE, an algorithmic method has been developed that uses the infinitesimal generators belonging to the Lie algebra of this symmetry group. A short introduction to this method is described below.

If one has a 1-parameter local Lie group G, then its elements can be generated through the exponential map $g_\epsilon = \exp(\epsilon \mathbf{v})$, where $\mathbf{v}$ is in the Lie algebra $\mathfrak{g}$ of G. For infinitesimal values of ϵ, the exponential map reduces to a linear transformation

$$g_\epsilon = 1 + \epsilon \mathbf{v} + O(\epsilon^2) \approx 1 + \epsilon \mathbf{v}. \tag{2.13}$$

Thus when G forms a local group of transformations when acting on a manifold $M \subseteq X \times U$, the transformed variables are found by $(\tilde{x}, \tilde{u}) = g_\epsilon \cdot (x, u)$, which can be written as ([8], p. 60)

$$\begin{aligned} \tilde{x}^i &= x^i + \epsilon \xi^i(x, u) + O(\epsilon^2) \\ \tilde{u} &= u + \epsilon \phi(x, u) + O(\epsilon^2), \end{aligned} \tag{2.14}$$

if $\mathbf{v}$, in its most general form, is written in the following basis

$$\mathbf{v} = \sum_{i=1}^{p} \xi^i(x, u) \frac{\partial}{\partial x^i} + \phi(x, u) \frac{\partial}{\partial u}. \tag{2.15}$$

For infinitesimal ϵ, $O(\epsilon^2)$ can be ignored which reduces the variable transformations to a linear transformation. The assumption of infinitesimal ϵ will remain from now on, and therefore only small variations in (x, u) will be certainly valid from this theory.

To find the symmetry group G_s of a given PDE, we have to restrict the functions ξ^i, ϕ such that the new solution $\tilde{u}(x)$ obtained from Equation 2.10 remains a solution of the original PDE. Finding the constraints that ξ^i, ϕ satisfy can be done by letting the $\mathbf{v}$ act on the PDE and making use of an important theorem later on. To let $\mathbf{v}$ act on the PDE requires it to be "prolonged" to work on the space where all PDEs are defined.

Definition 2.8 (Jet Space, Olver p. 96)**.** Let U_n denote the space of all n-th derivatives of $u \in U$ and let $U^{(n)} \equiv U \times U_1 \times ... \times U_n$. The space $X \times U^{(n)}$ is called the n-th order *jet space* of the space $X \times U$, whose coordinates represent the independent variables, dependent variables and all derivatives up to order n of the dependent variables. If only a part of the underlying space $M \subseteq X \times U$ is considered, we obtain

$$M^{(n)} \equiv M \times U_1 \times ... \times U_n. \tag{2.16}$$

Example 2.6. Consider a PDE with 2 independent variables (x, t) and 1 independent variable u. The space of all first derivatives U_1 is then $U_1 = (u_x, u_t)$, and $U_2 = (u_{xx}, u_{xt}, u_{tt})$. The total space of $U^{(2)}$ is given by $U^{(2)} = U \times U_1 \times U_2$, with coordinates

$$u^{(2)} = (u, u_x, u_t, u_{xx}, u_{xt}, u_{tt}). \tag{2.17}$$

Any PDE of order n is a function $\Delta(x, u^{(n)}) = 0$ which depends on the independent variables x and the dependent variable together with its derivatives $u^{(n)}$. The space of all PDEs is thus $X \times U^{(n)}$. The following theorem will show that the infinitesimal generator $\mathbf{v}$ can be used to obtain the symmetry group G_s of a PDE. As a transformation generated by $\mathbf{v}$ also transforms the original PDE into a different one, it must transform in such a way that the transformed PDE still holds, i.e. $\Delta(\tilde{x}, \tilde{u}^{(n)}) = 0$. Prolonging $\mathbf{v}$ is required to let it act on the space $X \times U^{(n)}$. To find the prolongation of an infinitesimal generator, some additional mathematical tools are introduced for notational purposes.

Definition 2.9. (Olver p. 95) Consider a smooth function $f(x)$, then the k-th partial derivative will be denoted as

$$\partial_{\mathbf{J}} f(x) = \frac{\partial^k f(x)}{\partial x^{j_1} \partial x^{j_2} ... \partial x^{j_k}}, \tag{2.18}$$

where $\mathbf{J} = (j_1, j_2, ..., j_k)$, with $1 \leq j_i \leq p$ for all $i = 1, ..., k$, denotes the integers w.r.t. each independent variable the function is differentiated over. The order of $j_1, ..., j_k$ is not important.

Proposition 2.2 (Total Derivative, Olver p. 109)**.** Given a function $P(x, u^{(n)})$ defined on $M^{(n)} \subseteq X \times U^{(n)}$, the *total derivative* of P w.r.t. x^i has the general form

$$D_i P = \frac{\partial P}{\partial x^i} + \sum_{\mathbf{J}} u_{\mathbf{J},i} \frac{\partial P}{\partial u_{\mathbf{J}}} \tag{2.19}$$

for $\mathbf{J} = (j_1, ..., j_k)$, where

$$u_{\mathbf{J},i} = \frac{\partial u_{\mathbf{J}}}{\partial x^i} = \frac{\partial^{k+1} u}{\partial x^i \partial x^{j_1} \cdots \partial x^{j_k}}. \tag{2.20}$$

The sum of $\mathbf{J}$ ranges over all possible combinations up until k, the length of $\mathbf{J}$, is equal to the highest order derivative n appearing in P.

Example 2.7. Consider a function $P(x, u^{(2)}) = 4x + 2u_x + uu_{xt}$ with independent variables (x, t). The total derivative of P w.r.t. x is found to be

$$\begin{aligned} D_x P &= \frac{\partial P}{\partial x} + u_x \frac{\partial P}{\partial u} + u_{xx} \frac{\partial P}{\partial u_x} + u_{xt} \frac{\partial P}{\partial u_t} + u_{xxx} \frac{\partial P}{\partial u_{xx}} + u_{xxt} \frac{\partial P}{\partial u_{xt}} + u_{xtt} \frac{\partial P}{\partial u_{tt}} \\ &= 4 + 2u_{xx} + u_x u_{xt} + uu_{xxt}. \end{aligned} \tag{2.21}$$

At last, the prolongation of $\mathbf{v}$ is ready to be discussed. The prolongation of $\mathbf{v}$ is defined as the infinitesimal generator of the prolonged 1-parameter group of $\exp(\epsilon \mathbf{v})$ acting on $(x, u^{(n)})$, instead of (x, u) as before.

Theorem 2.2 (Generator Prolongation, Olver p. 110)**.** Let $\mathbf{v}$ be a vector field as stated in Equation 2.15, defined on subset $M \subseteq X \times U$. The n-th order prolongation of $\mathbf{v}$ is the vector field

$$\mathrm{pr}^{(n)} \mathbf{v} = \mathbf{v} + \sum_{\mathbf{J}} \phi^{\mathbf{J}}(x, u^{(n)}) \frac{\partial}{\partial u_{\mathbf{J}}}, \tag{2.22}$$

defined on $M^{(n)} \subseteq X \times U^{(n)}$, where $\mathbf{J} = (j_1, j_2, ..., j_k)$ with $1 \leq j_k \leq p$ and $1 \leq k \leq n$. The coefficient functions $\phi^{\mathbf{J}}$ are given by

$$\phi^{\mathbf{J}}(x, u^{(n)}) = D_{\mathbf{J}} \left(\phi - \sum_{i=1}^{p} \xi^i \frac{\partial u}{\partial x^i} \right) + \sum_{i=1}^{p} \xi^i \frac{\partial u_{\mathbf{J}}}{\partial x^i}, \tag{2.23}$$

where $D_{\mathbf{J}}$ is the total derivative w.r.t. $\mathbf{J}$ and $u_{\mathbf{J}} = \frac{\partial u}{\partial x^{\mathbf{J}}}$.

The prolongation of a vector field becomes a lengthy expression rather quickly when considering many dependent and independent variables. The examples in the following sections will be straightforward exercises to become familiar with the method. Finally, we make use of the following theorem to determine the symmetry group G_s using the prolongation of $\mathbf{v}$.

Theorem 2.3 (Infinitesimal Criterion, Olver p. 104)**.** Suppose $\Delta(x, u^{(n)}) = 0$ is a differential equation defined over $M \subseteq X \times U$. If G is a local group of transformations acting on M and

$$\mathrm{pr}^{(n)}\mathbf{v}[\Delta(x, u^{(n)})] = 0 \tag{2.24}$$

whenever $\Delta(x, u^{(n)}) = 0$ for every infinitesimal generator $\mathbf{v}$ of G, then G is a symmetry group of the system.

Applying Theorem 2.3 provides conditions for the utility functions ξ^i and ϕ of Equation 2.15 and solving for these conditions gives the infinitesimal generators of the Lie algebra corresponding to the local symmetry group G_s.

Example 2.8. Consider a differential equation with independent variables (x, y) and dependent variable u. The most general vector field from Equation 2.15 then becomes

$$\mathbf{v} = \xi^1(x, y, u)\partial_x + \xi^2(x, y, u)\partial_y + \phi(x, t, u)\partial_u. \tag{2.25}$$

If Theorem 2.3 is used and the resulting conditions have been used to find the functions ξ^1, ξ^2 and ϕ, one could for some specific differential equation obtain $\xi^1 = -y$, $\xi^2 = x$ and $\phi = 0$. This gives the infinitesimal generator $\mathbf{v} = -y\partial_x + x\partial_y$. Applying the exponential map from Definition 2.5 and letting it act on the variables (x, y, u), results in

$$\begin{aligned}
e^{\epsilon \mathbf{v}} x &= \left(1 + \epsilon \mathbf{v} + \frac{\epsilon^2}{2!}\mathbf{v}^2 + ...\right) x = \left(x - \epsilon y - \frac{\epsilon^2}{2!}x + \frac{\epsilon^3}{3!}y + ...\right) = \cos(\epsilon)x - \sin(\epsilon)y \\
e^{\epsilon \mathbf{v}} y &= \left(1 + \epsilon \mathbf{v} + \frac{\epsilon^2}{2!}\mathbf{v}^2 + ...\right) y = \left(y + \epsilon x - \frac{\epsilon^2}{2!}y - \frac{\epsilon^3}{3!}x + ...\right) = \sin(\epsilon)x + \cos(\epsilon)y \\
e^{\epsilon \mathbf{v}} u &= \left(1 + \epsilon \mathbf{v} + \frac{\epsilon^2}{2!}\mathbf{v}^2 + ...\right) u = (u + 0 + 0 + ...) = u
\end{aligned} \tag{2.26}$$

The 1-parameter local group of transformations can be identified as

$$G : (\cos(\epsilon)x - \sin(\epsilon)y, \sin(\epsilon)x + \cos(\epsilon)y, u). \tag{2.27}$$

Such groups transformations are equal to rotating the x and y variables, which means that the symmetry group G_s is locally similar to the group $SO(2)$.

2.4 Extension of the Local Symmetry Group

Ultimately, the result we are after is to find the local group of transformations that contains all the elements which leave the set of solutions to a PDE invariant. The symmetry group defined by Definition 2.7 provides information about a local group of transformations G leaving the set of solutions invariant, but the prolongation technique from the previous section requires infinitesimal transformations. Therefore the symmetry groups found with Theorem 2.3 are only known to hold for infinitesimal ϵ, but what happens when we apply elements g_ϵ to a solution with non-infinitesimal ϵ?

The theory described by Olver and others contain little information about these extensions. What happens to the solutions when considering non-infinitesimal transformations will be explored in the following sections.

There are also Lie contact symmetries and Lie-Backlünd symmetries, which includes higher order derivatives of u as arguments in the utility functions ξ^i and ϕ of Equation 2.15. These will not be considered in this thesis.

3 Logistic Equation

The logistic equation is a first order 1-dimensional non-linear ordinary differential equation, introduced by Pierre-Francois Verhulst in 1838 to model population growth, and has the following form:

$$\frac{dP}{dt} = rP\left(1 - \frac{P}{k}\right) \tag{3.1}$$

where $P = P(t)$ is a function of the population size over time, and r, k are real constants referring to the growth rate and carrying capacity respectively.

For small values of P, the solution will behave like an exponential function, $P \sim e^{rt}$, while for large values of P the growth of the solution keeps diminishing by the non-linear term, up until $P = k$ where the growth stops. This growth can be seen when solving the ODE analytically to give the most general solution, in this case done with `MATHEMATICA`, yielding the solution

$$P(t) = \frac{kP_0e^{rt}}{(k - P_0) + P_0e^{rt}}, \tag{3.2}$$

where $P_0 = P(0)$. Knowledge of the solution is not required for finding the symmetry group of the ODE, however it will nicely illustrate the effects of each transformation when plotted.

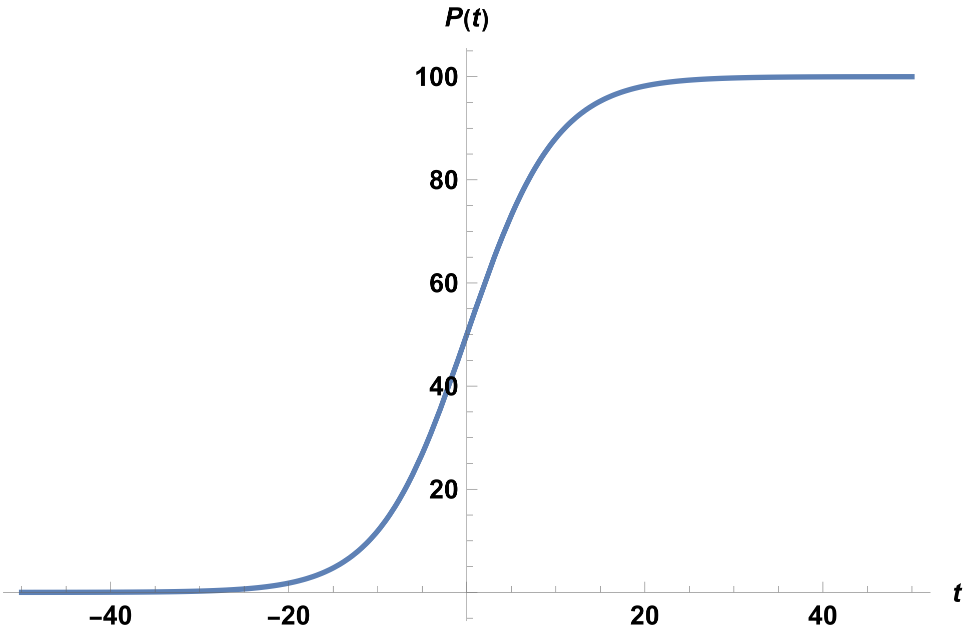


Figure 2: Plot of solution (Equation 3.2) of the logistic equation for $P_0 = 50$, $k = 100$ and $r = 0.2$.

The Lie point symmetry of this system is a local symmetry group G_s, where each element g in G_s transforms the dependent and independent coordinates such that the transformed solution will satisfy the ODE in the transformed coordinates. This is denoted as $g\cdot(t, P) \to (\tilde{t}, \tilde{P})$, where $\tilde{P}$ is a solution to the ODE in the new transformed coordinates, i.e. $\Delta(\tilde{t}, \tilde{P}) = 0$ if $\Delta(t, P) = 0$. The following sections will discuss the process of finding G_s by utilizing Theorem 2.3, as well as showing how these transformations can be used to discover transformations of the solutions to the original ODE, using Equation 2.10.

3.1 Deriving Lie Point Symmetries

The associated local group of transformations of the symmetry group G_s of the ODE can be found by prolonging the infinitesimal generators according to Theorem 2.3. Applying the prolongation on a general vector field and letting it act on the differential equation, will give the infinitesimal generators of G_s if the expression yields zero. Since transformations on the space (t, P), equivalent to $X \times U \cong \mathbb{R}^2$, are considered, note that P is no longer treated as a function of t in the derivation below of the infinitesimal generators.

The most general vector field corresponding to the Lie algebra of G_s is given by Equation 2.15

$$\mathbf{v} = \xi(t, P)\partial_t + \phi(t, P)\partial_P \tag{3.3}$$

where ∂_t denotes the partial derivative with respect to t. As Equation 3.1 only depends on the first order derivative of P, only the first order prolongation is required, written as

$$\mathrm{pr}^{(1)}\mathbf{v} = \mathbf{v} + \phi^t(t, P)\partial_{P_t}. \tag{3.4}$$

At this point Theorem 2.3 can be applied to find the conditions for the infinitesimal generators of G. Using the prolonged vector field from Equation 3.4, this yields

$$\begin{aligned}\mathrm{pr}^{(1)}\mathbf{v}[\Delta] &= (\xi\partial_t + \phi\partial_P + \phi^t\partial_{P_t})\left[P_t - rP + \frac{r}{k}P^2\right] \\ &= -r\phi + \frac{2r}{k}P + \phi^t = 0 \end{aligned} \tag{3.5}$$

Using the definition of the total derivative from Proposition 2.2, ϕ^t can be expanded into

$$\begin{aligned}\phi^t &= D_t(\phi - \xi P_t) + \xi P_{tt} \\ &= D_t(\phi) - P_t D_t(\xi) \\ &= \phi_t + P_t\phi_P - P_t\xi_t - {P_t}^2\xi_P\end{aligned}$$

Substituting this result into Equation 3.5 gives

$$\begin{aligned} r\phi - \frac{2r}{k}\phi P &= \phi_t + P_t\phi_P - P_t\xi_t - {P_t}^2\xi_P \\ r\phi - \frac{2r}{k}P &= \phi_t + (r\phi_P - r\xi_t)P - \left(\frac{r}{k}\phi_P - \frac{r}{k}\xi_t + r^2\xi_P\right)P^2 + \frac{2r^2}{k}\xi_P P^3 - \frac{r^2}{k^2}\xi_P P^4\end{aligned}$$

by substituting P_t with $rP - \frac{r}{k}P$ in the second step and ordering them by powers of P. The determining equations are given by each monomial of P, and are displayed below:

$$\text{(a)}\quad \phi_t = r\phi \qquad \text{(b)}\quad \frac{2r}{k}\phi = (r\phi_P - r\xi_t) \qquad \text{(c)}\quad -\frac{r}{k}\phi_P + \frac{r}{k}\xi_t - r^2\xi_P = 0$$

$$\text{(d)}\quad \frac{2r^2}{k}\xi_P = 0 \qquad \text{(e)}\quad \frac{r^2}{k^2}\xi_P = 0$$

Solving these differential equations gives the infinitesimal generators and in turn the local symmetries transformations. From (d), $\xi(t, P) = \xi(t)$. This sets $\phi_P = \xi_t$ in (c), but that means $\phi = 0$ from (b). Therefore $\xi(t)$ can only be constant in t, and thus the functions of the vector field are given by

$$\xi(t, P) = A, \qquad \phi(t, P) = 0,$$

where $A \in \mathbb{R}$. A is a free parameter, and therefore the simplest infinitesimal generator is found when $A = 1$. Plugging this result into Equation 3.3 gives a single infinitesimal generator

$$\mathbf{v_1} = \partial_t. \tag{3.6}$$

It turns out that the Lie algebra $\mathfrak{g}$ of the symmetry group of the logistic equation is spanned by only one infinitesimal generator.

From Definition 2.6, each generator generates a 1-parameter group of transformations by applying the exponential map on the space of independent and dependent variables (t, P), as done below:

$$e^{\epsilon \mathbf{v_1}} t = \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) t = t + \epsilon + 0 + 0 + ... = t + \epsilon$$
$$e^{\epsilon \mathbf{v_1}} P = \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) P = P + 0 + 0 + ... = P$$

The total transformation is thus $(\tilde{t}, \tilde{P}) = g_\epsilon \cdot (t, P) = (t + \epsilon, P)$ and forms the following local 1-parameter group of transformations:

$$G_1 : (t + \epsilon, P)$$

As the group only adds a constant term in the coordinate, it is commonly called the translational group, which will also be apparent from the transformation on the solution displayed in the next section.

3.2 Finding Global Symmetry

From Theorem 2.3, the group given above locally forms the symmetry group G_s, i.e. for small ϵ such that the elements are close to the identity. The question of interest is whether this symmetry exists for larger ϵ, and possibly even all ϵ such that the symmetry group G_s is actually a global symmetry group.

To confirm whether the transformation holds for larger ϵ, the transformed solution must be found and be plugged back into the logistic equation. If the symmetry is a global one, the equation should still hold under non-infinitesimal values of ϵ.

Using Equation 2.10, the transformation yields $\Phi_g(t) = 1$ and $\Xi_g(t) = t + \epsilon$. The inverse $\Xi_g^{-1}(t)$ is $\Xi_g^{-1}(t) = t - \epsilon$, which leads to a new solution of the form $\tilde{P}(t) = P(\Xi_g^{-1}(t)) = P(t - \epsilon)$, where t is the original coordinate. Using $P(t - \epsilon)$ on Equation 3.2 and substituting it in the logistic equation, the ODE still vanishes for all ϵ. Therefore the local symmetry group G_1 of the logistic equation is actually a global symmetry group.

Since the prolongation technique only leaves one possible infinitesimal generator, the global group G_1 forms the total symmetry group G_s of the logistic equation. This group is known as the time translation group, which can be clearly understood from looking at Figure 3. Each value of P of the original solution is shifted by some constant factor ϵ, thus being a translation in time.

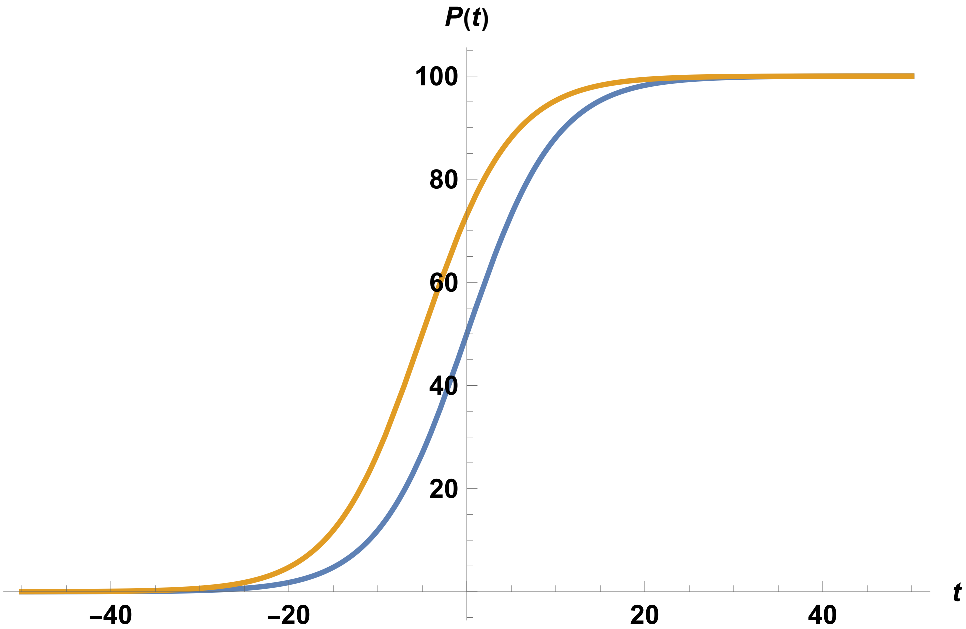


Figure 3: Plot of $P(t)$ *(blue)* and $P(t+5)$ *(orange)* from Equation 3.2, both with $P_0 = 50$, $k = 100$ and $r = 0.2$.

Numerical analysis can also be performed to show that $P(t-\epsilon)$ holds for large values of ϵ. Figure 4 shows the cumulative absolute difference between the left and right hand side of Equation 3.1 for $P(t+\epsilon)$ and $P(e^{\epsilon}t)$ for different ϵ in $t \in [-50, 50]$. $P(e^{\epsilon}t)$ represent a transformation obtained when using the generator $\mathbf{v} = t\partial_t$. As this transformation is not found using the prolongation technique, it does not map the set of solutions to solutions, and therefore the error increases when increasing ϵ.

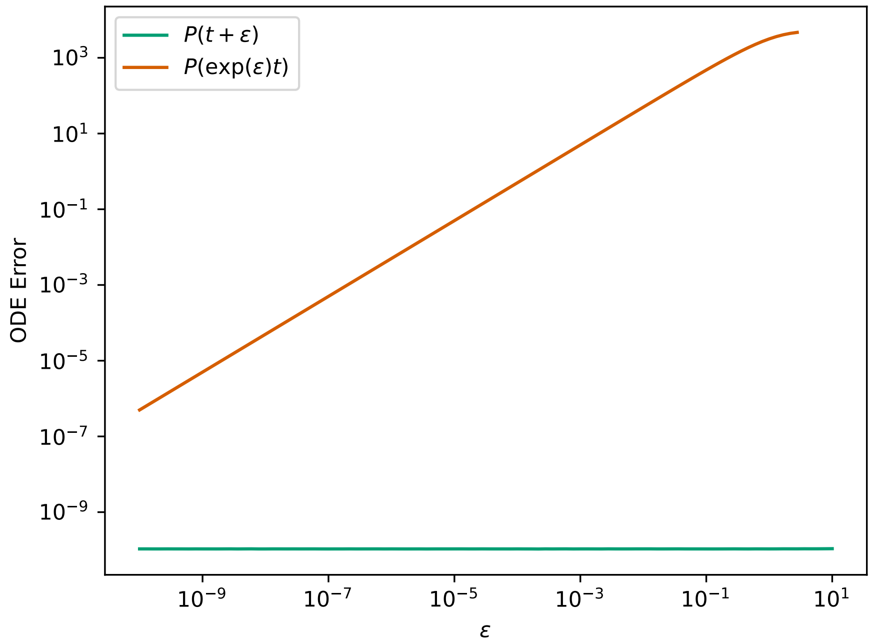


Figure 4: Plot of the cumulative absolute difference between the right and left hand side of the logistic equation for $P(t+\epsilon)$ *(green)* and $P(\exp(\epsilon)t)$ *(red)* for different ϵ with 5000 evenly spaced points between $t \in [-50, 50]$.

4 Heat Equation

The method of prolongation is applicable to both ordinary and partial differential equations. This section shows the method for a (1+1) dimensional linear partial differential equation of second order. The heat equation is a linear PDE, and models how heat diffuses through space over time. In one spatial dimension, the heat equation is given by

$$u_t(x,t) = u_{xx}(x,t). \tag{4.1}$$

A general solution can be found using Fourier series and performing a separation of variables. Such a solution consist of an infinite sum of sine and cosine terms, complicating the application of some transformations to the coordinate variables and performing numerical calculations. Therefore a solution of the form

$$u(x,t) = 1 + \sinh(c_1 + c_2 x + c_2^2 t) + \cosh(c_1 + c_2 x + c_2^2 t) = 1 + e^{c_1 + c_2 x + c_2^2 t}, \tag{4.2}$$

where c_1, c_2 are constants, is applied when performing numerical checks later on in this chapter. The solution above provides easier transformations while not loosing too much complexity over the Fourier solution and does not depend on infinite sums.

4.1 Deriving Lie Point Symmetries

The vector field contains an additional spatial dimension compared to the logistic equation and thus can be written most generally in the following form:

$$\mathbf{v} = \xi^1(x,t,u)\partial_x + \xi^2(x,t,u)\partial_t + \phi(x,t,u)\partial_u. \tag{4.3}$$

The heat equation is a second order PDE and therefore requires a second order prolongation, which together with the infinitesimal criterion yields

$$\mathrm{pr}^{(2)}\mathbf{v}[\Delta] = \phi^t - \phi^{xx} = 0 \tag{4.4}$$

where ϕ^i is obtained from Equation 2.23, as shown below:

$$\begin{aligned}
\phi^t &= D_t(\phi - \xi^1 u_x - \xi^2 u_t) + \xi^1 u_{tx} + \xi^2 u_{tt} \\
&= D_t(\phi) - u_x D_t(\xi^1) - u_t D_t(\xi^2) \\
&= \phi_t - \xi^1_t u_x + (\phi_u - \xi^2_t) u_t - \xi^1_u u_x u_t - \xi^2_u u_t^2
\end{aligned}$$

and similarly for ϕ^{xx}

$$\begin{aligned}
\phi^{xx} &= D_x(D_x(\phi - \xi^1 u_x - \xi^2 u_t)) + \xi^1 u_{xxx} + \xi^2 u_{xxt} \\
&= D_x^2(\phi) - u_x D_x^2(\xi^1) - u_t D_x^2(\xi^2) - 2u_{xx} D_x(\xi^1) - 2u_{xt} D_x(\xi^2) \\
&= \phi_{xx} + (2\phi_{xu} - \xi^1_{xx}) u_x - \xi^2_{xx} u_t + (\phi_{uu} - 2\xi^1_{xu}) u_x^2 - 2\xi^2_{xu} u_x u_t - \xi^1_{uu} u_x^3 \\
&\quad - \xi^2_{uu} u_x^2 u_t + (\phi_u - 2\xi^1_x) u_{xx} - 2\xi^2_x u_{xt} - 3\xi^1_u u_x u_{xx} - \xi^2_u u_t u_{xx} - 2\xi^2_u u_x u_{xt}
\end{aligned}$$

Using the condition from Equation 4.4, and the fact that $u_t = u_{xx}$, we obtain an overdetermined system of 10 differential equations for ϕ, ξ^1 and ξ^2 when equating derivatives of u. These equations are

$$\begin{array}{llllll}
\text{(a)} & \phi_t = \phi_{xx} & \text{(b)} & -\xi^1_t = 2\phi_{xu} - \xi^1_{xx} & \text{(c)} & \phi_u - \xi^2_t = -\xi^2_{xx} + \phi_u - 2\xi^1_x \\
\text{(d)} & 0 = \phi_{uu} - 2\xi^1_{xu} & \text{(e)} & -\xi^1_u = -2\xi^2_{xu} - 3\xi^1_u & \text{(f)} & -\xi^2_u = -\xi^2_u \\
\text{(h)} & 0 = -\xi^1_{uu}, & \text{(i)} & 0 = -\xi^2_u & \text{(j)} & 0 = -2\xi^2_x
\end{array}$$

where $\xi^2_u = 0$ appears multiple times. These conditions provide the necessary restrictions to determine solutions for ξ^1, ξ^2 and ϕ.

Let us denote $\xi^1 = f(x,t,u)$, $\xi^2 = g(x,t,u)$ and $\phi = h(x,t,u)$. From (i,j),

$$\xi^2 = g(t). \tag{4.5}$$

Plugging this into (e) sets $\xi^1 = f(x,t)$.
From (c), $-\xi^2_t = -2\xi^1_x$, which can be converted to $-\xi^2_{tx} = -2\xi^1_{xx}$ with the first coefficient being 0. Therefore $\xi^1 = \mu(t)x + \nu(t)$. From (d), $\phi_{uu} = 0$ and therefore

$$\phi = \beta(x,t)u + \alpha(x,t). \tag{4.6}$$

From (c), the new definition of ξ^1 gives $g_t(t) = 2\mu(t)$, hence we have $\mu(t) = \frac{1}{2}g_t(t)$ which can be substituted back in ξ^1 to obtain

$$\xi^1 = \frac{1}{2}g_t(t)x + \nu(t). \tag{4.7}$$

From (b), $-\xi^1_t = 2\phi_{xu}$. This gives $-\frac{1}{2}g_{tt}(t)x + \nu_t(t) = \beta_x(x,t)$. Solving for β gives

$$\beta(x,t) = -\frac{1}{4}g_{tt}(t)x^2 + \nu_t(t)x + k(t),$$

where $k(t)$ is any function of t.

Finally, use (a) to get $-\frac{1}{4}g_{ttt}(t)x^2u + \nu_{tt}(t)xu + k_t(t)u + \alpha_t = -\frac{1}{2}g_{tt}(t)u + \alpha_{xx}$. If $\alpha(x,t)$ is a solution to the heat equation, $-\frac{1}{4}g_{ttt}(t)x^2u + \nu_{tt}(t)xu + k_t(t)u = -\frac{1}{2}g_{tt}(t)u$ remains. The most general solution can be found by solving

$$-\frac{1}{4}g_{ttt}(t)x^2 + \nu_{tt}(t)x + k_t(t) = -\frac{1}{2}g_{tt}(t).$$

The expression has to hold for all x and therefore $g_{ttt}(t) = 0$, $\nu_{tt}(t) = 0$ and $k_t(t) = -\frac{1}{2}g_{tt}(t)$. The first condition gives $g(t) = c_1t^2 + c_2t + c_3$ and the second one yields $\nu(t) = c_4t + c_5$. Lastly, $k_t(t) = -\frac{1}{2}(2c_1) = -c_1$ and thus $k(t) = -c_1t + c_6$. Plugging these back into Equations 4.5, 4.6 and 4.7, the following functions are found

$$\begin{aligned}
\xi^1(x,t,u) &= c_1tx + \frac{1}{2}c_2x + c_4t + c_5 \\
\xi^2(x,t,u) &= c_1t^2 + c_2t + c_3 \\
\phi(x,t,u) &= \left(-\frac{1}{2}c_1x^2 + c_4x - c_1t + c_6\right)u + \alpha(x,t)
\end{aligned}$$

where c_i are arbitrary constants and $\alpha(x,t)$ is any function satisfying the heat equation. Since the ordering and size of the constants is not important, they can be redefined into the following, allowing for a nice order of the generators and simpler calculations later on.

$$\begin{aligned}
\xi^1(x,t,u) &= c_1 + c_4x + 2c_5t + 4c_6xt \\
\xi^2(x,t,u) &= c_2 + 2c_4t + 4c_6t^2 \\
\phi(x,t,u) &= (c_3 - c_5x - c_6(x^2 + 2t))u + \alpha(x,t)
\end{aligned}$$

The infinitesimal generators can be found by plugging in the functions above in Equation 4.3 and grouping all terms containing a specific constant c_i. Seven generators are obtained,

$$\mathbf{v_1} = \partial_x \tag{4.8a}$$
$$\mathbf{v_2} = \partial_t \tag{4.8b}$$
$$\mathbf{v_3} = u\partial_u \tag{4.8c}$$
$$\mathbf{v_4} = x\partial_x + 2t\partial_t \tag{4.8d}$$
$$\mathbf{v_5} = 2t\partial_x - xu\partial_u \tag{4.8e}$$
$$\mathbf{v_6} = 4tx\partial_x + 4t^2\partial_t - (x^2 + 2t)u\partial_u \tag{4.8f}$$
$$\mathbf{v}_\alpha = \alpha(x,t)\partial_u \tag{4.8g}$$

where the first six infinitesimal generators form a finite dimensional Lie algebra and the final generator is an infinite dimensional Lie subalgebra.

Applying the exponential map on the variables $e^{\epsilon\mathbf{v_i}}(x,t,u) = (\tilde{x},\tilde{t},\tilde{u})$ for $i = 1,...,6,\alpha$, the following 1-parameter groups of transformations are found

$$G_1: \quad (x+\epsilon, t, u) \tag{4.9a}$$
$$G_2: \quad (x, t+\epsilon, u) \tag{4.9b}$$
$$G_3: \quad (x, t, e^{\epsilon}u) \tag{4.9c}$$
$$G_4: \quad (e^{\epsilon}x, e^{2\epsilon}t, u) \tag{4.9d}$$
$$G_5: \quad (x+2\epsilon t, t, e^{-\epsilon x-\epsilon^2 t}u) \tag{4.9e}$$
$$G_6: \quad \left(\frac{x}{1-4\epsilon t}, \frac{t}{1-4\epsilon t}, \sqrt{1-4\epsilon t}\exp\left(-\frac{\epsilon x^2}{1-4\epsilon t}\right)u\right) \qquad \text{for } |\epsilon t| < \frac{1}{4} \tag{4.9f}$$
$$G_\alpha: \quad (x, t, u+\epsilon\alpha(x,t)) \tag{4.9g}$$

where the specific derivation of G_6 can be found in the appendix (subsection A). The other groups are found similarly as done in section 3.

4.2 Finding Global Symmetries

All local 1-parameter transformation groups except G_6 are defined for all ϵ and are thus also global groups of transformations. It also turns out that for these global transformation groups, the transformed solution of Equation 4.2 obtained by applying Equation 2.10 always yields new solutions that satisfy the heat equation. So even though the prolongation technique only provides the generators for infinitesimal transformations, the global transformations groups are global symmetry groups.

An example of G_5 applied to the solution from Equation 4.2 is shown in Figure 5, where ϵ is varied up until large values, well above the limit of what can be considered infinitesimal. Numerical calculations are done by choosing a solution, preferably the most general solution if available, transforming it with Equation 2.10 and symbolically calculating the derivatives of the transformed solution. The numerical difference between the right and left hand side is calculated for all points in a range, repeated for different values of ϵ and then plotted.

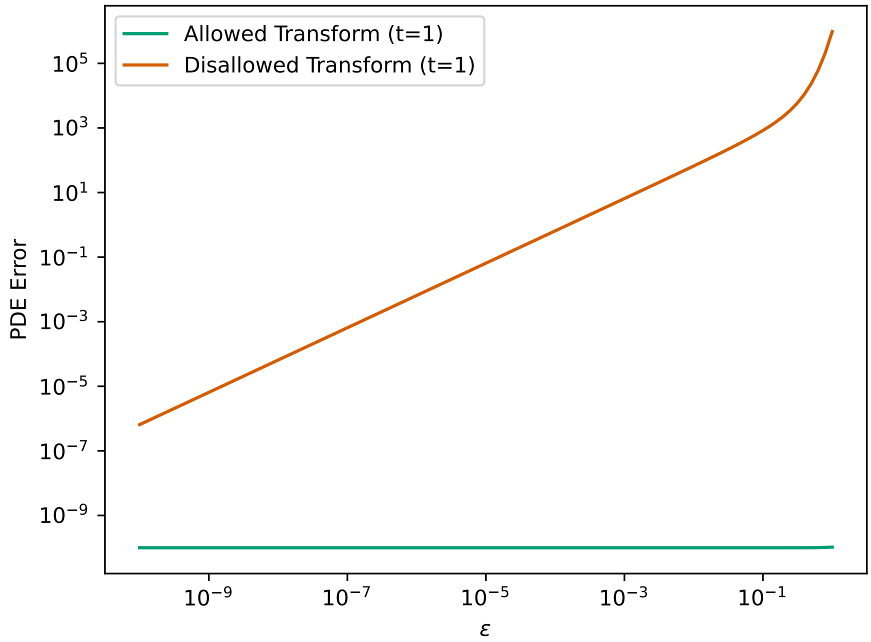


Figure 5: Plot of the cumulative absolute value of $u_t - u_{xx}$ for the transformed solution from G_5 *(green)* and the slightly different transformation $(x + 2\epsilon t, t, \exp(-\epsilon x + \epsilon^2 t)u)$ *(orange)* which does not form a symmetry group, using $t = 1$ and 5000 evenly spaced points of $x \in [-5, 5]$.

In Figure 5, a clear distinction is visible between the allowed transformation and the disallowed transformation. For smaller values of ϵ the disallowed transformation might be within floating point error range, but the error clearly rises for larger ϵ. The allowed transformations sometimes has a small error due to floating point inaccuracies.

The 1-parameter transformation group G_6 does however have a restriction on the values ϵ can attain. For $|\epsilon t| \geq \frac{1}{4}$, the geometric series can no longer be used and there exists no closed-form expression for G_6 above this limit. The group G_6 is thus the first example of a truly local group of transformations, which also restricts the total symmetry group G_s of the heat equation.
If the solution given in Equation 4.2 is transformed with Equation 2.10 and the derivatives are calculated with a program like `MATHEMATICA`, the difference between the right and left hand side does give zero regardless of value of ϵ and t, even for $|\epsilon t| > \frac{1}{4}$. The restriction thus comes purely from the local transformation group. This makes G_6 a symmetry group of the heat equation, but only up to $|\epsilon t| < \frac{1}{4}$. Due to the upper bound being restricted by both the group (ϵ) and the domain of the PDE (t), this makes for an interesting symmetry group as its domain $\mathscr{U}$ is dependent on the range of possible t values of the PDE that is considered.

When combining these symmetry groups, the resulting total symmetry group will be restricted by the local symmetry group created by G_6. Something interesting about its domain $\mathscr{U}$ is that it depends on the amount of products of the exponential map that are taken. For example, if we just consider elements $g_\epsilon = \exp(\epsilon_i)\mathbf{v_i}$, for any i, acting on M, the domain $\mathscr{U}$ is given by

$$(\epsilon_1, ..., \epsilon_5, \epsilon_6) \in \left(\mathbb{R}, ..., \mathbb{R}, |\epsilon_6 t| < \frac{1}{4}\right),$$

where x, t can be any value as long as $|\epsilon_6 t| < \frac{1}{4}$. The moment we start considering elements that consist of products of $\exp(\epsilon_i \mathbf{v_i})$ and $\exp(\epsilon_6 \mathbf{v_6})$, the domain shrinks further. For instance, first scaling the independent variables with $\exp(\epsilon_4 \mathbf{v_4})$ and then applying $\exp(\epsilon_6 \mathbf{v_6})$, the domain is only defined for $|\epsilon_6 \exp(2\epsilon_4)t| < \frac{1}{4}$. Performing the same operations but in reverse order leaves the domain unchanged at $|\epsilon_6 t| < \frac{1}{4}$. The order of multiplication of elements thus also matters for the domain $\mathscr{U}$ of the total symmetry group.

4.3 Lie Algebra and Global Group Equivalent

As the heat equation has multiple generators, the Lie algebra contains useful information about its corresponding Lie group structure. The infinitesimal generators give rise to the following commutator table. The generator $\mathbf{v}_\alpha$ is an infinite-dimensional generator, as $\alpha(x,t)$ is any function satisfying the heat equation. Calculating $[\mathbf{v_i}, \mathbf{v}_\alpha]$ for $i = 1,..,6$ returns a generator which belongs to the infinite-dimensional generator, while $[\mathbf{v_i}, \mathbf{v_j}]$ for $i, j = 1, ..., 6$ always returns a generator $\mathbf{v_k}$ with $k = 1, ..., 6$ and therefore the infinite-dimensional generator can be kept separate from the other generators. The Lie algebra can be seen as a *semidirect sum* between the finite-dimensional Lie algebra spanned by $\{\mathbf{v_1}, ..., \mathbf{v_6}\}$ and the infinite-dimensional Lie algebra spanned by $\mathbf{v}_\alpha$. Note that the infinite-dimensional generator is only present in linear PDEs.

	$\mathbf{v_1}$	$\mathbf{v_2}$	$\mathbf{v_3}$	$\mathbf{v_4}$	$\mathbf{v_5}$	$\mathbf{v_6}$	$\mathbf{v}_\alpha$
$\mathbf{v_1}$	0	0	0	$\mathbf{v_1}$	$-\mathbf{v_3}$	$2\mathbf{v_5}$	$\mathbf{v}_{\alpha_\mathbf{x}}$
$\mathbf{v_2}$	0	0	0	$2\mathbf{v_2}$	$2\mathbf{v_1}$	$4\mathbf{v_4} - 2\mathbf{v_3}$	$\mathbf{v}_{\alpha_\mathbf{t}}$
$\mathbf{v_3}$	0	0	0	0	0	0	$-\mathbf{v}_\alpha$
$\mathbf{v_4}$	$-\mathbf{v_1}$	$-2\mathbf{v_2}$	0	0	$\mathbf{v_5}$	$2\mathbf{v_6}$	$\mathbf{v}_{\alpha'}$
$\mathbf{v_5}$	$\mathbf{v_3}$	$-2\mathbf{v_1}$	0	$-\mathbf{v_5}$	0	0	$\mathbf{v}_{\alpha''}$
$\mathbf{v_6}$	$-2\mathbf{v_5}$	$-4\mathbf{v_4} + 2\mathbf{v_3}$	0	$-2\mathbf{v_6}$	0	0	$\mathbf{v}_{\alpha'''}$
$\mathbf{v}_\alpha$	$-\mathbf{v}_{\alpha_\mathbf{x}}$	$-\mathbf{v}_{\alpha_\mathbf{t}}$	$\mathbf{v}_\alpha$	$-\mathbf{v}_{\alpha'}$	$-\mathbf{v}_{\alpha''}$	$-\mathbf{v}_{\alpha'''}$	0

Table 1: Commutator table of $[\mathbf{v_i}, \mathbf{v_j}]$, with row i and column j, of the infinitesimal generators from the heat equation

Studying the table reveals that $\mathbf{v_1}$, $\mathbf{v_3}$ and $\mathbf{v_5}$ form a subalgebra. This subalgebra is isomorphic to Heisenberg algebra $\mathfrak{h}_3$, which satisfies $[X,Y] = Z, [X,Z] = 0, [Y,Z] = 0$. This isomorphism can be realized when performing the transformations $\mathbf{v_1} \to -Y$, $\mathbf{v_3} \to -Z$, $\mathbf{v_5} \to X$.

The three remaining generators can be transformed into a Lie algebra isomorphic to $\mathfrak{sl}(2,\mathbb{R})$, but requires an additional transformation. The commutation relations of this algebra are $[H,A] = 2A, [H,B] = -2B, [A,B] = H$. However, Table 1 shows that $[\mathbf{v_2}, \mathbf{v_6}] = 4\mathbf{v_4} - 2\mathbf{v_3}$, and $\mathbf{v_3}$ belongs to the $\mathfrak{h}_3$ algebra. Defining the new generator $\mathbf{v_4}' = \mathbf{v_4} - \frac{1}{2}\mathbf{v_3}$, the following table is obtained.

	$\mathbf{v_1}$	$\mathbf{v_2}$	$\mathbf{v_3}$	$\mathbf{v_4}'$	$\mathbf{v_5}$	$\mathbf{v_6}$	$\mathbf{v}_\alpha$
$\mathbf{v_1}$	0	0	0	$\mathbf{v_1}$	$-\mathbf{v_3}$	$2\mathbf{v_5}$	$\mathbf{v}_{\alpha_\mathbf{x}}$
$\mathbf{v_2}$	0	0	0	$2\mathbf{v_2}$	$2\mathbf{v_1}$	$4\mathbf{v_4}'$	$\mathbf{v}_{\alpha_\mathbf{t}}$
$\mathbf{v_3}$	0	0	0	0	0	0	$-\mathbf{v}_\alpha$
$\mathbf{v_4}'$	$-\mathbf{v_1}$	$-2\mathbf{v_2}$	0	0	$\mathbf{v_5}$	$2\mathbf{v_6}$	$\mathbf{v}_{\alpha'}$
$\mathbf{v_5}$	$\mathbf{v_3}$	$-2\mathbf{v_1}$	0	$-\mathbf{v_5}$	0	0	$\mathbf{v}_{\alpha''}$
$\mathbf{v_6}$	$-2\mathbf{v_5}$	$-4\mathbf{v_4}'$	0	$-2\mathbf{v_6}$	0	0	$\mathbf{v}_{\alpha'''}$
$\mathbf{v}_\alpha$	$-\mathbf{v}_{\alpha_\mathbf{x}}$	$-\mathbf{v}_{\alpha_\mathbf{t}}$	$\mathbf{v}_\alpha$	$-\mathbf{v}_{\alpha'}$	$-\mathbf{v}_{\alpha''}$	$-\mathbf{v}_{\alpha'''}$	0

Table 2: Commutator table of the infinitesimal generators from

The generators $\mathbf{v_2}$, $\mathbf{v_4}'$ and $\mathbf{v_6}$ now also form a subalgebra. This subalgebra is isomorphic to $\mathfrak{sl}(2,\mathbb{R})$ when transforming the generators as $\mathbf{v_2} \to 2A$, $\mathbf{v_4}' \to -H$ and $\mathbf{v_6} \to -2B$. The commutator $[\mathbf{v_i}, \mathbf{v_j}]$, where $\mathbf{v_i}$ is any generator from $\mathfrak{sl}(2,\mathbb{R})$ and $\mathbf{v_j}$ any generator from $\mathfrak{h}_3$, always returns an element from $\mathfrak{h}_3$. This makes the subalgebra $\mathfrak{h}_3$ also known as an *ideal.* The finite dimensional part of the Lie algebra $\mathfrak{g}$ of the heat equation is therefore denoted as $\mathfrak{g} = \mathfrak{h}_3 \niplus \mathfrak{sl}(2,\mathbb{R})$.

A well known Lie group which carries the same Lie algebra is known as the Schrödinger group, and has the following structure [9]

$$G = H_3 \rtimes SL(2,\mathbb{R}). \tag{4.10}$$

The Schrödinger group is a semidirect product of the Heisenberg and special linear group, where the special linear group acts with outer automorphisms on the Heisenberg group. Unfortunately, proving that the heat equation has the same Lie algebra and therefore the exact same local group is not sufficient to know that it also carries the Schrödinger group as its global symmetry group, according to Theorem 2.1.

Craddock found the same result of the group structure being similar to $H_3 \rtimes SL(2,\mathbb{R})$. Additionally he proved mathematically using so called *intertwining* operators [10] that if only solutions in the space of $L^2(\mathbb{R})$ (space of square-integrable functions, i.e. $\int\int |f(x,t)|^2 dxdt < \infty$) are considered, the symmetry groups do form a global symmetry group together. The solution from Equation 4.2 does not satisfy this property, however a solution of the form

$$f(x,t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right), \qquad t > 0 \tag{4.11}$$

satisfies the heat equation and is in $L^2(\mathbb{R})$. The transformation when applying $\mathbf{v_6}$ gives

$$\tilde{f}(x,t) = f(x,t),$$

with detailed derivation found in the appendix (subsection B). $f(x,t)$ is said to be an *invariant solution* w.r.t. $\mathbf{v_6}$, and because all other transformation groups are global, solutions of this form do have a global symmetry group.

One problem with this approach is that by restricting the set of possible solutions, it can no longer be treated as the same system. The restriction leads to the addition of another PDE or constraint that the solutions satisfy, and the combined system might no longer have the local 1-parameter transformation group G_6 as a result. In that case it makes sense that the remaining symmetry groups are global as the only non-global symmetry group has been eliminated by inclusion of this additional condition. Note that the restriction to $L^2(\mathbb{R})$ functions makes sense when studying the Schrödinger equation, but there is little reason to restrict functions for the heat equation. Without restricting the solution space, the local group of transformations given by $\mathbf{v_6}$ remains a bound on the domain of $\mathscr{U}$ and therefore the total symmetry group cannot said to be global. One thus either restricts the solution space to obtain a global symmetry group or sticks to the total solution space which can only be described by a local symmetry group.

5 Filtration Equation

In this section a nonlinear potential filtration equation is considered. Specifically, this equation is a nonlinear variant of the heat equation and will also lead to an interesting discussion of what a global symmetry group is. The differential equation is defined as

$$u_t = 3(u_{xx})^{\frac{1}{3}}. \tag{5.1}$$

Similarly to the heat equation, general solutions provide difficulties for numerical analysis. Furthermore, a very simple solution in this case will suffice to show how transformations can lead to undefined functions from a specific infinitesimal generator. This solution is a simple linear function which vanishes on both sides of the differential equation,

$$u(x,t) = ax + b \tag{5.2}$$

where a, b are real constants.

5.1 Lie Point Symmetries

The infinitesimal generators of the Lie point symmetries have been determined by [11].

$$\mathbf{v_1} = \partial_x \tag{5.3a}$$
$$\mathbf{v_2} = \partial_t \tag{5.3b}$$
$$\mathbf{v_3} = \partial_u \tag{5.3c}$$
$$\mathbf{v_4} = x\partial_x + 2t\partial_t + 2u\partial_u \tag{5.3d}$$
$$\mathbf{v_5} = \frac{2}{3}t\partial_x + u\partial_u \tag{5.3e}$$
$$\mathbf{v_6} = x\partial_u \tag{5.3f}$$
$$\mathbf{v_7} = u\partial_x \tag{5.3g}$$

Some of these generators have been covered in the examples before, like ∂_x. Generator $\mathbf{v_7}$ depends on u while acting on the x variable, which has not been covered in a previous example and is the generator of interest. Applying the exponential map the following 1-parameter group is found

$$G_7 = (x + \epsilon u, t, u), \tag{5.4}$$

which is defined for all ϵ and is therefore a global transformation group.

5.2 Finding Global Symmetry

Using the solution displayed in Equation 5.2, the transformation for this particular solution becomes $(x + \epsilon(ax + b), t, u)$, which remains a global transformation group. All that is left is to find the inverse of this operation (denoted as $\Xi_g^{-1}(x,t)$), found by taking $\tilde{x} = (1 + \epsilon a)x + \epsilon b$ and expressing it in terms of $\tilde{x}$. Using Equation 2.10, $\Xi_g^{-1}(x,t) = (\frac{x-\epsilon b}{1+\epsilon a}, t)$, which can be applied to the original solution

$$\tilde{u}(x,t) = a\frac{x - \epsilon b}{1 + \epsilon a} + b = \frac{ax + b}{1 + \epsilon a} = \tilde{a}x + \tilde{b}. \tag{5.5}$$

with $\tilde{a} = a/(1 + \epsilon a)$ and $\tilde{b} = b/(1 + \epsilon a)$. This solution is not defined for $\epsilon = -\frac{1}{a}$. According to Sepanski [11], this result means that the action of $g_\epsilon \in G_7$ applied to a solution does not lead to a global action. However, according to Definition 2.7 an element of the symmetry group G_s only needs to transform a solution into a solution if $g_\epsilon \cdot f(x)$ exists. The action of g_ϵ holds both infinitesimally and globally, only for each solution with some chosen value of a, there exists one ϵ where the product $g_\epsilon \cdot f(x)$ is not defined. Thus we can still consider global actions of g_ϵ and the transformation group G_7 still forms a symmetry group for all ϵ according to Definition 2.7.

This example differs from the heat equation, where the transformation group given by $\mathbf{v_6}$ was only locally defined. This could not be circumvented and therefore the symmetry group of the heat equation also remains local. In the case of the filtration equation the issue arises when applying the global transformation to a function, which in some cases is not defined.

Furthermore, as not all $g_\epsilon \cdot f(x)$ are defined one could argue that some transformed solutions do not have an inverse and therefore the symmetry group is not a group. Definition 2.7 however does not require that each transformed solutions created by $g \in G$ has an inverse, only that the underlying transformation group G has an inverse element such that $g^{-1} \cdot (g \cdot (x, u)) = (x, u)$ for $g \in G$. In this case, the inverse element of transformation group G_7 is given by $g_e^{-1} \cdot (x, u) = (x - \epsilon u, u)$. All definitions are satisfied, and the transformation group G_7 is thus also a global symmetry group.

The previous sections have shown what can be accomplished using the prolongation method and what kind of symmetries arise from the Lie algebra found using the method. The concepts of local Lie groups, local transformation groups and local symmetry groups are not always familiar when one is used to global Lie groups. To discover more information about the symmetry group and its structure, we will take a look at another method that can be used to find discrete symmetries of the same partial differential equation.

6 Discrete Symmetries Framework

The prolongation method provided the infinitesimal generators which in turn allowed us to find the continuous Lie point symmetries locally around the identity. It turns out that these infinitesimal generators can also be used to find discrete point symmetries, specifically by utilizing the Lie algebra that they form.

6.1 Hydon's Method

In the articles written by Hydon, he describes a method to find the discrete point symmetries of a differential equation, working for both ODEs [3] and PDEs [4]. Even though the infinitesimal generators of a Lie point symmetry group G_s only provide information about infinitesimal transformations, they can still be used to find discrete symmetries. Hydon's method, outlined in his articles, is described below.

6.1.1 Finding Possible Transformations

Consider a PDE $\Delta(x, u^{(n)}) = 0$, which has an r-dimensional symmetry group G_s with corresponding infinitesimal generators $\mathbf{v_i}$ with $i = 1, ..., r$. These generators form a Lie algebra and therefore the generators satisfy

$$[\mathbf{v_i}, \mathbf{v_j}] = c_{ij}^k \mathbf{v_k}, \tag{6.1}$$

where c_{ij}^k are known as the *structure constants*. Furthermore, each generator generates a 1-parameter group $G_i = \exp(\epsilon \mathbf{v_i})$. Note that these and all upcoming indices in this section follow the rules of Einstein summation. Now consider a PDE that has any (discrete or continuous) point symmetry Γ mapping (x, u) to $(\tilde{x}, \tilde{u})$, where $x = (x^1, x^2, ..., x^p)$. Then this symmetry can form a continuous 1-parameter symmetry group $\tilde{G}_i$ as follows

$$\tilde{G}_i = \Gamma G_i \Gamma^{-1} = \exp(\epsilon \Gamma \mathbf{v_i} \Gamma^{-1}), \tag{6.2}$$

with $\tilde{\mathbf{v}}_\mathbf{i} = \Gamma \mathbf{v_i} \Gamma^{-1}$ being the generator of this group. Using the generator basis from Equation 2.15, and the fact that $\Gamma^{-1} : (\tilde{x}, \tilde{u}) \to (x, u)$, we obtain that

$$\begin{aligned} \tilde{\mathbf{v}}_\mathbf{i} \tilde{x}^j &= \Gamma \mathbf{v_i} x^j = \Gamma \xi_i^j(x, u) = \xi_i^j(\tilde{x}, \tilde{u}) \\ \tilde{\mathbf{v}}_\mathbf{i} \tilde{u} &= \Gamma \mathbf{v_i} u = \Gamma \phi_i(x, u) = \phi_i(\tilde{x}, \tilde{u}) \end{aligned} \tag{6.3}$$

Therefore each new generator $\tilde{\mathbf{v}}_\mathbf{i}$ can be expressed in the basis

$$\tilde{\mathbf{v}}_\mathbf{i} = \sum_{j=1}^{p} \xi_i^j(\tilde{x}, \tilde{u}) \partial_{\tilde{x}^j} + \phi_i(\tilde{x}, \tilde{u}) \partial_{\tilde{u}}. \tag{6.4}$$

Each new generator has the exact same expression as the regular generators, except that it is defined w.r.t. $(\tilde{x}, \tilde{u})$. These new generators also form a basis for the same Lie algebra, which implies that

$$[\tilde{\mathbf{v}}_\mathbf{i}, \tilde{\mathbf{v}}_\mathbf{j}] = c_{ij}^k \tilde{\mathbf{v}}_\mathbf{k}, \tag{6.5}$$

where the structure constants are equal to the ones appearing in Equation 6.1.

Because the Lie algebra is a vector space spanned by the generators, the generators can be rewritten into a new basis using a transformation matrix B, or in component notation

$$\mathbf{v_i} = b_i^l \tilde{\mathbf{v}}_\mathbf{l} \qquad i, l = 1, ..., r. \tag{6.6}$$

Additionally, we require the transformations to be invertible, which requires $\det(B) \neq 0$. Transforming the set of infinitesimal generators to a different basis using B is known as an *automorphism*. An automorphism is a linear map from $\mathfrak{g}$ to $\mathfrak{g}$, such that it has an inverse mapping. In this case the mapping is done with the transformation matrix B with inverse B^{-1}.

To find the possible discrete transformations of a PDE, the possible configurations of the basis transformation matrix B must be found. Combining the results from Equation 6.1 and Equation 6.6, nonlinear conditions on the components b_i^l can be found satisfying

$$c_{lm}^n b_i^l b_j^m = c_{ij}^k b_k^n. \tag{6.7}$$

The nonlinearity makes solving these constraints often tedious to do by hand. The following section will explore a numerical method to find the values of B. Due to the structure constants being anti-symmetric, only solving equations with $i < j$ yields all necessary information.

Example 6.1. Consider a PDE with 3 continuous Lie point symmetries, generated by the following generators in its Lie algebra

$$\mathbf{v_1} = \partial_x, \quad \mathbf{v_2} = \partial_y, \quad \mathbf{v_3} = x\partial_y - y\partial_x. \tag{6.8}$$

The only non-zero commutation relations are

$$[\mathbf{v_1}, \mathbf{v_3}] = \mathbf{v_2}, \quad [\mathbf{v_2}, \mathbf{v_3}] = -\mathbf{v_1}. \tag{6.9}$$

The only non-zero structure constants are then $c_{13}^2 = 1$, $c_{23}^1 = -1$ and their reverse $c_{31}^2 = -1$, $c_{32}^1 = 1$. The most general transformation matrix B is given by

$$B = \begin{pmatrix} b_1^1 & b_1^2 & b_1^3 \\ b_2^1 & b_2^2 & b_2^3 \\ b_3^1 & b_3^2 & b_3^3 \end{pmatrix}. \tag{6.10}$$

Some of these parameters can be eliminated (i.e. set to zero) when solving the nonlinear constraints from Equation 6.7. The easiest conditions are obtained for $n = 3$, as there is no commutator which returns $\mathbf{v_3}$ as a result. For (i, j), we obtain three results

$$\begin{aligned} (1,2): &\quad 0 = 0 \\ (1,3): &\quad 0 = b_2^3 \\ (2,3): &\quad 0 = -b_1^3 \end{aligned} \tag{6.11}$$

These equations set $b_1^3 = b_2^3 = 0$. For $n = 1$, the following conditions are obtained

$$\begin{aligned} (1,2): &\quad -b_1^2 b_2^3 + b_1^3 b_2^2 = 0 \\ (1,3): &\quad -b_1^2 b_3^3 + b_1^3 b_3^2 = b_2^1 \\ (2,3): &\quad -b_2^2 b_3^3 + b_2^3 b_3^2 = -b_1^1 \end{aligned} \tag{6.12}$$

These equations can be simplified to provide constraints on some parameters, but no more parameters can be set to zero. The same goes for $n = 2$. To eliminate more parameters, the information covered next is required. The final transformation matrix now looks like

$$B = \begin{pmatrix} b_1^1 & b_1^2 & 0 \\ b_2^1 & b_2^2 & 0 \\ b_3^1 & b_3^2 & b_3^3 \end{pmatrix}. \tag{6.13}$$

Up until now, all possible transformations Γ have been considered to form new generators. To restrict transformations that can be found using only the continuous symmetries generated by the 1-parameter groups of $\mathbf{v_i}$, the adjoint action of the 1-parameter groups is used. The definitions are taken from Hall [12].

Definition 6.1 (Adjoint Map, Hall p. 63)**.** Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. Then for each $g \in G$, define the adjoint map $\mathrm{Ad}_g : \mathfrak{g} \to \mathfrak{g}$ by the formula

$$\mathrm{Ad}_g(\mathbf{v}) = g\mathbf{v}g^{-1}. \tag{6.14}$$

Definition 6.2 (Adjoint Action, Hall p. 81)**.** Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$. The *adjoint action* (or *adjoint representation*) of G is the map $\mathrm{Ad} : G \to GL(\mathfrak{g})$ given by $g \to \mathrm{Ad}_g$.

The adjoint action of the 1-parameter group generated by $\mathbf{v_j}$ is described by the matrix

$$A(j, \epsilon) = \exp(\epsilon C(j)), \tag{6.15}$$

where $(C(j))_i^k = c_{ij}^k$, with k denoting the column and i denoting the row of matrix j. The adjoint action can be used to generate equivalent groups using some other element g. The group generated by $\mathbf{v_i}$ is equivalent to, utilizing the element $g = \exp(\epsilon \mathbf{v_j})$, the group generated by

$$\hat{\mathbf{v}}_\mathbf{i} = \mathrm{Ad}_{\exp(\epsilon \mathbf{v_j})}(\mathbf{v_i}) = (A(j, \epsilon))_i^p \mathbf{v_p}. \tag{6.16}$$

This relation, combined with Equation 6.6, gives the following condition

$$\hat{\mathbf{v}}_\mathbf{i} = (A(j, \epsilon))_i^p b_p^l \tilde{\mathbf{v}}_\mathbf{l}. \tag{6.17}$$

This condition is equivalent, under the group generated by $\mathbf{v_j}$, to

$$\mathbf{v_i} = \hat{b}_i^l \tilde{\mathbf{v}}_\mathbf{l}, \tag{6.18}$$

with $\hat{b}_i^l = (A(j, \epsilon))_i^p b_p^l$.

This equation is like Equation 6.6, but the matrix B has been replaced with $A(j, \epsilon)B$. Both conditions (Equation 6.6 and Equation 6.18) should hold and therefore the parameters ϵ can be used to let $A(j, \epsilon)B = B$. Whenever ϵ is chosen such that an entry of $A(j, \epsilon)B$ is zero, the continuous symmetry generated by $\mathbf{v_j}$ is removed from the possible automorphisms determined by B. After the transformation matrix has been maximally reduced, all possible automorphisms of the Lie algebra have been found without those made possible by the continuous symmetries. These automorphisms are the same for all Lie algebras with the same structure constants. Now that the matrix B has been reduced, the remaining transformations corresponding to B need to be calculated and verified if they hold for a specific PDE.

Example 6.2. Consider the problem from the previous example (Example 6.1). More parameters can be eliminated by utilizing the adjoint action. The structure constant matrices $C(i)$ are given by

$$C(1) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \quad C(2) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad C(3) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{6.19}$$

Exponentiating these matrices results in the following three adjoint matrices

$$A(1,\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\epsilon & 1 \end{pmatrix}, \quad A(2,\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \epsilon & 0 & 1 \end{pmatrix}, \quad A(3,\epsilon) = \begin{pmatrix} \cos(\epsilon) & \sin(\epsilon) & 0 \\ -\sin(\epsilon) & \cos(\epsilon) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6.20}$$

Multiplying B with $A(1,\epsilon)$, we find

$$BA(1,\epsilon) = \begin{pmatrix} b_1^1 & b_1^2 & 0 \\ b_2^1 & b_2^2 & 0 \\ b_3^1 & b_3^2 - \epsilon b_3^3 & b_3^3 \end{pmatrix}. \tag{6.21}$$

The value of ϵ can be chosen to be anything, like $\epsilon = b_3^2/b_3^3$ since $b_3^3 \neq 0$. As the transformation matrix must remain the same under the adjoint action of $\mathbf{v_1}$, b_3^2 can be set to zero. Similarly, multiplying B with $A(2,\epsilon)$ yields

$$BA(2,\epsilon) = \begin{pmatrix} b_1^1 & b_1^2 & 0 \\ b_2^1 & b_2^2 & 0 \\ b_3^1 + \epsilon b_3^3 & 0 & b_3^3 \end{pmatrix}. \tag{6.22}$$

Which sets $b_3^1 = 0$ using $\epsilon = -b_3^1/b_3^3$. For the final adjoint matrix, multiplying with B gives the following matrix

$$BA(3,\epsilon) = \begin{pmatrix} b_1^1\cos(\epsilon) - b_1^2\sin(\epsilon) & b_1^2\cos(\epsilon) + b_1^1\sin(\epsilon) & 0 \\ b_2^1\cos(\epsilon) - b_2^2\sin(\epsilon) & b_2^2\cos(\epsilon) + b_2^1\sin(\epsilon) & 0 \\ 0 & 0 & b_3^3 \end{pmatrix}. \tag{6.23}$$

When looking at the top left entry, it is equal to zero when $\epsilon = \arctan(b_1^1/b_1^2)$. This means that $b_1^1 = 0$, unless $b_1^2 = 0$ such that ϵ is not defined. However, if $b_1^2 = 0$, b_1^1 must be nonzero to have $\det(B) \neq 0$. Two possible B configurations are obtained, those being

$$B_1 = \begin{pmatrix} b_1^1 & 0 & 0 \\ b_2^1 & b_2^2 & 0 \\ 0 & 0 & b_3^3 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 & b_1^2 & 0 \\ b_2^1 & b_2^2 & 0 \\ 0 & 0 & b_3^3 \end{pmatrix}. \tag{6.24}$$

6.1.2 Verifying PDE Transformations

To find out if these automorphisms lead to any discrete point transformations, we first have to how the (in)dependent variables are transformed. Recall that we want to find the discrete transformations given by:

$$\Gamma : (x,u) \to (\tilde{x}(x,u), \tilde{u}(x,u)) \tag{6.25}$$

The transformation matrix B will place restrictions on certain types of transformations. These restrictions can be found by letting $\mathbf{v_i}$ act on $\tilde{x}$, applying Equation 6.4 and Equation 6.6, to obtain

$$\begin{aligned} \mathbf{v_i}\tilde{x}^j &= b_i^l \tilde{\mathbf{v}}_\mathbf{l}\tilde{x}^j \\ &= b_i^l \xi_l^j(\tilde{x}, \tilde{u}). \end{aligned} \tag{6.26}$$

The generators $\mathbf{v_i}$ and the functions ξ_i^j are known, creating partial differential equations that can be solved to find $\tilde{x}^j$. Similarly, the new independent variable $\tilde{u}$ satisfies

$$\mathbf{v_i}\tilde{u} = b_i^l \phi_l(\tilde{x}, \tilde{u}). \tag{6.27}$$

All these equations can be put into the following matrix form:

$$\begin{pmatrix} \mathbf{v_1}\tilde{x}^1 & \mathbf{v_1}\tilde{x}^2 & ... & \mathbf{v_1}\tilde{x}^p & \mathbf{v_1}\tilde{u} \\ \mathbf{v_2}\tilde{x}^1 & \mathbf{v_2}\tilde{x}^2 & ... & \mathbf{v_2}\tilde{x}^p & \mathbf{v_2}\tilde{u} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{v_n}\tilde{x}^1 & \mathbf{v_n}\tilde{x}^2 & ... & \mathbf{v_n}\tilde{x}^p & \mathbf{v_n}\tilde{u} \end{pmatrix} = B \begin{pmatrix} \xi_1^1(\tilde{x}, \tilde{u}) & \xi_1^2(\tilde{x}, \tilde{u}) & ... & \xi_1^p(\tilde{x}, \tilde{u}) & \phi_1(\tilde{x}, \tilde{u}) \\ \xi_2^1(\tilde{x}, \tilde{u}) & \xi_2^2(\tilde{x}, \tilde{u}) & ... & \xi_2^p(\tilde{x}, \tilde{u}) & \phi_2(\tilde{x}, \tilde{u}) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \xi_n^1(\tilde{x}, \tilde{u}) & \xi_n^2(\tilde{x}, \tilde{u}) & ... & \xi_n^p(\tilde{x}, \tilde{u}) & \phi_n(\tilde{x}, \tilde{u}) \end{pmatrix} \tag{6.28}$$

These $(p+1)\times n$ differential equations determine the possible transformations for the (in)dependent variables. Once solved, the final step that must be taken is to confirm if a solution that is transformed according to these transformed variables remains a solution to the PDE. To do so, we make use of the following definitions from the book written by Hydon [13].

Definition 6.3 (Total Derivative Jacobian, Hydon p. 137)**.** Let the transformed independent variables $\tilde{x}^i$ with $i = 1, ..., p$ be functions of x^i and u. The Jacobian is then given by

$$J = \begin{vmatrix} D_{x^1}\tilde{x}^1 & D_{x^1}\tilde{x}^2 & ... & D_{x^1}\tilde{x}^p \\ D_{x^2}\tilde{x}^1 & D_{x^2}\tilde{x}^2 & ... & D_{x^2}\tilde{x}^p \\ \vdots & \vdots & \ddots & \vdots \\ D_{x^p}\tilde{x}^1 & D_{x^p}\tilde{x}^2 & ... & D_{x^p}\tilde{x}^p \end{vmatrix}. \tag{6.29}$$

The Jacobian matrix can be used to express how the transformed dependent variables $\tilde{u}$ are changed when differentiated w.r.t. $\tilde{x}^i$. Applying the chain rules gives

$$\begin{pmatrix} D_{x^1}\tilde{u} \\ D_{x^2}\tilde{u} \\ \vdots \\ D_{x^p}\tilde{u} \end{pmatrix} = J \begin{pmatrix} \tilde{u}_{\tilde{x}^1} \\ \tilde{u}_{\tilde{x}^2} \\ \vdots \\ \tilde{u}_{\tilde{x}^p} \end{pmatrix}. \tag{6.30}$$

By making use of Cramers rule, the vector on the right hand side can be expressed as stated in the following definition.

Definition 6.4 (Hydon p. 137)**.** Partial derivatives of $\tilde{u}$ w.r.t. $\tilde{x}^i$, expressed in terms of x^i, can be found using

$$\tilde{u}_{\tilde{x}^i} = \frac{1}{J} J_i(\tilde{u}), \tag{6.31}$$

where $J_i(\tilde{u})$ denotes the Jacobian, but with the ith column being replaced by full derivatives of $\tilde{u}$ w.r.t. x^i. The equation above can be used to recursively find higher order derivatives, as shown below

$$\tilde{u}_{\tilde{x}^i,\tilde{x}^j} = \frac{1}{J} J_j(\tilde{u}_{\tilde{x}^i}), \tag{6.32}$$

where the jth column is replaced with full derivatives of the result found in the equation above.

Finally all the tools have been presented to find out if the point transformation Γ is a point symmetry of a PDE. Consider a PDE $\Delta(x, u^{(n)}) = 0$. If $\Delta(\tilde{x}, \tilde{u}^{(n)}) = 0$, where $\Gamma : (x, u) \to (\tilde{x}, \tilde{u})$ and the derivatives are found using Definition 6.4, then Γ is a discrete point symmetry of the PDE.

Example 6.3. Consider the (1+1)-dimensional heat equation $\Delta(x, u^{(n)}) = u_{xx} - u_t = 0$ and suppose we want to know whether the transformation given by $\Gamma : (x, u) \to (-x, -t, u)$ is a discrete point symmetry of the PDE. To verify this, $\tilde{u}_{\tilde{x},\tilde{x}} - \tilde{u}_{\tilde{t}}$ should also be equal to zero. Employing Definition 6.3, we find

$$J = \begin{vmatrix} D_x\tilde{x} & D_x\tilde{t} \\ D_t\tilde{x} & D_t\tilde{t} \end{vmatrix} = \begin{vmatrix} -1 & 0 \\ 0 & -1 \end{vmatrix} = 1. \tag{6.33}$$

Now use this information to calculate the partial derivatives of the transformed independent variables, given by Definition 6.4:

$$\begin{aligned} \tilde{u}_{\tilde{x}} &= \frac{1}{J} \begin{vmatrix} D_x\tilde{u} & D_x\tilde{t} \\ D_t\tilde{u} & D_t\tilde{t} \end{vmatrix} = 1 \cdot \begin{vmatrix} u_x & 0 \\ u_t & -1 \end{vmatrix} = -u_x, \\ \tilde{u}_{\tilde{x}\tilde{x}} &= \frac{1}{J} \begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & D_x\tilde{t} \\ D_t\tilde{u}_{\tilde{x}} & D_t\tilde{t} \end{vmatrix} = 1 \cdot \begin{vmatrix} -u_{xx} & 0 \\ -u_{xt} & -1 \end{vmatrix} = u_{xx}. \end{aligned} \tag{6.34}$$

Similarly, for $\tilde{u}_{\tilde{t}}$ we find

$$\tilde{u}_{\tilde{t}} = \frac{1}{J} \begin{vmatrix} D_x\tilde{x} & D_x\tilde{u} \\ D_t\tilde{x} & D_t\tilde{u} \end{vmatrix} = 1 \cdot \begin{vmatrix} -1 & u_x \\ 0 & u_t \end{vmatrix} = -u_t. \tag{6.35}$$

Substituting these results into the heat equation, it can be shown that

$$\tilde{u}_{\tilde{x}\tilde{x}} - \tilde{u}_{\tilde{t}} = u_{xx} + u_t \neq 0. \tag{6.36}$$

Therefore the point transformation given by Γ is not a point symmetry of the PDE.

6.2 Gradient Descent

Finding the values of the transition matrix B can be found analytically, however this quickly escalates to solving many coupled nonlinear equations when considering equations with several generators. An alternative approach is to use an optimization algorithm to solve the conditions of Equation 6.7. The idea is as follows. Start with a random initial transition matrix B, make some small changes to the values such that the loss (right hand side minus left hand side of Equation 6.7) yields a lower value, and iterate through this process until the loss stagnates. The fundamentals of this process are described in this section. The main source of information is the excellent openly available book by Goodfellow et al. [14].

One such optimization algorithm is the gradient descent method. It makes use of the following definition.

Definition 6.5 (Gradient Descent, Goodfellow p. 83)**.** Let $f(\boldsymbol{x})$ with $\boldsymbol{x} = (x^1, x^2, ...)$ be a function with a local minimum at $\boldsymbol{x}^*$ and let $\boldsymbol{x_0}$ be a randomly chosen starting point. The method of *gradient descent* (steepest descent) entails calculating the equation

$$\boldsymbol{x_1} = \boldsymbol{x_0} - \epsilon \nabla f(\boldsymbol{x_0}), \tag{6.37}$$

substituting $\boldsymbol{x_0}$ with $\boldsymbol{x_1}$ and calculating the new point $\boldsymbol{x_2}$ and so on. For certain values of the *learning rate* ϵ, the algorithm approaches the local minimum at $\boldsymbol{x}^*$.

Gradient descent usually requires many steps to approach the minimum at $\boldsymbol{x}^*$, described by algorithm 1. Gradient descent is useful when there is a function $f(\boldsymbol{x})$ which needs to be min-

Algorithm 1: Gradient Descent

Data: learning rate $\epsilon > 0$
Data: stopping constant $c > 0$
$\boldsymbol{x} \in \mathcal{U}(-2, 2)$
$\boldsymbol{g} = \nabla f(\boldsymbol{x})$
$\boldsymbol{x'} = \boldsymbol{x} - \epsilon \boldsymbol{g}$
while $|\boldsymbol{x} - \boldsymbol{x'}| > c$ **do**
  $\boldsymbol{x} = \boldsymbol{x'}$
  $\boldsymbol{g} = f(\boldsymbol{x})$
  $\boldsymbol{x'} = \boldsymbol{x} - \epsilon \boldsymbol{g}$
end
return $\boldsymbol{x'}$.

imized, but finding the point $\boldsymbol{x}^*$ analytically is difficult. The function $f(\boldsymbol{x})$ that needs to be minimized is called the *loss function* and is denoted as $L(\boldsymbol{\theta})$, where $\boldsymbol{\theta} = (\theta^1, \theta^2, ...)$ are free parameters that are changed during the algorithmic procedure. Functions may contain multiple local and global minima, and the point that the gradient descent algorithm converges to depends both on the learning rate as well as the initial starting point $\boldsymbol{x_0}$. Methods that prevent getting stuck in a local minima will be covered later on. Preferably, loss functions are convex as there is only a single minimum.

The starting point $\boldsymbol{x_0}$ is chosen randomly, usually using either a uniform or Gaussian distribution. For all upcoming sections, a uniform distribution between -2 and 2 is chosen. A parameter b^i_j being equal to ± 1 occurs in many examples, thus the gradient descent algorithm should be able to reach this value with this initialization. Note that is also based on experimentation, so choosing a different domain might yield better or worse results.
For finding discrete symmetries, Equation 6.7 has to be solved, which can also be seen as a loss function subtracting one side from the other and taking the L^2 *norm*:

$$L(\boldsymbol{b}) = \sqrt{\sum_n \sum_i \sum_j \left(c^n_{lm} b^l_i b^m_j - c^k_{ij} b^n_k\right)^2}. \tag{6.38}$$

Minimizing this loss function gives the parameter values of $\boldsymbol{b}$ such that Equation 6.7 holds. To find these parameter values, gradient descent can be used. As the loss function contains a lot of variables, numerically calculated derivatives (calculated using `Python` package `JAX`) of the loss function are used. Currently, setting $b^i_j = 0$ for all i, j also minimizes the loss function. To implement the second condition of $\det(B) \neq 0$, Equation 6.38 can be changed into

$$L(\boldsymbol{b}) = \sqrt{\sum_n \sum_i \sum_j \left(c^n_{lm} b^l_i b^m_j - c^k_{ij} b^n_k\right)^2 + \frac{1}{\sigma} \exp\left(-\frac{1}{2}\left(\frac{\det(B)}{\sigma}\right)^2\right)}, \tag{6.39}$$

where σ is a small constant. The second term is like a normal distribution and for small values of σ will behave like a sharp peak at $\det(B) = 0$. The loss function will no longer equal zero when all $b^i_j = 0$ and therefore will no longer be a global minimum. Note that other functions can be chosen for the second term, as long as they have a defined first order derivative, peak when $\det(B) = 0$ and diminish when moving away from this point.

One problem with minimizing the loss using algorithm 1 is that the convergence to $\boldsymbol{b}^*$ starts to slow down tremendously when the gradient becomes less steep. This effect can be reduced by making use of momentum. To do so, an additional component is added alongside the gradient. When starting, there is some initial velocity $\boldsymbol{v_0}$. If the gradient is calculated and the velocity is added to this gradient, the new parameters can be found using $\boldsymbol{b_{n+1}} = \boldsymbol{b_n} + \boldsymbol{v_n}$. Using the following notation, we can express the same without the indices as $\boldsymbol{b} \leftarrow \boldsymbol{b} + \boldsymbol{v}$, with

$$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \nabla L(\boldsymbol{b}), \tag{6.40}$$

where $\alpha \in [0, 1]$. If $\boldsymbol{v}$ is a vector with all zeroes, then the first step is just like regular gradient descent. However, the second step carries over some of the gradient of the first step (hence the term momentum) as $\boldsymbol{v}$ is no longer zero. When the gradient starts to become smaller, the velocity $\boldsymbol{v}$ ensures that the convergence to $\boldsymbol{b}^*$ is faster. A nice example of this can be seen in the webpage application on `https://distill.pub/2017/momentum/`.

Another problem with using the loss function from Equation 6.39 is that for small values of σ, the gradient explodes when coming close to $\det(B)$. When the determinant is very close to zero, the parameters will be adjusted too much by the gradient, to the extent that the gradient descent might as well start all over again with new parameter values. Larger values of σ widens the function around $\det(B) = 0$, lowering the gradient but also increasing the loss when values of $\det(B)$ are further away from 0 which is not desired. This can be partially prevented using adaptive learning, which changes the effective learning rate based on the size of the gradient.

Let the parameters be updated with $\boldsymbol{b} \leftarrow \boldsymbol{b}+\Delta\boldsymbol{v}$, where the adapted momentum $\Delta\boldsymbol{v}$ is updated as

$$\begin{aligned} \boldsymbol{r} &\leftarrow \boldsymbol{r} + (\nabla L(\boldsymbol{b})) \odot (\nabla L(\boldsymbol{b})) \\ \Delta\boldsymbol{v} &\leftarrow \frac{-\epsilon}{\delta + \sqrt{\boldsymbol{r}}} \odot \boldsymbol{v}, \end{aligned} \tag{6.41}$$

where $\odot$ denotes element-wise multiplication (Hadamard product), δ is a very small ($\approx 10^{-7}$) stabilization constant and both division and square root are applied element-wise. Each direction has its own effective learning rate, which is lowered when the gradient is steep in that direction.

The algorithm used for determining the values of $\boldsymbol{b}$ in the following sections is known as adaptive moments (ADAM) gradient descent, proposed by Kingma et al. [15]. They claim it is suited for problems with many parameters and is applicable for noisy gradients. According to [16], the optimizer tends to skip over small local minima. Additionally, empirically it is found to perform well compared to other optimization variants of gradient descent ([15], [17]). That being said, the performance of the optimizer depends on the specific loss function.

The Adam optimizer makes use of the adapted momentum with bias correction. The algorithm is described by algorithm 2. The implementations of the ρ_1 and ρ_2 parameters converts $\mathbf{v}$ and $\mathbf{r}$ into their exponentially decaying average of the current and previous gradients, such that older gradients stored in $\mathbf{v}$ and $\mathbf{r}$ matter less after multiple iterations. Because both $\mathbf{v}$ and $\mathbf{r}$ are initialized at only values of zero, there is a bias for the optimizer towards zero. To minimize this effect, the bias corrected $\hat{\mathbf{v}}$ and $\hat{\mathbf{r}}$ variants are calculated.

Multiple distinct transformation matrices can be found using Hydon's method for a single set of infinitesimal generators. Performing a single simulation is therefore not enough to ensure that all possible transformation matrices are found. One method to try to prevent this is to perform N simulations, and taking the average of all results which have converged. If for example a parameter b_1^1 is zero in all transformation matrix configurations, then the averaged result of b_1^1 should also be close to zero. If b_1^2 in a configuration is non-zero, some simulations will end up with this parameter as non-zero and therefore the average result of this parameter will be greater than that of b_1^1. Doing a small amount of simulations, we are not guaranteed to encounter all different configurations, which can occur when one configuration is significantly more likely to descent to than some other configuration or when there are many different configurations. The upcoming examples only have one or two different transformation matrix configurations, thus choosing to do $N = 30$ simulations makes these problems unlikely to occur.

In practice, the Adam algorithm is best used to determine which parameters b_j^i can be set to zero. Doing so one might find that only one parameter in a row/column remains, which must then be nonzero and can be used to set some other parameter to zero using the adjoint matrices.

Algorithm 2: Adam Gradient Descent, Goodfellow p. 306

Data: Learning rate $\epsilon > 0$
Data: Stopping constant $c > 0$
Data: Momentum decay rates ρ_1, $\rho_2 \in [0, 1]$
Data: Small numerical stabilization constant δ
Result: $\boldsymbol{b}^*$
$\boldsymbol{b} \in \mathcal{N}(0, 1)$
$\boldsymbol{v}$, $\boldsymbol{r} = 0$
$t = 0$
while $L(\boldsymbol{b}) > c$ **do**
  $\boldsymbol{g} = \nabla L(\boldsymbol{b})$
  $t \leftarrow t + 1$
  $\boldsymbol{v} \leftarrow \rho_1 \boldsymbol{v} + (1 - \rho_1)\boldsymbol{g}$
  $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2)\boldsymbol{g} \odot \boldsymbol{g}$
  $\hat{\boldsymbol{v}} \leftarrow \boldsymbol{v}/(1 - \rho_1^t)$
  $\hat{\boldsymbol{r}} \leftarrow \boldsymbol{r}/(1 - \rho_2^t)$
  $\Delta \boldsymbol{v} = -\epsilon/(\sqrt{\hat{\boldsymbol{r}}} + \delta) \odot \hat{\boldsymbol{v}}$
  $\boldsymbol{b} \leftarrow \boldsymbol{b} + \Delta \boldsymbol{v}$
end
return $\boldsymbol{b}$.

Algorithm 3: Transformation Matrix Algorithm

Data: Learning rate $\epsilon > 0$
Data: Stopping constant $c > 0$
Data: Number of simulations $N \geq 1$
Data: Number of iterations $I \geq 1$
$\boldsymbol{b_{sum}} = O_{d \times d}$
$i = 0$
for n *in* N **do**
  $\boldsymbol{b_0} \in \mathcal{U}(-2, 2)_{d \times d}$
  $\boldsymbol{b^*_{est}} \leftarrow \text{Adam}(\boldsymbol{b_0}, \epsilon, I)$
  if $\nabla L(\boldsymbol{b^*_{est}}) < c$ **then**
    $\boldsymbol{b_{sum}} \leftarrow \boldsymbol{b_{sum}} + \boldsymbol{b^*_{est}}$
    $i \leftarrow i + 1$
  end
end
$\boldsymbol{b_{avg}} = \boldsymbol{b_{sum}}/i$
return $\boldsymbol{b_{avg}}$

7 Spherical Burgers Equation

The spherical Burgers' equation is a special form of the generalized Korteweg-de Vries-Burgers equation, and used by Hydon in [4] to showcase the method to find the discrete symmetries of this PDE. The spherical Burgers' equation is given by

$$u_t + \frac{u}{t} + uu_x = u_{xx}. \tag{7.1}$$

The symmetry group of this equation has a corresponding Lie algebra with three infinitesimal generators, found in [18],

$$\begin{aligned}
\mathbf{v_1} &= -x\partial_x - 2t\partial_t + u\partial_u \\
\mathbf{v_2} &= \ln(t)\partial_x + \frac{1}{t}\partial_u \\
\mathbf{v_3} &= \partial_x.
\end{aligned}$$

The first and last generators are also found in the symmetry group of the heat equation. The transformation created by applying the exponential map on $\mathbf{v_2}$ gives

$$G_3 : \left(x + \epsilon \ln(t), t, u + \frac{\epsilon}{t}\right).$$

To find the discrete symmetries, we apply Hydon's method described in subsection 6.1. The method consist of two phases, starting with finding all possible transformations given by the transformation matrix B.

7.1 Finding Transformation Matrix

The transition matrix B is found by solving the constraints given in Equation 6.7. To do so the structure constants have to be found. These are given by the commutator relations $[\mathbf{v_1}, \mathbf{v_2}] = \mathbf{v_2} - 2\mathbf{v_3}$ and $[\mathbf{v_1}, \mathbf{v_3}] = \mathbf{v_3}$, i.e.

$$c^2_{12} = 1, \quad c^3_{12} = -2, \quad c^3_{13} = 1 \text{ and } c^2_{21} = -1, \quad c^3_{21} = 2, \quad c^3_{31} = -1. \tag{7.2}$$

The last three structure constants are due to anti-symmetry of the commutator. The process starts with eliminating some of the variables present in the transformation matrix B. In its most general form, it is given by

$$B = \begin{pmatrix} b^1_1 & b^2_1 & b^3_1 \\ b^1_2 & b^2_2 & b^3_2 \\ b^1_3 & b^2_3 & b^3_3 \end{pmatrix}.$$

Applying the conditions of Equation 6.7 will be done both analytically and computationally, making use of gradient descent. Doing so allows the methods to be compared side by side, displaying their benefits and drawbacks.

7.1.1 Analytical Solving Method

Some values of these variables can be found by applying Equation 6.7 with the structure constants given by Equation 7.2. This equation has 3 free variables to choose from, those being i, j and n. When a generator does not appear as a result of commutating any two generators, choosing that value for n provides the simplest starting position. In this equation, $\mathbf{v_1}$ never appears as a result, thus $n = 1$ provides the best starting point. Because, as we can see for $n = 1$, the left hand side of Equation 6.7 is zero and this yields the conditions

$$\begin{aligned} 0 &= c_{ij}^k b_k^1 \\ &= c_{ij}^1 b_1^1 + c_{ij}^2 b_2^1 + c_{ij}^3 b_3^1 \end{aligned}$$

The values of b_k^1 can be found by going over the pairs (i, j) and solving the equations. For $(i, j) = (1, 3)$, the only nonzero structure constant is $c_{13}^3 = 1$, while $(1, 2)$ has 2 nonzero structure constants, giving the following conditions

$$\begin{aligned} (1,2):& \qquad 0 = b_2^1 - 2b_3^1 \\ (1,3):& \qquad 0 = b_3^1 \\ (2,3):& \qquad 0 = 0. \end{aligned}$$

Solving these equations gives $b_3^1 = 0$, $b_2^1 = 0$ and lastly, as B is nonsingular, $b_1^1 \neq 0$.

Now consider $n = 2$ and use the results above. The conditions are now given by

$$\begin{aligned} c_{lm}^2 b_i^l b_j^m &= c_{ij}^k b_k^2 \\ b_i^1 b_j^2 &= c_{ij}^1 b_1^2 + c_{ij}^2 b_2^2 + c_{ij}^3 b_3^2. \end{aligned}$$

Going over the pairs (i, j), the following results can be found

$$\begin{aligned} (1,2):& \qquad b_1^1 b_2^2 = b_2^2 - 2b_3^2 \\ (1,3):& \qquad b_1^1 b_3^2 = b_3^2, \end{aligned}$$

which are only consistent when $b_3^2 = 0$. As $b_3^1 = 0$, $b_3^2 = 0$ and B is nonsingular, $b_3^3 \neq 0$.

Finally consider $n = 3$ together with the results above. Applying Equation 6.7 the following conditions are found:

$$\begin{aligned} c_{lm}^3 b_i^l b_j^m &= c_{ij}^k b_k^3 \\ -2b_i^1 b_j^2 + b_i^1 b_j^3 &= c_{ij}^1 b_1^3 + c_{ij}^2 b_2^3 + c_{ij}^3 b_3^3. \end{aligned}$$

Going over the pairs (i, j), the following results can be found

$$\begin{aligned} (1,2):& \qquad -2b_1^1 b_2^2 + b_1^1 b_2^3 = b_2^3 - 2b_3^3 \\ (1,3):& \qquad -2b_1^1 b_3^2 + b_1^1 b_3^3 = b_3^3, \end{aligned}$$

Since $b_3^2 = 0$ and $b_3^3 \neq 0$, the second equation only holds when $b_1^1 = 1$. Reducing the first equation with this information leads to $-2b_2^2 + b_2^3 = b_2^3 - 2b_3^3$, setting $b_2^2 = b_3^3$. After solving these equations for all values of n, the transformation matrix B has been reduced to

$$B = \begin{pmatrix} 1 & b_1^2 & b_1^3 \\ 0 & b_2^2 & b_2^3 \\ 0 & 0 & b_2^2 \end{pmatrix}.$$

Additional variables can be eliminated using the adjoint matrices. The structure constants given in Equation 7.2 lead to the following matrices

$$C(1) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 2 \\ 0 & 0 & -1 \end{pmatrix}, \qquad C(2) = \begin{pmatrix} 0 & 1 & -2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad C(3) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Exponentiating the matrices $\epsilon C(i)$ leads to the following adjoint matrices

$$A(1,\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-\epsilon} & 2\epsilon e^{-\epsilon} \\ 0 & 0 & e^{-\epsilon} \end{pmatrix}, \qquad A(2,\epsilon) = \begin{pmatrix} 1 & \epsilon & -2\epsilon \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad A(3,\epsilon) = \begin{pmatrix} 1 & 0 & \epsilon \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{7.3}$$

The derivation can be found in the appendix (subsection C), or alternatively by using `MATHEMATICA` (see subsection E). Multiplying any of these matrices with B and choosing a value of ϵ such that any entry becomes zero is equal to setting the variable in that entry equal to zero. For example, multiplying B with $A(3,\epsilon)$ results in

$$BA(3,\epsilon) = \begin{pmatrix} 1 & b_1^2 & b_1^3 + \epsilon \\ 0 & b_2^2 & b_2^3 \\ 0 & 0 & b_3^3 \end{pmatrix},$$

therefore allowing to set $b_1^3 = 0$ using $\epsilon = -b_1^3$. The parameter ϵ of each adjoint matrix can only be used once. Likewise,

$$BA(2,\epsilon) = \begin{pmatrix} 1 & b_1^2 + \epsilon & -2 \\ 0 & b_2^2 & b_2^3 \\ 0 & 0 & b_3^3 \end{pmatrix} \quad \text{and} \quad BA(1,\epsilon) = \begin{pmatrix} 1 & e^{-\epsilon} b_1^2 & 2\epsilon e^{-\epsilon} b_1^2 \\ 0 & e^{-\epsilon} b_2^2 & 2\epsilon e^{-\epsilon} b_2^2 - e^{-\epsilon} b_2^3 \\ 0 & 0 & e^{-\epsilon} b_3^3 \end{pmatrix}.$$

Choosing $\epsilon = -b_1^2$ for the second adjoint matrix sets $b_1^2 = 0$ and $\epsilon = b_2^3/(2b_2^2)$ for the first adjoint matrix sets $b_2^3 = 0$. Note that dividing by b_2^2 is now allowed as setting $b_1^2 = 0$ means that $b_2^2 \neq 0$ to prevent B from being nonsingular. The transformation matrix has been further reduced to

$$B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & b_2^2 & 0 \\ 0 & 0 & b_2^2 \end{pmatrix}.$$

Also note that if $A(2,\epsilon)$ is applied first of all the three adjoint matrices, it can also be used to eliminate b_1^3, which leaves $A(3,\epsilon)$ unable to remove any parameter. As b_3^1 also does not appear in any of the nonlinear conditions, this new information cannot be used to eliminate b_1^2. Hence the order in which the adjoint matrices are used and what parameter they set to zero does matter.

Letting $b_2^2 = b \neq 0$, the transformation matrix has been maximally reduced to

$$B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{pmatrix}. \tag{7.4}$$

Which transformations arise from this transformation matrix will be covered in subsection 7.2, but first we will show how the same transformation matrix can be found using the gradient descent method.

7.1.2 Computational Solving Method

The transformation matrix B found in the previous section can also be found using the gradient descent method. The spherical Burger's equation can be solved analytically without too much hassle, but differential equations involving a larger amount of generators will quickly become cumbersome. This section will showcase what the optimizer returns. The code with explanation can be found at `https://github.com/TomR21/MSc-Thesis-Code`.

Similarly to the previous method, the starting point is a transformation matrix filled with variables b^i_j. Using the Adam optimizer described in section 6, the algorithm can be run to find B without considering any adjoint matrices yet. The results can be seen in Figure 6. Clearly, $b^1_2 = b^1_3 = b^2_3 = 0$, which agrees with the analytical analysis from the previous section.

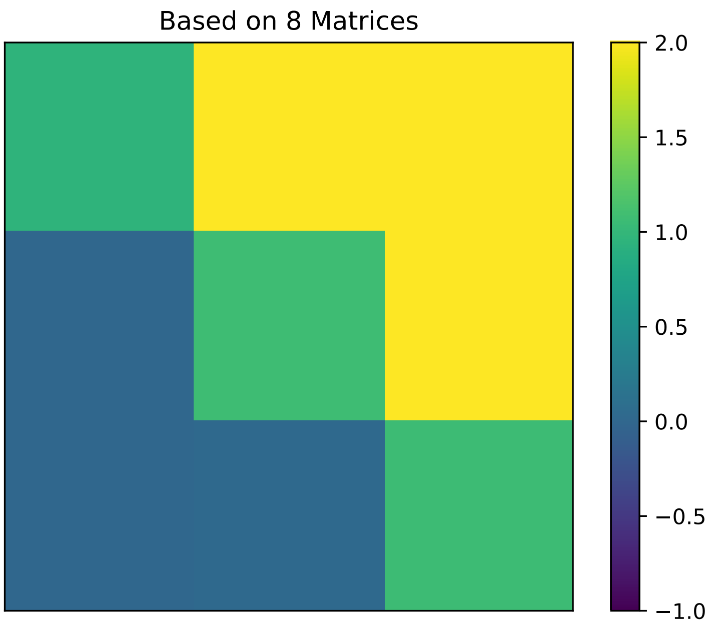


Figure 6: Resulting values of the transformation matrix B doing 10 simulations. Two matrices had a high loss and thus were not considered.

The adjoint matrices can be found symbolically using `MATHEMATICA` (using functions from appendix subsection E), which gives the same matrices as those of Equation 7.3. Multiplying these with B, the same values of ϵ can be chosen as those in the analytical section to obtain $b^2_1 = b^3_1 = b^3_2 = 0$. This leaves just the diagonal matrix with variables

$$B = \begin{pmatrix} b^1_1 & 0 & 0 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix}.$$

To see if there are any further restrictions, these values must be used for solving the nonlinear conditions of Equation 6.7. The obtained transformation matrix is the same matrix as the one obtained from the analytical solving method in Equation 7.4.

For differential equations with a small amount of generators, the computational solving method offers little benefit over the analytical solving method. Differential equations with a larger amount of infinitesimal generators benefit more from this approach, as the nonlinear coupled conditions generally become harder to solve. This will become apparent in later sections when looking at other differential equations.

7.2 Finding PDE Symmetries

Now that all possible transformations of the Lie algebra have been found, it is time to verify if they form discrete transformations of the solutions of the PDE. First the transformations of the independent and dependent variables must be found. Let $\tilde{x} = f(x,t,u)$, $\tilde{t} = g(x,t,u)$ and $\tilde{u} = h(x,t,u)$. Using Equation 6.28, the following PDEs must be solved

$$\begin{pmatrix} \mathbf{v_1}\tilde{x} & \mathbf{v_1}\tilde{t} & \mathbf{v_1}\tilde{u} \\ \mathbf{v_2}\tilde{x} & \mathbf{v_2}\tilde{t} & \mathbf{v_2}\tilde{u} \\ \mathbf{v_3}\tilde{x} & \mathbf{v_3}\tilde{t} & \mathbf{v_3}\tilde{u} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b \end{pmatrix} \begin{pmatrix} -\tilde{x} & -2\tilde{t} & \tilde{u} \\ \ln(\tilde{t}) & 0 & 1/\tilde{t} \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} -\tilde{x} & -2\tilde{t} & \tilde{u} \\ b\ln(\tilde{t}) & 0 & b/\tilde{t} \\ b & 0 & 0 \end{pmatrix}$$

There are 9 differential equations that the transformed variables must satisfy, which can be solved using regular methods, shown in the appendix (subsection D) to keep it brief. The transformations are given by

$$(\tilde{x},\ \ \tilde{t},\ \ \tilde{u}) = \left(b(x + \ln(c_1)tu + c_3\sqrt{t}),\ \ c_1 t,\ \ \frac{b}{c_1}u + c_2\frac{1}{\sqrt{t}} \right),$$

where c_i are real constants with $c_1 \neq 0$. To determine these constants, we will have to see for which values the differential equation still holds, i.e.

$$\tilde{u}_{\tilde{t}} + \frac{\tilde{u}}{\tilde{t}} + \tilde{u}\tilde{u}_{\tilde{x}} = \tilde{u}_{\tilde{x}\tilde{x}}, \tag{7.5}$$

given that Equation 7.1 holds. Using Definition 6.3 and Definition 6.4, the transformed variables are found to be

$$\begin{aligned} J &= \begin{vmatrix} D_x\tilde{x} & D_x\tilde{t} \\ D_t\tilde{x} & D_t\tilde{t} \end{vmatrix} = bc_1 \\ \tilde{u}_{\tilde{x}} &= \begin{vmatrix} D_x\tilde{u} & D_x\tilde{t} \\ D_t\tilde{u} & D_t\tilde{t} \end{vmatrix} = \frac{1}{c_1}u_x \\ \tilde{u}_{\tilde{x}\tilde{x}} &= \begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & D_x\tilde{t} \\ D_t\tilde{u}_{\tilde{x}} & D_t\tilde{t} \end{vmatrix} = \frac{1}{bc_1}u_{xx} \\ \tilde{u}_{\tilde{t}} &= \begin{vmatrix} D_x\tilde{x} & D_x\tilde{u} \\ D_t\tilde{x} & D_t\tilde{u} \end{vmatrix} = \frac{b}{c_1^2}u_t - \frac{1}{2}\frac{c_2}{c_1}t^{-3/2} - \frac{b}{c_1}\ln(c_1)uu_x - \frac{1}{2}\frac{bc_3}{c_1^2}t^{-1/2}u_x. \end{aligned}$$

Substituting these values into the symmetry condition of Equation 7.5 yields

$$\frac{b}{c_1^2}u_t + \frac{b}{c_1^2}\frac{u}{t} + \frac{b}{c_1^2}(1 - \ln(c_1))uu_x + \frac{1}{2}\frac{c_2}{c_1}t^{-3/2} + \left(\frac{c_2}{c_1} - \frac{1}{2}b\frac{c_3}{c_1^2}\right)u_x t^{-1/2} = \frac{1}{bc_1}u_{xx}.$$

The only known information is that the original PDE of Equation 7.1 holds, thus the $t^{-3/2}$ and $u_x t^{-1/2}$ terms must disappear, setting $c_2 = c_3 = 0$. The remaining terms on the right hand side should have the same prefactor, setting $c_1 = 1$. The equation then represents the old PDE when $b = \frac{1}{b}$, which leads to $b = \pm 1$. For other values of these constants the symmetry condition is not met and solutions are not mapped to other solutions of the PDE. As $b = 1$ returns the identity transformation, the only new discrete symmetry transformation is therefore given by

$$\Gamma : (x, t, u) \to (-x, t, -u).$$

The spherical Burgers equation has a single discrete point symmetry, which returns to the identity transformation when applied twice. The continuous symmetry transformations given by $\mathbf{v_1}$, $\mathbf{v_2}$ and $\mathbf{v_3}$ are not able to generate the transformation given by Γ, confirming that it does generate new transformations.

The strength of Hydon's method not only lies in the ability to find the discrete symmetry transformations, but to also establish that there exist no other discrete point symmetries. The symmetry found above could have also been found by inspection of the PDE, but ruling out that there are any other symmetries is significantly more difficult. Now that Hydon's method has been applied to this example, we will apply it to a PDE seen before. The logistic equation only has a single generator in its Lie algebra, meaning that there exists no automorphisms and therefore no discrete point symmetries can be found. The heat equation does have multiple generators and will be covered in the next section.

8 Heat Equation

Now consider the (1+1)-dimensional heat equation given by Equation 4.1. The generators were found in section 4, with the structure constants being displayed in Table 1. Finding the possible automorphisms is again the first step towards the discrete point symmetries of the heat equation.

8.1 Finding Transformation Matrix

The transformation matrix in its most general form is given by

$$B = \begin{pmatrix} b_1^1 & b_1^2 & \dots & b_1^6 \\ b_2^1 & b_2^2 & \dots & b_2^6 \\ \vdots & \vdots & \ddots & \vdots \\ b_6^1 & b_6^2 & \dots & b_6^6 \end{pmatrix}.$$

Both analytical and computational analysis will be done, but the analytical analysis will prove more difficult than the spherical Burger's equation.

8.1.1 Analytical Solving Method

Each generator can be created by commuting two generators, thus there is no n which simplifies the nonlinear conditions. Each condition contains at least a product of two different variables, making them difficult to solve analytically. There is an alternative method to determine which variables are zero, suggested by Gray ([19], §7.7).

By observing the Lie algebra, one can see that $\mathbf{v_3}$ commutes with every generator and therefore $c_{3j}^k = 0$. Using Equation 6.5, we see that $\tilde{\mathbf{v}}_\mathbf{3}$ must also commute with all other new generators $\mathbf{v}_i$. As $\tilde{\mathbf{v}}_\mathbf{3} = b_3^1 \mathbf{v_1} + ... + b_3^6 \mathbf{v_6}$, the only possible way to ensure that it commutes with all other new generators is when $b_3^i = 0$ for $i \neq 3$. Together with $\det(B) \neq 0$, we also know that $b_3^3 \neq 0$. This information can be used when applying the adjoint matrices.

Also, as found in the discussion of the Lie algebra of the heat equation, $\mathbf{v_1}, \mathbf{v_3}, \mathbf{v_5}$ form an ideal. Similarly as above, the transformed generators $\tilde{\mathbf{v}}_\mathbf{1}$, $\tilde{\mathbf{v}}_\mathbf{3}$ and $\tilde{\mathbf{v}}_\mathbf{5}$ will also have to map to itself when taking the commutator with any other transformed generator. Each generator $\mathbf{v_i}$ appears at least once in one of the new generators, and therefore ($\tilde{\mathbf{v}}_\mathbf{1}$, $\tilde{\mathbf{v}}_\mathbf{3}$ and $\tilde{\mathbf{v}}_\mathbf{5}$) cannot depend on $\mathbf{v_2}$, $\mathbf{v_4}$ or $\mathbf{v_6}$. Consequently, $b_1^2 = b_1^4 = b_1^6 = 0$ and $b_5^2 = b_5^4 = b_5^6 = 0$. To reduce the transformation matrix further, we take a look at the adjoint matrices given below

$$A(1,\epsilon) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -\epsilon & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \epsilon & 0 & 1 & 0 \\ 0 & 0 & -\epsilon^2 & 0 & -2\epsilon & 1 \end{pmatrix}, \quad A(2,\epsilon) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -2\epsilon & 0 & 1 & 0 & 0 \\ -2\epsilon & 0 & 0 & 0 & 1 & 0 \\ 0 & 4\epsilon^2 & 2\epsilon & -4\epsilon & 0 & 1 \end{pmatrix}$$

$$A(3,\epsilon) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad A(4,\epsilon) = \begin{pmatrix} e^{\epsilon} & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{2\epsilon} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-\epsilon} & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-2\epsilon} \end{pmatrix}$$

$$A(5,\epsilon) = \begin{pmatrix} 1 & 0 & -\epsilon & 0 & 0 & 0 \\ 2\epsilon & 1 & -\epsilon^2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \epsilon & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad A(6,\epsilon) = \begin{pmatrix} 1 & 0 & 0 & 0 & 2\epsilon & 0 \\ 0 & 1 & -2\epsilon & 4\epsilon & 0 & 4\epsilon^2 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 2\epsilon \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The adjoint matrices $A(3,\epsilon)$ and $A(4,\epsilon)$ are not able to eliminate any parameters, so they can only be used to rescale some parameters at the end. There are only four adjoint matrices left, and therefore only four parameters that can be eliminated. Multiplying $A(1,\epsilon)$ and $A(5,\epsilon)$ with B allows us to set b_5^3 and b_1^3 to zero respectively, by using the fact that $b_3^3 \neq 0$. Although both $A(i,\epsilon)B$ and $BA(i,\epsilon)$ can be calculated to eliminate a parameter, they lead to different equations in each entry. For example, $A(1,\epsilon)B$ leads to equations involving b_3^3, which is known to be nonzero, while $BA(1,\epsilon)$ does not, thus changing the placement might help in certain systems.

Making use of the other two adjoint matrices requires an assumption to be made. For example, multiplying $A(2,\epsilon)$ with B gives

$$\begin{pmatrix} b_1^1 & 0 & 0 & 0 & b_1^5 & 0 \\ b_2^1 & b_2^2 & b_2^3 & b_2^4 & b_5^2 & b_2^6 \\ 0 & 0 & b_3^3 & 0 & 0 & 0 \\ b_4^1 - 2\epsilon b_2^1 & b_4^2 - 2\epsilon b_2^2 & b_4^3 - 2\epsilon b_2^3 & b_4^4 - 2\epsilon b_2^4 & b_4^5 - 2\epsilon b_2^5 & b_4^6 - 2\epsilon b_2^6 \\ b_5^1 - 2\epsilon b_1^1 & 0 & 0 & 0 & b_5^5 - 2\epsilon b_1^5 & 0 \\ b_6^1 - 4\epsilon b_4^1 + 4\epsilon^2 b_2^1 & b_6^2 - 4\epsilon b_4^2 + 4\epsilon^2 b_2^2 & b_6^{3\prime} & b_6^{4\prime} & b_6^{5\prime} & b_6^{6\prime} \end{pmatrix},$$

with $b_6^{i\prime} = b_6^1 - 4\epsilon b_4^i + 4\epsilon^2 b_2^i$. The only value known to be nonzero is b_3^3, which can not be used here to eliminate a parameter. To go forward, an entry has to be picked, like $b_4^2 - 2\epsilon b_2^2$. An assumption has to be made, either $b_2^2 = 0$ or $b_2^2 \neq 0$, where the latter allows b_4^2 to be set to zero using $\epsilon = b_4^2/(2b_2^2)$. Either assumption creates a different transformation matrix B. Let B_1 be the transformation corresponding to $b_2^2 \neq 0$ and B_2 to $b_2^2 = 0$.

Matrix $\boldsymbol{B_1}$:
By setting $b_4^2 = 0$ and $b_2^2 \neq 0$, evaluating the nonlinear conditions will provide more information. For example, for (n, i, j) we obtain

$$(2,2,4) : -2b_2^2 b_4^4 = -2b_2^2 \quad \rightarrow \quad b_4^4 = 1.$$

Substituting this result into B_1 and reevaluating the nonlinear conditions allows to solve for more parameters. Continuing this process and using $A(6, \epsilon)$ to eliminate another parameter, the following transformation matrix is obtained, where a is a real or complex constant. The ϵ_4 parameter comes from multiplying $A(4, \epsilon_4)$ with B, as this adjoint matrix has not yet been accounted for.

$$B_1 = \begin{pmatrix} ae^{\epsilon_4} & 0 & 0 & 0 & 0 & 0 \\ 0 & a^2e^{2\epsilon_4} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{a}e^{-\epsilon_4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{a^2}e^{-2\epsilon_4} \end{pmatrix}. \tag{8.1}$$

Matrix $\boldsymbol{B_2}$:
For this case, we assume $b_2^2 = 0$ but the ϵ parameter from $A(2, \epsilon)$ has not yet been used to eliminate any value. This new information can be used to solve some of the nonlinear conditions, which sets other parameters to zero. Continuing to do so, using the remaining adjoint matrices $A(2, \epsilon)$ and $A(6, \epsilon)$ to eliminate two more values and multiplying B with $A(4, \epsilon_4)$, the final transformation matrix is given by

$$B_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & ae^{\epsilon_4} & 0 \\ 0 & 0 & 0 & 0 & 0 & a^2e^{2\epsilon_4} \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ -\frac{1}{a}e^{-\epsilon_4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{a^2}e^{-2\epsilon_4} & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{8.2}$$

8.1.2 Computational Solving Method

The procedure to find the transformation matrices of the heat equation analytically requires insight into the structure of the Lie algebra and how this affects the parameters of the transformations. The computational solving method can be used to acquire the same results without having to find this information. Running the Adam algorithm requires only the structure constants, with its results being shown in Figure 7.

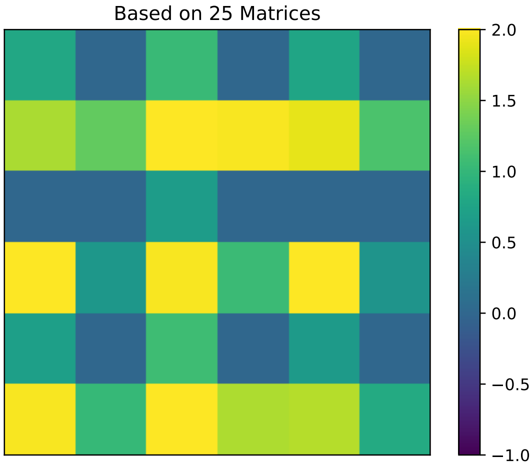


Figure 7: Average B values after Adam optimization using 25 simulations, learning rate of 1e-3, and 20.000 iterations

The parameters found to be zero are the same ones as found by Gray. Further optimization requires the adjoint matrices. Only four adjoint matrices can be used to eliminate parameters, so the Adam optimizer will be run each time an adjoint matrix is applied, to see if setting 1 parameter to zero leads to other parameters being zero. Just as the analytical case, start with $A(1, \epsilon)$ and $A(5, \epsilon)$ to eliminate b_5^3 and b_1^3. Rerunning the optimizer gives Figure 8.

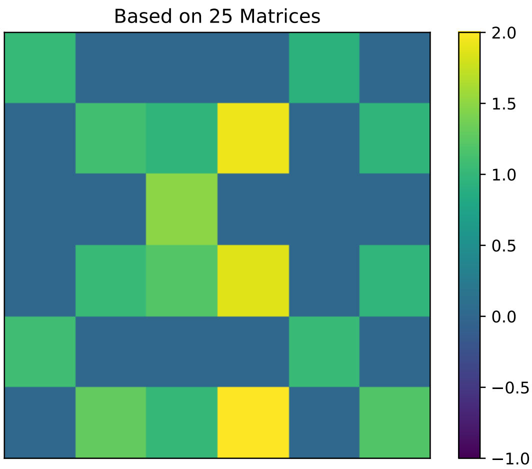


Figure 8: Average B values after Adam optimization using 25 simulations, learning rate of 1e-3, and 20.000 iterations

The figure reveals that using just using $A(1, \epsilon)$ and $A(5, \epsilon)$ to eliminate two parameters also sets other parameters to zero. Finding these values with solving the nonlinear conditions analytically was harder to do, as most equations still contained multiple nonlinear terms. Despite the additional information, an assumption still has to be made about a certain parameter to use the remaining adjoint matrices. The choice of parameter does not matter, so this time we will assume that either $b_1^1 \neq 0$ or $b_1^1 = 0$. Let B_1 correspond to the first choice and B_2 to the second.

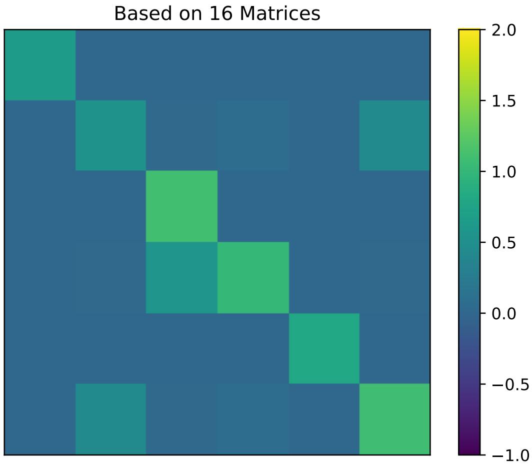


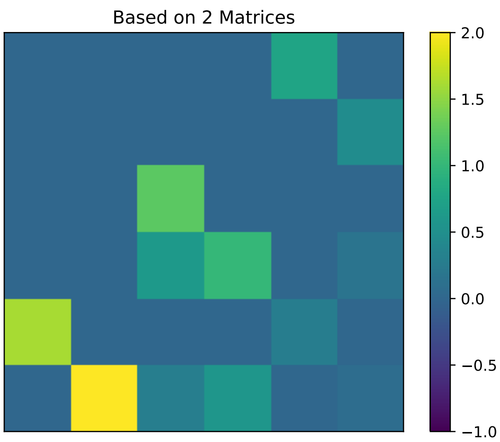
Figure 9: Final averaged matrix values assuming $b_1^1 \neq 0$, using 25 simulations, learning rate of 1e-3 and 25.000 iterations.

Option 1: $\boldsymbol{b_1^1} \neq 0$

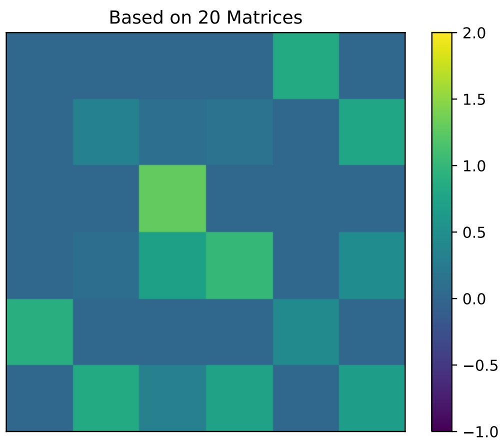
This assumption allows to set $b_5^1 = 0$ using $A(2, \epsilon)$. Running the optimizer again and using the final adjoint matrix, the final averaged output of the optimizer is shown in Figure 9. The final output is not yet sufficient to find the maximally reduced transformation matrix, thus the nonlinear conditions have to be reevaluated one last time. Doing so one obtains that the off-diagonal values like b_6^2 must be zero, and that the resulting matrix is equal to that of Equation 8.1.

Option 2: $\boldsymbol{b_1^1} = 0$

Implementing this change gives an insight into one of the difficulties when running the Adam optimizer to find which parameters can be put to zero. Not all starting configurations will converge nicely to a low loss value, so a decision has to be made for which loss values to stop adding the final found configuration $\boldsymbol{b^*_{est}}$, named the *cutoff* value.



(a) Using a cutoff value of 1



(b) Using a cutoff value of 5

Figure 10: Final averaged matrix values $\boldsymbol{b_{avg}}$ assuming $b_1^1 = 0$ using different cutoff values, with 25 simulations, learning rate of 1e-3 and 25.000 iterations.

When considering two different cutoff values, as done in Figure 10, the final results vary greatly. Many starting configurations do not seem to be able to go below a loss value of 3 to 5, which might be due to the algorithm not being able to leave its local minimum.

However, when continuing with a cutoff value of 5, no additional information will be found aside from the eliminated parameters using the adjoint matrices. The analysis will continue using the lower cutoff value of 1. Using the two remaining adjoint matrices and rerunning the Adam optimizer gives the final result shown in Figure 11. Lastly, the nonlinear conditions need to be reevaluated. Solving these and multiplying the resulting matrix with $A(4, \epsilon)$ yields the same solution as the one found in Equation 8.2.

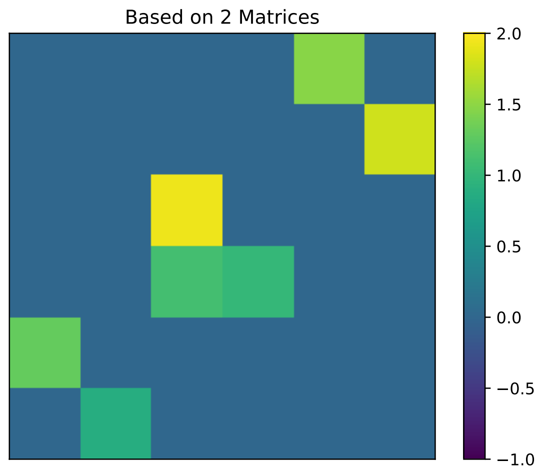


Figure 11: Final averaged matrix values $\boldsymbol{b_{avg}}$ assuming $b_1^1 = 0$ using cutoff of 1, with 25 simulations, learning rate of 1e-3 and 25.000 iterations.

Something interesting to note is that this problem of selecting the right cutoff value is more important for this option than the other one. Furthermore, when no parameters were eliminated, the optimizer converges more often than when multiple parameters were kept at zero. This might become a problem for differential equations with more parameters, thus additional experimentation of the cutoff value might be required depending on which PDE and transformation matrix is being studied.

8.2 Finding PDE Symmetries

To convert the transformation matrix into possible transformations of the (in)dependent variables, use Equation 6.28. Both transformation matrices will lead to different transformations and are therefore treated separately.

Matrix $\boldsymbol{B_1}$
Starting with B_1, the PDEs are given by

$$\begin{pmatrix} \mathbf{v_1}\tilde{x} & \mathbf{v_1}\tilde{t} & \mathbf{v_1}\tilde{u} \\ \mathbf{v_2}\tilde{x} & \mathbf{v_2}\tilde{t} & \mathbf{v_2}\tilde{u} \\ \mathbf{v_3}\tilde{x} & \mathbf{v_3}\tilde{t} & \mathbf{v_3}\tilde{u} \\ \mathbf{v_4}\tilde{x} & \mathbf{v_4}\tilde{t} & \mathbf{v_4}\tilde{u} \\ \mathbf{v_5}\tilde{x} & \mathbf{v_5}\tilde{t} & \mathbf{v_5}\tilde{u} \\ \mathbf{v_6}\tilde{x} & \mathbf{v_6}\tilde{t} & \mathbf{v_6}\tilde{u} \end{pmatrix} = \begin{pmatrix} ae^{\epsilon_4} & 0 & 0 \\ 0 & a^2e^{2\epsilon_4} & 0 \\ 0 & 0 & \tilde{u} \\ \tilde{x} & 2\tilde{t} & 0 \\ \frac{2}{a}e^{\epsilon_4}\tilde{t} & 0 & -\frac{1}{a}e^{\epsilon_4}\tilde{x}\tilde{u} \\ \frac{4}{a^2}e^{2\epsilon_4}\tilde{x}\tilde{t} & \frac{4}{a^2}e^{2\epsilon_4}\tilde{t}^2 & -\frac{1}{a^2}e^{2\epsilon_4}(\tilde{x}^2+2\tilde{t})\tilde{u} \end{pmatrix}$$

From $\mathbf{v_1}$, $\mathbf{v_2}$ and $\mathbf{v_3}$, the transformations are already restricted to $\tilde{x} = ae^{\epsilon_4}x + c_1$, $\tilde{t} = a^2e^{\epsilon_4}x + c_2$ and $\tilde{u} = bu$. Lastly, using the PDEs from $\mathbf{v_4}$ sets $c_1 = c_2 = 0$. The PDEs from $\mathbf{v_5}$ and $\mathbf{v_6}$ do not give any further restriction and the transformations can be written as:

$$(\tilde{x},\ \ \tilde{t},\ \ \tilde{u}) = \left(ae^{\epsilon_4}x,\ \ a^2e^{2\epsilon_4}t,\ \ be^{\epsilon_3}u\right), \tag{8.3}$$

The $\exp(\epsilon_3)$ factor in front of u stems from the continuous symmetry generated by $\mathbf{v_3}$, which has not yet been removed as its adjoint matrix is simply the identity matrix. To account for this symmetry, which is responsible for the scaling of u, the factor $\exp(\epsilon_3)$ is multiplied with u. All adjoint matrices have now been accounted for, so the symmetry condition can be calculated. The symmetry condition of $\tilde{u}_{\tilde{t}} = \tilde{u}_{\tilde{x}\tilde{x}}$, found by applying Definition 6.4, gives the following equation

$$\frac{be^{\epsilon_3}}{a^2e^{\epsilon_4}}u_t = \frac{be^{\epsilon_3}}{a^2e^{\epsilon_4}}u_{xx},$$

which is satisfied for all values except $a = 0$. In Hydon's method, the parameters ϵ_3 and ϵ_4 can either be real or complex. Furthermore, we can divide the discrete point symmetries into real symmetries ($\tilde{x}$, $\tilde{t}$, $\tilde{u}$ are real-valued functions) and complex symmetries.

If ϵ_3 and ϵ_4 are real constants, than the scaling created by both $\exp(\epsilon_3)$ and $\exp(\epsilon_4)$ ranges between $(0, \infty)$. The real discrete point symmetries up to the adjoint action of the real Lie groups of scaling, are generated by

$$\Gamma_1 : (x, t, u) \to (-x, t, u) \qquad \Gamma_2 : (x, t, u) \to (x, t, -u). \tag{8.4}$$

Going from x to $-x$ cannot be realized by the real scaling from $\mathbf{v_3}$ and therefore forms a discrete point symmetry. With generators Γ_1, Γ_2 and the real scaling from ϵ_3 and ϵ_4, all transformations of Equation 8.3 can be created. This makes Γ_1 and Γ_2 the only discrete point generators. The group structure of these generators is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$.

When considering complex symmetries, the transformations can be represented by $(\tilde{x}, \tilde{t}, \tilde{u}) = (\lambda x, \lambda^2 t, \mu u)$ with $\lambda, \mu \in \mathbb{C}$. Up to the real scaling done by $\exp(\epsilon_3\mathbf{v_3})$ and $\exp(\epsilon_4\mathbf{v_4})$, the following options remain: $\lambda = p \pm i$ and $\mu = k \pm i$ with $p, k \in \mathbb{R}$. There are thus an infinite amount of discrete symmetries when only considering real scaling. If one restricts λ and μ to only values found on either the imaginary or real axis, then the complex discrete point symmetries, up to the adjoint action of the real Lie group of scaling, are generated by

$$\Gamma_3 : (x, t, u) \to (ix, -t, u) \qquad \Gamma_4 : (x, t, u) \to (x, t, iu). \tag{8.5}$$

These two form an abelian group, with a group structure isomorphic to $\mathbb{Z}_4 \times \mathbb{Z}_4$, which has 16 distinct elements.

If ϵ_3 and ϵ_4 are complex constants, then the real symmetries up to the adjoint action of the complex Lie group of scaling are given by only the identity map as all transformations from Equation 8.3 can be realized by only choosing a different complex value of ϵ_3 and ϵ_4. Similarly, the complex symmetries up to the complex Lie group of scaling also reduce to the identity map.

Matrix B_2

For the other matrix B_2, the PDEs are given by

$$\begin{pmatrix} \mathbf{v_1}\tilde{x} & \mathbf{v_1}\tilde{t} & \mathbf{v_1}\tilde{u} \\ \mathbf{v_2}\tilde{x} & \mathbf{v_2}\tilde{t} & \mathbf{v_2}\tilde{u} \\ \mathbf{v_3}\tilde{x} & \mathbf{v_3}\tilde{t} & \mathbf{v_3}\tilde{u} \\ \mathbf{v_4}\tilde{x} & \mathbf{v_4}\tilde{t} & \mathbf{v_4}\tilde{u} \\ \mathbf{v_5}\tilde{x} & \mathbf{v_5}\tilde{t} & \mathbf{v_5}\tilde{u} \\ \mathbf{v_6}\tilde{x} & \mathbf{v_6}\tilde{t} & \mathbf{v_6}\tilde{u} \end{pmatrix} = \begin{pmatrix} 2ae^{\epsilon_4}\tilde{t} & 0 & -ae^{\epsilon_4}\tilde{x}\tilde{u} \\ 4a^2e^{2\epsilon_4}\tilde{x}\tilde{t} & 4a^2e^{2\epsilon_4}\tilde{t}^2 & -a^2e^{2\epsilon_4}(\tilde{x}^2+2\tilde{t})\tilde{u} \\ 0 & 0 & \tilde{u} \\ -\tilde{x} & -2\tilde{t} & \tilde{u} \\ -\frac{1}{a}e^{\epsilon_4} & 0 & 0 \\ 0 & \frac{1}{a^2}e^{2\epsilon_4} & 0 \end{pmatrix}$$

By considering the PDEs of the first three generators acting on $\tilde{t}$, it is restricted to $\tilde{t} = 1/(c - 4a^2\exp(2\epsilon_4)t)$. Using $\mathbf{v_6}\tilde{t} = \frac{1}{a^2}e^{2\epsilon_4}$ sets $c = 0$. For $\tilde{x}$, use $\mathbf{v_6}\tilde{x} = 0$ to derive the following:

$$\begin{aligned} 0 &= 4xt\partial_x\tilde{x} + 4t^2\partial_t\tilde{x} \\ &= 8ae^{\epsilon_4}xt\tilde{t} + 16a^2e^{2\epsilon_4}t^2\tilde{x}\tilde{t} \\ &= -\frac{2}{a}xt - 4e^{\epsilon_4}t^2\tilde{x}, \end{aligned}$$

where the final line can be rewritten to give $\tilde{x} = -x/(2a\exp(\epsilon_4)t)$. To find the transformations of u, consider first $\mathbf{v_3}\tilde{u} = \tilde{u}$, which sets $\tilde{u} = f(x,t)u$. Evaluating $\mathbf{v_1}$ and $\mathbf{v_2}$ on $\tilde{u}$ gives the conditions

$$\partial_x f(x,t) = \frac{x}{2t}f(x,t) \qquad \partial_t f(x,t) = \left(\frac{1}{2t} - \frac{x^2}{4t^2}\right)f(x,t).$$

The first condition only allows solutions $f(x,t) = \exp(x^2/(4t^2))g(t)$, with the second condition narrowing it down to $g(t) = b\sqrt{t}$ where b is a real or complex constant. The final transformations are given by

$$(\tilde{x},\ \tilde{t},\ \tilde{u}) = \left(\frac{-x}{ae^{\epsilon_4}2t},\ \frac{-1}{a^2e^{2\epsilon_4}4t},\ be^{\epsilon_3}\sqrt{t}\exp\left(\frac{x^2}{2t}\right)u\right), \tag{8.6}$$

where $\exp(\epsilon_3)$ is once again added to account for the scaling of u created by $\mathbf{v_3}$. All the other PDEs do not provide any further restrictions on $(\tilde{x},\tilde{t},\tilde{u})$. Next up is to determine whether all the transformation satisfy the symmetry condition. The derivation can be found in the appendix (subsection F), where it turns out that it always holds placing no further constraints on a and b.

If ϵ_3 and ϵ_4 are real constants, then the real symmetries, up to the adjoint action of the real Lie group of scaling, are generated by

$$\Gamma_5^{\pm} : \left(\pm\frac{x}{2t},\ -\frac{1}{4t},\ \sqrt{t}\exp\left(\frac{x^2}{2t}\right)u\right), \quad \Gamma_6^{\pm} : \left(\pm\frac{x}{2t},\ -\frac{1}{4t},\ -\sqrt{t}\exp\left(\frac{x^2}{2t}\right)u\right). \tag{8.7}$$

When taking Γ_1 and Γ_2 from Equation 8.4 into account, all real discrete point symmetries can be generated by Γ_1, Γ_2 and

$$\Gamma_5 : \left(\frac{x}{2t}, \ -\frac{1}{4t}, \ \sqrt{t} \exp\left(\frac{x^2}{2t} \right) u \right) \tag{8.8}$$

Note that although Γ_5 generates a real discrete symmetry, applying the generator twice yields

$$\Gamma_5^2 : \left(-x, t, \frac{iu}{2} \right), \tag{8.9}$$

which gives a complex transformation for $\tilde{u}$. Hence these generators do not have a group structure for real symmetries.

When considering complex symmetries, let $ae^{\epsilon_4} = \lambda$ and $be^{\epsilon_3} = \mu$ with $\lambda, \mu \in \mathbb{C}$. Once again the complex symmetries, up to the adjoint action of the real Lie group of scaling, are given by $\lambda = p \pm i$ and $\mu = k \pm i$ with $p, k \in \mathbb{R}$ and thus there are an infinite amount of them. If restricting to λ and μ to only values lying on the real/imaginary axis, then all the complex discrete point symmetries can be generated by Γ_3 and Γ_4 from Equation 8.5 and Γ_5 from Equation 8.8. From Equation 8.9, it can be seen that the identity map is recovered when applying the transformation generated by Γ_5 8 times, thus Γ_5 on its own forms the cyclic group of order 8. Note that Γ_3 and Γ_5 are not commutative and therefore the group structure is more complicated. The size group contains at least 32 distinct elements, namely the 16 elements generated by Γ_3 and Γ_4 and another 16 by first applying Γ_5 and then applying any of the 16 elements the previous group of elements.

If ϵ_3 and ϵ_4 are complex constants, then only the transformation created by Γ_5 is needed to create all possible symmetries up to the adjoint action of the complex Lie groups of scaling. Higher order discrete symmetries, like

$$\Gamma_5^3 : \left(-\frac{x}{2t}, \ \frac{1}{4t}, \ \frac{i}{2} \sqrt{t} \exp\left(\frac{x^2}{2t} \right) u \right), \tag{8.10}$$

can simply be created from Γ_5 and using complex scaling. Therefore both the real and complex discrete point symmetries up to the adjoint of complex scaling consist only of generator Γ_5 and the identity map.

To find new solutions of the heat equations that are realized by Γ_5, we first calculate the inverse transformation, given by

$$\Gamma_5^{-1} : \left(-\frac{x}{2t}, \ -\frac{1}{4t}, \ \frac{1}{\sqrt{t}} \exp\left(-\frac{x^2}{2t} \right) u \right). \tag{8.11}$$

Applying Equation 2.10, if $u = f(x, t)$ is a solution to the heat equation, so is

$$\tilde{f}(x, t) = \frac{i}{2\sqrt{t}} \exp\left(-\frac{x^2}{2t} \right) f\left(-\frac{x}{2t}, -\frac{1}{4t} \right). \tag{8.12}$$

The transformed solution is a complex function, even though the transformation generated by Γ_5 is a real-valued transformation. This discrete symmetry therefore should not be considered when only treating real solutions to the heat equation.

8.3 Application to Total Symmetry Group

The real discrete point symmetries have been found for the heat equation for both real scaling generated by $\mathbf{v_3}$ and $\mathbf{v_4}$ and complex scaling. For real scaling, the symmetries are generated by Γ_1 and Γ_2 from Equation 8.4 and Γ_5 from Equation 8.8. Applying Γ_5 twice however results in a complex transformation, and therefore the three generators do not form a group structure together. Nevertheless, the transformations from Γ_1, Γ_2 and Γ_5 remain valid discrete point symmetries as long as Γ_5 is only applied once. If one is only interested in real solutions to the heat equation, symmetries generated by Γ_5 should not be considered as it transforms real-valued functions into complex functions.
For complex scaling, the only symmetry that remains is the identity transformation and Γ_5.

For complex discrete point symmetries with real scaling, we found that there are an infinite amount of generators. If one restricts the complex values to lie on either the real or imaginary axis, the discrete point symmetries are generated using Γ_3 and Γ_4 from Equation 8.5 and again Γ_5. By allowing the discrete point symmetries to be complex the generators now do form a group structure. The group is non-abelian and contains at least 32 distinct elements, but an isomorphic group structure has not been found.

The continuous Lie point symmetries that have been covered in the previous chapters have been real transformations, so observing the real discrete point symmetries with real valued ϵ_3 and ϵ_4, we see that the heat equation must have at least 4 connected components. Allowing the discrete point symmetries to be complex increases the amount of connected components significantly.

9 Laplace Equation

The final differential equation that will be treated is the three dimensional Laplace equation in Cartesian coordinates, given by

$$u_{xx} + u_{yy} + u_{zz} = 0. \tag{9.1}$$

This equation is commonly studied as its solutions are the harmonic functions, found often in electrical or gravitational potential problems. The Laplace equation is a nice example to showcase the benefits of the computational solving method for finding the transformation matrix B. The Lie algebra of the symmetry group of the Laplace equation is spanned by 11 infinitesimal generators, put forward by Sattinger ([20], p. 84), excluding the infinite dimensional generator that arises from the linearity of the PDE.

$$\begin{aligned}
\mathbf{v_1} &= \partial_x \\
\mathbf{v_2} &= \partial_y \\
\mathbf{v_3} &= \partial_z \\
\mathbf{v_4} &= y\partial_z - z\partial_y \\
\mathbf{v_5} &= z\partial_x - x\partial_z \\
\mathbf{v_6} &= x\partial_y - y\partial_x \\
\mathbf{v_7} &= u\partial_u \\
\mathbf{v_8} &= (x^2 - y^2 - z^2)\partial_x + 2xy\partial_y + 2xz\partial_z - xu\partial_u \\
\mathbf{v_9} &= 2yx\partial_x + (-x^2 + y^2 - z^2)\partial_y + 2yz\partial_z - yu\partial_u \\
\mathbf{v_{10}} &= 2zx\partial_x + 2zy\partial_y + (-x^2 - y^2 + z^2)\partial_z - zu\partial_u \\
\mathbf{v_{11}} &= x\partial_x + y\partial_y + z\partial_z
\end{aligned}$$

Most of the transformations caused by these generators have been covered in previous examples, except for the ones generated by $\mathbf{v_8}$, $\mathbf{v_9}$ and $\mathbf{v_{10}}$. The transformations caused by these generators are known as the special conformal transformations. Such transformations are interesting because they are known to be equal to the symmetry transformation caused by an inversion ($x^i \to \frac{x^i}{\sum_j x^j x^j}$), translating x^i with some constant value and then doing another inversion.

Let $P_{1,2,3} = \mathbf{v_{1,2,3}}$, $J_{1,2,3} = \mathbf{v_{4,5,6}}$, $S = \mathbf{v_7}$, $K_{1,2,3} = \mathbf{v_{8,9,10}}$ and $D = \mathbf{v_{11}}$. The commutation relations are given by

$$[D, P_i] = -P_i, \quad [D, K_i] = K_i, \quad [J_i, J_j] = \epsilon_{ijk} J_k, \quad [J_i, K_j] = -\epsilon_{ijk} K_k$$

and

$$[P_i, K_j] = -2\epsilon_{ijk} J_k + 2\delta^i_j D - \delta^i_j S.$$

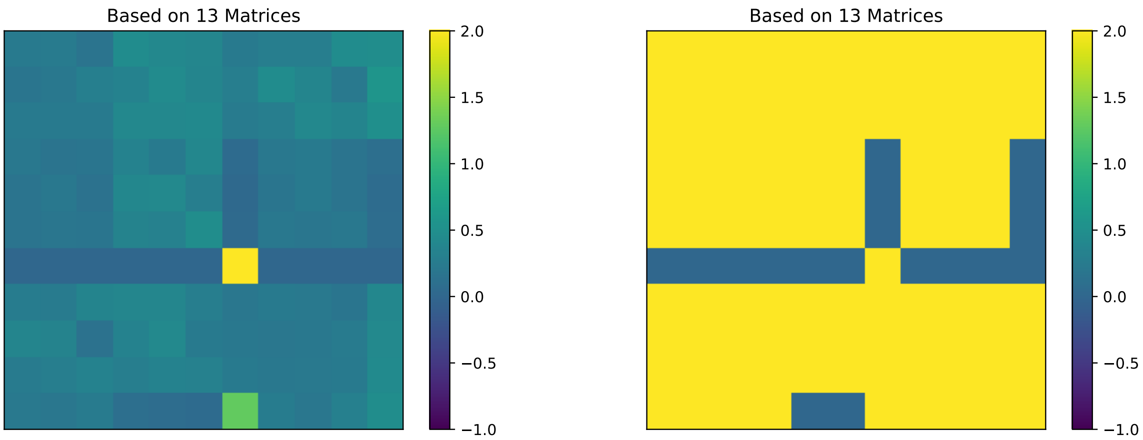
9.1 Finding Transformation Matrix

9.1.1 Analytical Solving Method

Finding the transformation matrices that form automorphisms analytically is a lot more difficult than the previous two examples. Not only does the transformation matrix exists of 121 parameters, there is also no smaller ideal of the Lie algebra. Furthermore, any infinitesimal generator can be created by commuting two specific infinitesimal generators, which means that there is no value of n for which the nonlinear conditions simplify to linear conditions. Solving this system analytically would take considerable amount of time, hence we move forth onto the computational method.

9.1.2 Computational Solving Method

Tackling this problem will require some initial information of what parameters b_j^i can be set to zero. Letting the Adam optimizer run without any additional constraints gives rise to Figure 12.



(a) Final averaged matrix values $\boldsymbol{b_{avg}}$. (b) Display which variables are zero using $\delta = 0.1$.

Figure 12: Plot for the first run without utilizing any adjoint matrix, using 30 simulations, learning rate of 4e-6 and 20.000 iterations.

Observing which parameters are close to zero and which ones are not yet close enough to set them to zero becomes harder when more parameters are involved. To circumvent this, we require the parameter to be below some threshold value δ to set it equal to zero. Note that this value is based on experimentation and might be case dependent. For example, if one chooses $\delta = 0.1$, the figure on the right of Figure 12 provides a clearer picture of which variables should be set to zero.

An assumption has to be made to further restrict the matrix. Choosing b_8^1 as the value which either is or is not zero, we again get two options. This specific parameter is chosen as it allows use 3 adjoint matrices to set values to zero.

Option 1: $\boldsymbol{b_8^1} \neq 0$
Using this information, b_8^{11}, b_8^6 and b_8^5 can be set to zero using the 8th, 9th and 10th adjoint matrix respectively. Setting the first parameter to zero, running the algorithm and putting in the next value for all three gives the result from Figure 13.

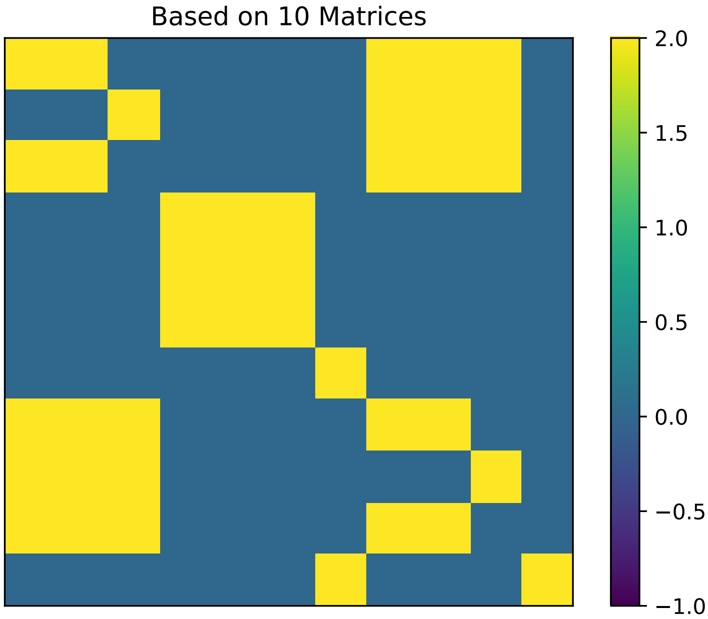


Figure 13: Matrix values $\boldsymbol{b_{avg}}$ using 30 simulations, learning rate of 6e-4 and 20.000 iterations.

The optimizer does not find any further zeroes, so we take a look again at the nonlinear conditions. These set b_{11}^{11} equal to -1, which sets multiple other values to zero such that only the three 3x3 blocks remain together with b_7^7 and b_{11}^7. The final matrix, before multiplying the unused adjoint matrices, looks like

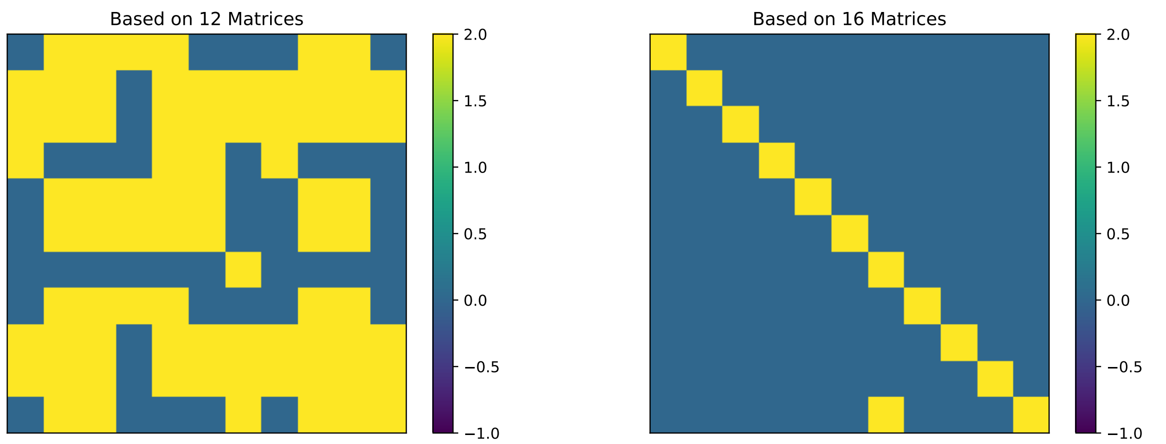
$$B_1 = \begin{pmatrix} & & & & & & & b_1^8 & b_1^9 & b_1^{10} & \\ & & & & & & & b_2^8 & b_2^8 & b_2^{10} & \\ & & & & & & & b_3^8 & b_3^9 & b_3^{10} & \\ & & & b_4^4 & b_4^5 & b_4^6 & & & & & \\ & & & b_5^4 & b_5^5 & b_5^6 & & & & & \\ & & & b_6^4 & b_6^5 & b_6^6 & & & & & \\ & & & & & & b_7^7 & & & & \\ b_8^1 & b_8^2 & b_8^3 & & & & & & & & \\ b_9^1 & b_9^2 & b_9^3 & & & & & & & & \\ b_{10}^1 & b_{10}^2 & b_{10}^3 & & & & & & & & \\ & & & & & & b_{11}^7 & & & & -1 \end{pmatrix}. \tag{9.2}$$

The 5th and 6th adjoint matrix can be used to set b_8^3 and b_8^2 to zero using $\epsilon = \arctan(b_8^3/b_8^1)$ and $\epsilon = \arctan(-b_8^2/b_8^1)$ respectively. The 4th can be used when making an another assumption. If $b_9^2 \neq 0$, then b_9^3 can be set to zero, and if $b_9^2 = 0$ then $b_{10}^2 \neq 0$ which can be used to set $b_{10}^3 = 0$. There are thus two solutions, each with a slightly different choice of three variables out of each 3x3 block. If one takes $b_9^2 \neq 0$, the nonlinear conditions can be solved to give

$$B_1 = \begin{pmatrix} & & & & & & & e^{-\epsilon}/\alpha & & & \\ & & & & & & & & abe^{-\epsilon}/\alpha & & \\ & & & & & & & & & be^{-\epsilon}/\alpha & \\ & & & a & & & & & & & \\ & & & & b & & & & & & \\ & & & & & ab & & & & & \\ & & & & & & \beta & & & & \\ e^{\epsilon}\alpha & & & & & & & & & & \\ & abe^{\epsilon}\alpha & & & & & & & & & \\ & & be^{\epsilon}\alpha & & & & & & & & \\ & & & & & & (1+\beta)/2 & & & & -1 \end{pmatrix}. \tag{9.3}$$

What happens when choosing $b_9^2 = 0$ will be explained after the PDEs have been solved that arise from B_1 above in the next section.

Option 2: $\boldsymbol{b_8^1} = 0$
Setting this value leads to $b_1^8 = b_4^3 = b_{11}^4 = 0$. Another assumption must be made to use the remaining the adjoint matrices. One option would be to assume either b_1^1 is zero or not. Making the assumption that $b_1^1 \neq 0$ and using the adjoint matrix to eliminate one parameter, the left figure of Figure 14 is obtained. This figure shows that $b_1^1 = 0$ and therefore the inconsistency would mean that there is no solution for $b_1^1 \neq 0$.



(a) $\boldsymbol{b_{avg}}$ assuming $b_1^1 \neq 0$. (b) $\boldsymbol{b_{avg}}$ with different initial information.

Figure 14: Plot of $\boldsymbol{b_{avg}}$ both assuming $b_1^1 \neq 0$, using 30 simulations, learning rate of 4e-6 and 20.000 iterations.

The Laplace equation does however have a discrete transformation which requires $b_1^1 \neq 0$. The identity matrix is always a valid automorphism, although a trivial one. Nevertheless, it is a solution that satisfies the nonlinear constraints. The optimization algorithm is thus not always able to find all the solutions, depending on the information it starts with.

For example, from the structure of the Laplace equation we can see that $\tilde{u} = -u$ should also be a discrete symmetry that cannot be created from the continuous symmetries. If we assume the $\tilde{u} = c_1 u^{c_2}$ where c_1, c_2 are real constants, then $b_i^7 = 0$ for $i \neq 7, 11$, $b_j^8 = 0$ for $j \neq 8, 11$, $b_k^9 = 0$ for $k \neq 9, 11$ and $b_l^{10} = 0$ for $l \neq 10, 11$, to satisfy the PDEs from Equation 6.28. Plugging this information into the optimizer, we obtain the right hand figure from Figure 14. Solving the nonlinear conditions and multiplying with the final adjoint matrix gives the final matrix below, where α, β are real constants and $a, b = \pm 1$.

$$B_2 = \begin{pmatrix} \alpha e^{\epsilon} &&&&&&&&&& \\ & ab\alpha e^{\epsilon} &&&&&&&&& \\ && a\alpha e^{\epsilon} &&&&&&&& \\ &&& b &&&&&&& \\ &&&& a &&&&&& \\ &&&&& ab &&&&& \\ &&&&&& \beta &&&& \\ &&&&&&& e^{-\epsilon}/\alpha &&& \\ &&&&&&&& abe^{-\epsilon}/\alpha && \\ &&&&&&&&& ae^{-\epsilon}/\alpha & \\ &&&&&& (\beta-1)/2 &&&& 1 \end{pmatrix}. \tag{9.4}$$

Unfortunately, this also means that the optimizer cannot always find all solutions in its current implementation, and further refinement is necessary to be able find solutions like these.

If one assumes both $b_8^1 = b_1^1 = 0$ and assumes another value of $b_i^1 \neq 0$, no more solutions have been found that have a different structure than Equation 9.2 or Equation 9.4 and therefore B_1 and B_2 are the only known possible transformation matrices when using the optimizer algorithm.

9.2 Finding Possible Transformations

Once again we have two different transformation matrices that create the automorphisms of the Lie algebra. To determine the possible transformations, the PDEs determined by these transformation matrices have to be solved first. The second transformation matrix is easier to solve and will be covered first.

Matrix B_2
Using the matrix from the Equation 9.4, the following PDEs can be used to find the transformations of x, y and z

$$\partial_x \tilde{x} = \alpha e^{\epsilon}, \quad \partial_y \tilde{y} = ab\alpha e^{\epsilon}, \quad \partial_z \tilde{z} = a\alpha e^{\epsilon}, \quad u\partial_u \tilde{x}^i = 0.$$

The only solutions that satisfy these equations are the functions

$$\tilde{x} = \alpha e^{\epsilon} x + c_1, \quad \tilde{y} = ab\alpha e^{\epsilon} y + c_2, \quad \tilde{z} = a\alpha e^{\epsilon} z + c_3.$$

Using the PDEs generated by $\mathbf{v_{11}}$, we can see that $c_1 = c_2 = c_3 = 0$. The solutions satisfy all the other PDEs and can therefore not be further reduced. To find $\tilde{u}$, we make use of the following PDEs

$$u\partial_u \tilde{u} = \beta \tilde{u}, \quad (x\partial_x + y\partial_y + z\partial_z)\tilde{u} = \frac{\beta - 1}{2}\tilde{u}.$$

The first equation sets $\tilde{u} = \delta u^\beta$. The second one only holds when $\beta = 1$. The remaining PDEs do not provide any further restrictions on a, b or α, δ. The final transformations are given by

$$\tilde{x} = \alpha e^\epsilon x, \quad \tilde{y} = ab\alpha e^\epsilon y, \quad \tilde{z} = a\alpha e^\epsilon z, \quad \tilde{u} = \delta e^{\epsilon_2} u, \tag{9.5}$$

where e^{ϵ_2} is added for the scaling of u which has not yet been accounted for. Calculation of the symmetry condition shows that there are no further constraints on a, b or α, δ, shown in the appendix (subsection G, 2nd part).

To keep this brief, we only consider real values of ϵ and ϵ_2. If real point transformations are considered, the discrete symmetries are generated by, up to scaling generated by $\mathbf{v_7}$ and $\mathbf{v_{11}}$, map (x, y, z, u) to

$$\Gamma_1 : (-x, y, z, u), \;\; \Gamma_2 : (x, -y, z, u), \;\; \Gamma_3 : (x, y, -z, u), \;\; \Gamma_4 : (x, y, z, -u). \tag{9.6}$$

The group is abelian and is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$.

When complex point transformations are considered, there will be an infinite amount of discrete generators when all complex transformations are allowed, just like the heat equation. Restricting to complex values lying on the real/imaginary axis, we obtain a subset of these generators, which up to scaling of x, y, z and u, are given by

$$\Gamma_1 : (ix, y, z, u), \;\; \Gamma_2 : (x, iy, z, u), \;\; \Gamma_3 : (x, y, iz, u), \;\; \Gamma_4 : (x, y, z, iu). \tag{9.7}$$

This group is also abelian and is isomorphic to $\mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4$.

Matrix B_1

The transformation matrix B_1 is given in Equation 9.3. The PDEs determining the possible transformations of the (in)dependent variables can now be solved. The necessary PDEs determining $\tilde{x}$ are given by

$$u\partial_u \tilde{x} = 0, \quad \partial_y \tilde{x} = 2\frac{ab}{\alpha e^\epsilon}\tilde{y}\tilde{x}, \quad \partial_z \tilde{x} = 2\frac{b}{\alpha e^\epsilon}\tilde{z}\tilde{x}, \quad y\partial_z \tilde{x} - z\partial_y \tilde{x} = 0.$$

The first equation makes $\tilde{x}$ independent of u. Substituting the second and third equations into the latter, we obtain that $\tilde{z} = a\frac{z}{y}\tilde{y}$. Following the same procedure for $\tilde{y}$, we find the following PDEs

$$u\partial_u \tilde{y} = 0, \quad \partial_x \tilde{y} = \frac{2}{\alpha e^\epsilon}\tilde{x}\tilde{y}, \quad \partial_z \tilde{y} = 2\frac{b}{\alpha e^\epsilon}\tilde{z}\tilde{y}, \quad z\partial_x \tilde{y} - x\partial_z \tilde{y} = 0.$$

Substituting the second and third equations again in the latter equation yields a condition on $\tilde{x}$, namely $\tilde{z} = b\frac{z}{x}\tilde{x}$. Using the first relation, $\tilde{x} = ab\frac{x}{y}\tilde{y}$. All that is left is to find a solution for $\tilde{y}$ utilizing another PDE, given below

$$\partial_y \tilde{y} = \frac{ab}{\alpha e^\epsilon}(-\tilde{x}^2 + \tilde{y}^2 - \tilde{z}^2)$$

Using symbolic software like `MATHEMATICA`, we find that the only function that holds for all three partial derivatives of $\tilde{y}$ is the function

$$\tilde{y} = -ab\alpha e^{\epsilon}\frac{y}{x^2+y^2+z^2},$$

which only satisfies all three derivatives when $a = b$, setting $ab = 1$. The transformations of the independent variables are thus given by

$$\tilde{x} = -\alpha e^{\epsilon}\frac{x}{x^2+y^2+z^2}, \quad \tilde{y} = -\alpha e^{\epsilon}\frac{y}{x^2+y^2+z^2}, \quad \tilde{z} = -a\alpha e^{\epsilon}\frac{z}{x^2+y^2+z^2}. \tag{9.8}$$

To find the transformations of u, we make use of the following PDEs generated by the transformation matrix:

$$u\partial_u\tilde{u} = \beta\tilde{u}, \quad \partial_x\tilde{u} = -\frac{1}{\alpha e^{\epsilon}}\tilde{x}\tilde{u}, \quad \partial_y\tilde{u} = -\frac{ab}{\alpha e^{\epsilon}}\tilde{y}\tilde{u}, \quad \partial_z\tilde{u} = -\frac{b}{\alpha e^{\epsilon}}\tilde{z}\tilde{u}.$$

The first equation sets $\tilde{u} = u^{\beta}f(x,y,z)$. The last three equations, using the transformations from Equation 9.8 and solving with numerical software, makes only the following transformations possible

$$\tilde{u} = \delta(x^2+y^2+z^2)^{1/2}u^{\beta},$$

where δ is a real constant. Lastly, a constraint can be found on β by making use of yet another PDE, given by

$$(x^2-y^2-z^2)\partial_x\tilde{u} + 2yx\partial_y\tilde{u} + 2zx\partial_z\tilde{u} - xu\partial_u\tilde{u} = 0.$$

Plugging in all the transformations found so far and calculating the derivatives, one finds that it only holds when $\beta = 1$. The transformations are therefore given by Equation 9.8 and

$$\tilde{u} = \delta e^{\epsilon_2}(x^2+y^2+z^2)^{1/2}u, \tag{9.9}$$

where e^{ϵ_2} comes from the scaling in u that could not be accounted for using the adjoint matrices. The following step is to find out if the symmetry condition provides any further constraints on a, b or α. The derivation for the symmetry condition can be found in the appendix (subsection G), which provides no further constraints for any of the variables.

Again only real values of ϵ and ϵ_2 are considered. The distinction between real and complex discrete point transformations will still be made. If the discrete points symmetries are real, up to scaling created by $\mathbf{v_7}$ and $\mathbf{v_{11}}$, the generators map (x,y,z,u) to

$$\begin{aligned}\Gamma^+_{5,\pm z} &: \left(\frac{x}{x^2+y^2+z^2}, \frac{y}{x^2+y^2+z^2}, \frac{\pm z}{x^2+y^2+z^2}, (x^2+y^2+z^2)^{1/2}u\right), \\ \Gamma^+_{6,\pm z} &: \left(\frac{-x}{x^2+y^2+z^2}, \frac{-y}{x^2+y^2+z^2}, \frac{\pm z}{x^2+y^2+z^2}, (x^2+y^2+z^2)^{1/2}u\right).\end{aligned} \tag{9.10}$$

Similarly, $\Gamma^-_{1,\pm z}$ denotes the same as the above but with a minus sign before the transformation of u. Note that any of these generators applied twice in a row returns the identity mapping. The fact that only the z variable can change minus sign independently is curious, but might be caused by the choice of $b_8^2 = b_8^3 = b_9^3 = 0$ that was done earlier. Using the generators Γ_1 to Γ_4 already found in Equation 9.6, the only new generator is given by

$$\Gamma_5 : \left(\frac{x}{x^2+y^2+z^2}, \frac{y}{x^2+y^2+z^2}, \frac{z}{x^2+y^2+z^2}, (x^2+y^2+z^2)^{1/2}u\right). \tag{9.11}$$

If complex discrete point symmetries are considered, than all discrete symmetries can be generated using Γ_1 to Γ_4 from Equation 9.7 and Γ_5 given above.

We can now consider what happens when choosing $b_9^2 = 0$ and $b_9^3 \neq 0$, such that the structure of B_1 in Equation 9.3 is different. When solving the nonlinear conditions, the transformation matrix has the form

$$B_3 = \begin{pmatrix} &&&&&&& e^{-\epsilon}/\alpha &&& \\ &&&&&&&&& -be^{-\epsilon}/\alpha & \\ &&&&&&&& abe^{-\epsilon}/\alpha && \\ &&& a &&&&&&& \\ &&&&& -ab &&&&& \\ &&&& b &&&&&& \\ &&&&&& \beta &&&& \\ e^{\epsilon}\alpha &&&&&&&&&& \\ && -be^{\epsilon}\alpha &&&&&&&& \\ & abe^{\epsilon}\alpha &&&&&&&&& \\ &&&&&& (\beta-1)/2 &&&& -1 \end{pmatrix}. \tag{9.12}$$

The values of the matrix are very similar to that of B_1, except for the swapped entries with one additional minus sign. When following the same procedure taken for B_1, we will find that the transformations realized by this matrix are of the form

$$\Gamma : \left(\frac{x}{x^2+y^2+z^2}, \frac{z}{x^2+y^2+z^2}, \frac{y}{x^2+y^2+z^2}, (x^2+y^2+z^2)^{1/2} u \right). \tag{9.13}$$

This is equal to the taking the generator Γ_5 and permuting the y and z variables, i.e. first applying Γ_5 and then applying

$$\Gamma_6 : (x, y, z, u) \to (x, z, y, u). \tag{9.14}$$

Similarly, if instead of assuming $b_8^1 \neq 0$ at the beginning we assume $b_9^1 \neq 0$ or $b_{10}^1 \neq 0$ and use the optimizer to reduce the transformation matrix further, other permutations between x, y and z can be found.

Lastly, the transformation of a solution to the Laplace equation $u = f(x, y, z)$ created by Γ_5 will be found. As Γ_5 is its own inverse, Equation 2.10 can be applied immediately to find new solutions with

$$\tilde{f}(x, y, z) = \frac{1}{\sqrt{x^2+y^2+z^2}} f\left(\frac{x}{x^2+y^2+z^2}, \frac{y}{x^2+y^2+z^2}, \frac{z}{x^2+y^2+z^2} \right). \tag{9.15}$$

This is a real solution and the discrete point transformation is therefore usable when considering either real or complex solutions to the Laplace equation.

9.3 Application to Total Symmetry Group

As stated in the introduction of the Laplace equation, the continuous special conformal symmetries are similar to an inversion, translation and another inversion. The inversions have been found using the optimizer and assuming $b_8^1 \neq 0$ and is given as Γ_5 in Equation 9.10. The generator remains the same whether considering real or complex discrete symmetries.

For real discrete point symmetries, the other generators are Γ_1, Γ_2, Γ_3 and Γ_4 from Equation 9.6. If the discrete point symmetries are allowed to be complex and are restricted to complex values on the real/imaginary axis, the generators are given by Γ_1, Γ_2, Γ_3 and Γ_4 from Equation 9.7. Furthermore, both real and complex discrete point symmetries have all permutations between x, y and z as discrete point symmetries. Permutations are not commutative, so the total discrete point symmetry group is also not abelian.

The group of real discrete point symmetries contains 16 elements from Γ_1 to Γ_4 and another 16 when first transforming with Γ_5 and then with any of those 16 transformations, as those are all unique. Hence the total group structure contains at least 32 distinct elements, excluding all possible permutations between x, y and z.
For the group of complex discrete point symmetries, it contains 32 elements from Γ_1 to Γ_4 and at least another 32 when multiplying Γ_5 with each of these transformations, since these are also all unique. The total group structure contains at least 64 distinct elements excluding permutations between x, y and z. It likely contains more as for complex Γ_1 to Γ_4, they no longer commute with Γ_5.

The transformation matrix B_2, corresponding to Γ_1 to Γ_4, was only found with the optimizer when observing that $u \to -u$ should be a valid transformation, so further improvement might be necessary when applying this method to other differential equations. There might be different transformation matrices which also have not been found using the optimizer, thus the optimizer alone is not yet sufficient to determine the total discrete symmetry group of the Laplace equation.

10 Conclusion

The global Lie point symmetry group of partial differential equations like the heat equation are discussed, starting with the established theory of finding the local Lie point symmetries using the prolongation method. Local Lie point symmetries are based on local Lie groups, where multiplication and inversion are only defined on a certain domain. Elements of a local Lie group create transformations, which depend on some parameter ϵ and are defined either locally or globally. The prolongation method only provides the local Lie point symmetries, so multiple differential equations are investigated to find out if their local symmetries can be extended to global symmetries.

The logistic equation was found to have a single infinitesimal generator using the prolongation technique. The new solutions, found by applying the transformation created by this generator on the general solution, satisfied the logistic equation for all values of ϵ. The symmetry group of the logistic equation is therefore a global one.

The infinitesimal generators of the heat equation were also calculated, where it turns out that the heat equation has a Lie algebra isomorphic to the Lie algebra of the global group $H_3 \rtimes SL(2, R)$. However, one generator of the Lie algebra generates transformations that are only defined within a range of $|\epsilon t| < \frac{1}{4}$, depending on both the group (ϵ) and the domain of the PDE (t). Furthermore, taking products of this element which generates these local transformations with another element reduces the range where it is defined even further. The total symmetry group can therefore not be described as a global Lie group. Despite this, for the solutions tested in this thesis they, after being transformed, remained solutions to the heat equation, even beyond the range where this transformation is defined. If the set of solutions is restricted to $L^2(\mathbb{R})$, seen often when studying the Schrödinger equation, then the symmetry groups found do form a global group.

Another equation that was studied is the filtration equation. This equation only contains transformations that are globally defined. Calculating the transformed solutions does however lead to functions that are not defined, due to division by zero. According to the definitions used by Olver, the total symmetry group remains global, as there is a distinction between local transformations that are defined within a certain domain and global transformations which lead to new solutions that are not defined. Using Olver's definition therefore does mean that not every transformations has to provide defined solutions.

Additionally, discrete point symmetries were found using the method described by Hydon, utilizing the Lie algebra of the local symmetry group found with the prolongation method. By considering automorphisms of the Lie algebra via linear basis transformations, excluding those created by the continuous symmetries, new transformations can be found that are unable to be created using just the continuous transformations. Although all steps of Hydon's method can be calculated analytically, systems with many generators become difficult to solve. An algorithm based on gradient descent, specifically the Adam optimizer, was used to find the automorphisms of the Lie algebra. The algorithm was able to find all transformation matrices that could be find analytically. It was unable to find one transformation matrix for the Laplace equation, which could only be found analytically by making large assumptions.

The spherical Burgers equation was first examined to find the discrete point symmetries. It only has a single discrete point transformation, which returns to the identity map when applied twice.

The heat equation had a greater variety of discrete symmetries, depending on whether the discrete symmetries were allowed to be complex or not. For real symmetries, two obvious discrete symmetry generators were found together with a more complicated discrete symmetry generator. The latter turns into a complex transformation when applied twice and hence does not form a group together with the first two. The transformed solution it generates also turns real-valued functions into complex ones. If only the first two generators are taken, they form a group of 4 components isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$. Allowing complex symmetries changes the first two generators such that they form a group of 16 components isomorphic to $\mathbb{Z}_4 \times \mathbb{Z}_4$. The other generator, which returns the identity transformation when applied four times, now does form a group with the other generators, although a non-abelian one containing at least 32 components. The structure of the global symmetry group of the heat equation thus increases significantly when considering complex transformations.

Lastly, the Laplace equation was investigated to see if the algorithm fares well against a PDE containing many generators, eleven in this case. The discrete generators that were found consisted of 4 obvious ones, which are either $x^j \to -x^j$ or $x^j \to ix^j$ depending on whether real or complex transformations are considered respectively. Another generator is the inversion generator, which is the same for both real or complex symmetries. Lastly, both real and complex symmetries have a permutation symmetry between x, y and z. The first four generators have a group structure isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ or $\mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4 \times \mathbb{Z}_4$ for the real and complex generators respectively. Adding the inversion symmetry yields at least the same number of elements that the above mentioned group already has, excluding any permutations. The amount of discrete symmetries considering either real or complex transformations are numerous and the total global symmetry group must therefore have many connected components.

To conclude, obtaining a global symmetry group from a PDE comes with many caveats. The structure of a local Lie group and local transformations differ in important ways from regular Lie groups, and not all symmetry transformations lead to defined solutions. Additionally, the discrete point symmetries show that the amount of connected components a global symmetry group has can increase rapidly when considering multiple independent variables. Further research could look into the how the local Lie point symmetries and discrete point symmetries can be combined to include or exclude global symmetry group candidates. Moreover, further refinement of the algorithm and the Adam optimizer can be used to make Hydon's method applicable to treat systems with large amount of generators.

Appendices

A Heat Equation Exponential Map

Here we derive how the exponential map leads to the group transformations found in Equation 4.9. As a reminder, the first group formed from generator $\mathbf{v_1} = \partial_x$ is found by doing

$$\begin{aligned} e^{\epsilon \mathbf{v_1}} x &= \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) x = x + \epsilon + 0 + 0 + ... = x + \epsilon \\ e^{\epsilon \mathbf{v_1}} t &= \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) t = t + 0 + 0 + 0 + ... = t \\ e^{\epsilon \mathbf{v_1}} u &= \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) u = u + 0 + 0 + ... = u, \end{aligned}$$

which gives the group transformation $(x + \epsilon, t, u)$. The next generators $\mathbf{v_2}$, $\mathbf{v_3}$ and $\mathbf{v_4}$ can be calculated similarly as above.

The derivation of the transformations caused by $\mathbf{v_6}$ is slightly more involved and is therefore laid out in this appendix. For $\mathbf{v_6} = 4tx\partial_x + 4t^2\partial_t - (x^2 + 2t)u\partial_u$, the following transformations are done. For the transformation of x, the observations below will simplify the tasks.

$$\begin{aligned} \mathbf{v_6} x &= (4tx\partial_x + 4t^2\partial_t - (x^2 + 2t)u\partial_u)x = 4tx \\ \mathbf{v_6} \alpha x^n t^m &= 4\alpha n t^{m+1} x^n + 4\alpha m t^{m+1} x^n = 4\alpha(m+n) t^{m+1} x^n \end{aligned}$$

The second condition shows that acting with $\mathbf{v_6}$ yields a similar expression, and it can therefore be applied repeatedly.

$$(\mathbf{v_6})^k \alpha x^n t^m = \alpha x^n t^{m+k} \prod_{i=0}^{k-1} 4(m + n + i)$$

The final step is calculating the effect of $\mathbf{v_6}$ on x instead of the expression above. This can be done by using

$$\begin{aligned} \mathbf{v_6}^k x &= \mathbf{v_6}^{k-1} 4tx \\ &= 4xt^k \prod_{i=0}^{k-2} 4(2 + i) \\ &= 4^k x t^k k! \end{aligned}$$

The transformation on x is now complete.

$$e^{\epsilon \mathbf{v_6}} x = \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) x = x + (4\epsilon t)x + (4\epsilon t)^2 x + (4\epsilon t)^3 x + ... = \frac{x}{1 - 4\epsilon t} \text{ for } |4\epsilon t| < 1$$

Transformation of t can be done similarly, using the generator on t and utilizing the previously found formula.

$$\begin{aligned} \mathbf{v_6} t &= (4tx\partial_x + 4t^2\partial_t - (x^2 + 2t)u\partial_u)x = 4t^2 \\ \mathbf{v_6}^k t &= (4t)^k k! t \end{aligned}$$

Thus the following transformation is found for t

$$e^{\epsilon \mathbf{v_6}} t = \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) t = t + (4\epsilon t)t + (4\epsilon t)^2 t + (4\epsilon t)^3 t + ... = \frac{t}{1 - 4\epsilon t} \text{ for } |4\epsilon t| < 1$$

Both of these transformations are only valid when $|4\epsilon t| < 1$, and elsewhere the geometric series cannot be used.

The transformation of u is more complicated, and only the first two terms are calculated.

$$\begin{aligned}
\mathbf{v_6} u &= -(x^2 + 2t)u \\
\mathbf{v_6}^2 u &= -\mathbf{v_6}(x^2 + 2t)u = -8tx^2 u - 8t^2 u + (x^2 + 2t)^2 u = (x^4 - 4tx^2 - 4t^2)u
\end{aligned}$$

The generator can be applied repeatedly and a single term of u remains, with increasingly more factors of $t^n x^m$ appearing. These can be ordered as follows into a nice expression.

$$\begin{aligned}
e^{\epsilon \mathbf{v_6}} u &= \left(1 + \epsilon \mathbf{v_1} + \frac{\epsilon^2 \mathbf{v_1}^2}{2!} + ...\right) u \\
&= u - \epsilon(x^2 + 2t)u + \frac{\epsilon^2}{2!}(x^4 - 4tx^2 - 4t^2)u + ... \\
&= \left(1 - 2\epsilon t - 4\frac{\epsilon^2}{2!}t^2 - ...\right) \cdot \left(1 - \epsilon x^2 + \frac{\epsilon^2}{2!}x^4 - \frac{\epsilon^2}{2!}8x^2 t + ...\right) u \\
&= \sqrt{1 - 4\epsilon t} \cdot \left(1 - \epsilon x^2(1 + 4\epsilon t + ...) - \frac{\epsilon^2}{2!}x^4(1 + 8\epsilon t + ...) + ...\right) u \\
&= \sqrt{1 - 4\epsilon t} \cdot \left(1 - \epsilon x^2 \frac{1}{1 + 4\epsilon t} - \frac{\epsilon^2}{2!}x^4 \left(\frac{1}{1 + 4\epsilon t}\right)^2 + ...\right) u \\
&= \sqrt{1 - 4\epsilon t} \cdot \exp\left(\frac{-\epsilon x^2}{1 - 4\epsilon t}\right) u
\end{aligned}$$

Which concludes the transformation of u. All three transformations are thus found and agree with the result found in Equation 4.9.

B Derivation Invariance Craddock Solution

The transformations group of $\mathbf{v_6}$ leads to new solutions (Olver, p. 119)

$$\tilde{u}(x,t) = \frac{1}{\sqrt{1 + 4\epsilon t}} \exp\left(\frac{-\epsilon x^2}{1 + 4\epsilon t}\right) f\left(\frac{x}{1 + 4\epsilon t}, \frac{t}{1 + 4\epsilon t}\right).$$

where $u = f(x)$ is a solution to the heat equation. Using the solution

$$f(x,t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right), \qquad t > 0$$

and substituting it in into the equation above, we get

$$\begin{aligned}
\tilde{u}(x,t) &= \frac{1}{\sqrt{1+4\epsilon t}} \exp\left(\frac{-\epsilon x^2}{1+4\epsilon t}\right) \frac{1}{\sqrt{4\pi t/(1+4\epsilon t)}} \exp\left(-\left(\frac{x}{1+4\epsilon t}\right)^2 \left(\frac{4t}{1+4\epsilon t}\right)^{-1}\right) \\
&= \frac{1}{\sqrt{4\pi t}} \exp\left(\frac{-\epsilon x^2}{1+4\epsilon t}\right) \exp\left(-\frac{x^2}{4t(1+4\epsilon t)}\right) \\
&= \frac{1}{\sqrt{4\pi t}} \exp\left(\frac{-x^2(1+4\epsilon t)}{4t(1+4\epsilon t)}\right) \\
&= \frac{1}{\sqrt{4\pi t}} \exp\left(\frac{-x^2}{4t}\right) \\
&= f(x,t)
\end{aligned}$$

Hence the solution did not change under this transformation.

C Derivation Adjoint Matrices Burgers

The derivation of the three adjoint matrices of the spherical burgers equation is given below. The adjoint matrices are given by

$$A(i,\epsilon) = \sum_{n=0}^{\infty} \frac{\epsilon^n}{n!} C(i)^n = I + \sum_{n=1}^{\infty} \frac{\epsilon^n}{n!} C(i)^n$$

where $C(i)^n$ is the nth matrix product of $C(i)$ with $C(i)^0 = I$.

Starting of with $i = 1$, the starting matrix is

$$C(1) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 2 \\ 0 & 0 & -1 \end{pmatrix}.$$

The following matrix products are

$$C(1)^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -4 \\ 0 & 0 & 1 \end{pmatrix}, \qquad C(1)^3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 6 \\ 0 & 0 & -1 \end{pmatrix}.$$

Following this pattern, the nth matrix product can be written as

$$C(1)^n = \begin{pmatrix} 0 & 0 & 0 \\ 0 & (-1)^n & (-1)^{n+1}2n \\ 0 & 0 & (-1)^n \end{pmatrix} = (-1)^n \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -2n \\ 0 & 0 & 1 \end{pmatrix}$$

Substituting this result into the equation for the adjoint matrix results in the following

$$
\begin{aligned}
A(1,\epsilon) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \sum_{n=1}^{\infty} \frac{\epsilon^n}{n!}(-1)^n \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -2n \\ 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1+\sum_{n=1}^{\infty} \frac{(-\epsilon)^n}{n!} & \sum_{n=1}^{\infty} \frac{(-\epsilon)^n}{n!} \cdot -2n \\ 0 & 0 & 1+\sum_{n=1}^{\infty} \frac{(-\epsilon)^n}{n!} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{(-\epsilon)^n}{n!} & 2\epsilon \sum_{n=1}^{\infty} \frac{(-\epsilon)^{n-1}}{(n-1)!} \\ 0 & 0 & \sum_{n=0}^{\infty} \frac{(-\epsilon)^n}{n!} \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-\epsilon} & 2\epsilon e^{-\epsilon} \\ 0 & 0 & e^{-\epsilon} \end{pmatrix}.
\end{aligned}
$$

For $i = 2$, the starting matrix is

$$
C(2) = \begin{pmatrix} 0 & 1 & -2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
$$

The following matrix product is

$$
C(1)^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},
$$

which makes all higher order matrix products also zero matrices. Finding the adjoint matrix becomes rather straightforward

$$
\begin{aligned}
A(2,\epsilon) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \epsilon \begin{pmatrix} 0 & 1 & -2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \sum_{n=2}^{\infty} \frac{\epsilon^n}{n!} C(2)^n \\
&= \begin{pmatrix} 1 & \epsilon & -2\epsilon \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{aligned}
$$

Similarly, the final matrix for $i = 3$ also gives a zero matrix for matrix products of 2 or higher, as shown below

$$
C(3) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad C(2)^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}
$$

The adjoint matrix therefore becomes

$$A(3,\epsilon) = \begin{pmatrix} 1 & 0 & \epsilon \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

D PDEs Burgers Equation

Let $\tilde{x} = f(x,t,u)$, $\tilde{t} = g(x,t,u)$ and $\tilde{u} = h(x,t,u)$. The PDEs generated by $\mathbf{v_3}$, the ones formed in the third row, are

$$\partial_x \tilde{x} = b, \quad \partial_x \tilde{t} = 0, \quad \partial_x \tilde{u} = 0.$$

These equations set $\tilde{x} = f(t,u) + bx$ $\tilde{t} = g(t,u)$ and $\tilde{u} = h(t,u)$. The PDEs generated by $\mathbf{v_1}$ and $\mathbf{v_2}$ acting on $\tilde{t}$ are respectively

$$(-x\partial_x - 2t\partial_t + u\partial_u)\tilde{t} = -2\tilde{t}, \quad (\ln(t)\partial_x + \frac{1}{t})\tilde{t} = 0.$$

The second sets $\tilde{t} = g(t)$ and the first one then gives $\tilde{t} = c_1 t$. Knowing one solution simplifies the other PDEs. Looking at $\mathbf{v_1}$ and $\mathbf{v_2}$ acting on $\tilde{u}$, we obtain

$$(-x\partial_x - 2t\partial_t + u\partial_u)\tilde{u} = \tilde{u}, \quad (\ln(t)\partial_x + \frac{1}{t})\tilde{u} = \frac{b}{\tilde{t}}.$$

The second equation leads to $\tilde{u} = \frac{b}{c_1}u + h(t)$. Substituting this into the first equation, we remain with $-2t\partial_t h(t) = h(t)$, which sets $h(t) = \frac{c_2}{\sqrt{t}}$. All that remains is to solve for $\tilde{x}$. The differential equations are given by

$$(-x\partial_x - 2t\partial_t + u\partial_u)\tilde{x} = -\tilde{x}, \quad (\ln(t)\partial_x + \frac{1}{t})\tilde{x} = b\ln(\tilde{t}).$$

The second equation reduces to $\partial_u f(t,u) = b\ln(c_1)t$, setting $f(t,u) = b\ln(c_1)tu + f(t)$. Using this result for the first equation leaves us with $-2t\partial_t f(t) = -f(t)$, gives the final condition $f(t) = c_3\sqrt{t}$. The three transformation are therefore given by

$$\tilde{x} = b(x + \ln(c_1)tu + c_3\sqrt{t}), \quad \tilde{t} = c_1 t, \quad \tilde{u} = \frac{b}{c_1}u + \frac{c_2}{\sqrt{t}}.$$

E Mathematica Commands

The use of symbolical software for this topic can be invaluable when taking a look at systems with many generators or dimensions. The code used for calculations in this thesis can be found on GitHub (`https://github.com/TomR21/MSc-Thesis-Code`). Additional information is provided on the webpage on how to make use of `MATHEMATICA` to quickly calculate adjoint matrices or print out all nonlinear conditions.

To find the adjoint matrices, in this example for a 3x3 matrix, use the following commands:

```
m1 = {{1,0,2},{0,1,2},{0,1,0}};
MatrixExp[e*m1]
```

F Symmetry Condition Heat Equation

The transformations of the (in)dependent variables is given by

$$(\tilde{x}, \tilde{t}, \tilde{u}) = \left(-\frac{x}{2a\exp(\epsilon_4)t}, -\frac{1}{4a^2\exp(2\epsilon_4)t}, be^{\epsilon_4}\sqrt{t}\exp\left(\frac{x^2}{4t}\right) u \right).$$

The Jacobian is calculated by

$$J = \begin{vmatrix} D_x\tilde{x} & D_x\tilde{t} \\ D_t\tilde{x} & D_t\tilde{t} \end{vmatrix} = \begin{vmatrix} -1/(2a\exp(\epsilon_4)t) & 0 \\ x/(2a\exp(\epsilon_4)t^2) & 1/(4a^2\exp(2\epsilon_4)t^2) \end{vmatrix} = -\frac{1}{8a^3\exp(3\epsilon_4)t^3}.$$

The transformed variables can then be found using this result.

$$\begin{aligned}
\tilde{u}_{\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u} & D_x\tilde{t} \\ D_t\tilde{u} & D_t\tilde{t} \end{vmatrix} = -8a^3\exp(3\epsilon_4)t^3 \begin{vmatrix} D_x\tilde{u} & 0 \\ D_t\tilde{u} & 1/(4a^2\exp(2\epsilon_4)t^2) \end{vmatrix} \\
&= -2ae^{\epsilon_4}tD_x\tilde{u} \\
&= -abe^{\epsilon_4}\exp\left(\frac{x^2}{4t}\right)(xt^{1/2}u + 2t^{3/2}u_x) \\
\tilde{u}_{\tilde{x}\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & D_x\tilde{t} \\ D_t\tilde{u}_{\tilde{x}} & D_t\tilde{t} \end{vmatrix} = -8a^3\exp(3\epsilon_4)t^3 \begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & 0 \\ D_t\tilde{u}_{\tilde{x}} & 1/(4a^2\exp(2\epsilon_4)t^2) \end{vmatrix} \\
&= -2ae^{\epsilon_4}tD_x\tilde{u}_{\tilde{x}} \\
&= a^2be^{2\epsilon_4}\exp\left(\frac{x^2}{4t}\right)(2t^{3/2}u + x^2t^{1/2}u + 4xt^{3/2}u_x + 4t^{5/2}u_{xx}).
\end{aligned}$$

Doing the same procedure for t we obtain

$$\begin{aligned}
\tilde{u}_{\tilde{t}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{x} & D_x\tilde{u} \\ D_t\tilde{x} & D_t\tilde{u} \end{vmatrix} = -8a^3e^{3\epsilon_4}t^3 \begin{vmatrix} -1/(2a\exp(\epsilon_4)t) & D_x\tilde{u} \\ x/(2a\exp(\epsilon_4)t^2) & D_t\tilde{u} \end{vmatrix} \\
&= 4a^2e^{2\epsilon_4}(t^2D_t\tilde{u} + xtD_x\tilde{u}) \\
&= a^2be^{2\epsilon_4}\exp\left(\frac{x^2}{4t}\right)\left(2t^{3/2}u + x^2t^{1/2}u + 4t^{5/2}u_t + 4t^{3/2}xu_x\right)
\end{aligned}$$

Substituting these results into the original heat equation, the symmetry condition is equal to

$$\begin{aligned}
0 &= \tilde{u}_{\tilde{x}\tilde{x}} - \tilde{u}_{\tilde{t}} \\
&= a^2be^{2\epsilon_4}\exp\left(\frac{x^2}{4t}\right)(4t^{5/2}u_{xx} - 4t^{5/2}u_t) \\
&= 4a^2be^{2\epsilon_4}t^{5/2}\exp\left(\frac{x^2}{4t}\right)(u_{xx} - u_t).
\end{aligned}$$

This holds for all values of a, b and ϵ_4, thus there is no further restriction from the symmetry condition.

G Symmetry Condition Laplace Equation

Let $\alpha \equiv \alpha e^{\epsilon}$ and $\delta \equiv \delta e^{\epsilon_2}$. The Jacobian is given by

$$J = \begin{vmatrix} \alpha\frac{x^2-y^2-z^2}{(x^2+y^2+z^2)^2} & 2\alpha\frac{xy}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{xz}{(x^2+y^2+z^2)^2} \\ 2\alpha\frac{xy}{(x^2+y^2+z^2)^2} & \alpha\frac{-x^2+y^2-z^2}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{yz}{(x^2+y^2+z^2)^2} \\ 2\alpha\frac{xz}{(x^2+y^2+z^2)^2} & 2\alpha\frac{yz}{(x^2+y^2+z^2)^2} & a\alpha\frac{-x^2-y^2+z^2}{(x^2+y^2+z^2)^2} \end{vmatrix} = \frac{a\alpha^3}{(x^2+y^2+z^2)^3}.$$

Now the three derivatives $\tilde{u}_{\tilde{x}\tilde{x}}, \tilde{u}_{\tilde{y}\tilde{y}}$ and $\tilde{u}_{\tilde{z}\tilde{z}}$ have to be found.

$$\begin{aligned}
\tilde{u}_{\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u} & 2\alpha\frac{xy}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{xz}{(x^2+y^2+z^2)^2} \\ D_y\tilde{u} & \alpha\frac{-x^2+y^2-z^2}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{yz}{(x^2+y^2+z^2)^2} \\ D_z\tilde{u} & 2\alpha\frac{yz}{(x^2+y^2+z^2)^2} & a\alpha\frac{-x^2-y^2+z^2}{(x^2+y^2+z^2)^2} \end{vmatrix} \\
&= \frac{1}{J}[a\alpha^2(-x^2+y^2+z^2)(x^2+y^2+z^2)^{-3}(D_x\tilde{u}) + 2a\alpha^2 xy(x^2+y^2+z^2)^{-3}(D_y\tilde{u}) \\
&+ 2a\alpha^2 xz(x^2+y^2+z^2)^{-3}(D_z\tilde{u})]. \\
&= \frac{1}{\alpha}(-x^2+y^2+z^2)(D_x\tilde{u}) + \frac{2}{\alpha}xy(D_y\tilde{u}) + \frac{2}{\alpha}xz(D_z\tilde{u}) \\
&= \frac{\delta}{\alpha}(x^2+y^2+z^2)^{1/2}((-x^2+y^2+z^2)u_x + 2xyu_y + 2xzu_z) \\
&+ \frac{\delta}{\alpha}u(x^2+y^2+z^2)^{-1/2}(-x^3+3x(y^2+z^2)).
\end{aligned}$$

This expression is used to find the second derivative of $\tilde{u}$ w.r.t. $\tilde{x}$, given by

$$\begin{aligned}
\tilde{u}_{\tilde{x}\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & 2\alpha\frac{xy}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{xz}{(x^2+y^2+z^2)^2} \\ D_y\tilde{u}_{\tilde{x}} & \alpha\frac{-x^2+y^2-z^2}{(x^2+y^2+z^2)^2} & 2a\alpha\frac{yz}{(x^2+y^2+z^2)^2} \\ D_z\tilde{u}_{\tilde{x}} & 2\alpha\frac{yz}{(x^2+y^2+z^2)^2} & a\alpha\frac{-x^2-y^2+z^2}{(x^2+y^2+z^2)^2} \end{vmatrix} \\
&= \frac{1}{\alpha}(-x^2+y^2+z^2)(D_x\tilde{u}_{\tilde{x}}) + \frac{2}{\alpha}xy(D_y\tilde{u}_{\tilde{x}}) + \frac{2}{\alpha}xz(D_z\tilde{u}_{\tilde{x}})
\end{aligned}$$

All terms depend on δ/α^2 when substituting the total derivatives. Similarly, all terms of $\tilde{u}_{\tilde{y}\tilde{y}}$ and $\tilde{u}_{\tilde{z}\tilde{z}}$ will also depend on δ/α^2 and therefore there will no be no further condition on a, α and δ, because $\delta \neq 0$ and $\alpha \neq 0$.

Matrix B2
The transformed variables are found to be

$$(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{u}) = (\alpha e^{\epsilon}x, ab\alpha e^{\epsilon}y, a\alpha e^{\epsilon}z, \delta e^{\epsilon_2}u)\,.$$

The Jacobian is given by

$$J = \begin{vmatrix} \alpha e^{\epsilon} & 0 & 0 \\ 0 & ab\alpha e^{\epsilon} & 0 \\ 0 & 0 & a\alpha e^{\epsilon} \end{vmatrix} = a^2 b\alpha^3 e^{3\epsilon} = b\alpha^3 e^{3\epsilon}.$$

Now the three derivatives $\tilde{u}_{\tilde{x}\tilde{x}}, \tilde{u}_{\tilde{y}\tilde{y}}$ and $\tilde{u}_{\tilde{z}\tilde{z}}$ have to be found.

$$\begin{aligned}
\tilde{u}_{\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u} & 0 & 0 \\ D_y\tilde{u} & ab\alpha e^{\epsilon} & 0 \\ D_z\tilde{u} & 0 & a\alpha e^{\epsilon} \end{vmatrix} \\
&= \frac{1}{b\alpha^3 e^{3\epsilon}} \cdot a^2 b\alpha^2 e^{2\epsilon}(D_x\tilde{u}) \\
&= \frac{1}{\alpha e^{\epsilon}}\delta e^{\epsilon_2} u_x
\end{aligned}$$

The second order derivative w.r.t. $\tilde{x}$ is then found to be

$$\begin{aligned}
\tilde{u}_{\tilde{x}\tilde{x}} &= \frac{1}{J}\begin{vmatrix} D_x\tilde{u}_{\tilde{x}} & 0 & 0 \\ D_y\tilde{u}_{\tilde{x}} & ab\alpha e^{\epsilon} & 0 \\ D_z\tilde{u}_{\tilde{x}} & 0 & a\alpha e^{\epsilon} \end{vmatrix} \\
&= \frac{1}{\alpha e^{\epsilon}}(D_x\tilde{u}_{\tilde{x}}) \\
&= \frac{1}{\alpha^2 e^{2\epsilon}}\delta e^{\epsilon_2} u_{xx}.
\end{aligned}$$

The other two second order derivatives w.r.t. $\tilde{y}$ and $\tilde{z}$ can be found using the same procedure, which obtains the following

$$\begin{aligned}
\tilde{u}_{\tilde{y}} &= \frac{a}{b\alpha e^{\epsilon}}\delta e^{\epsilon_2} u_y \\
\tilde{u}_{\tilde{y}\tilde{y}} &= \frac{1}{\alpha^2 e^{2\epsilon}}\delta e^{\epsilon_2} u_{yy} \\
\tilde{u}_{\tilde{z}} &= \frac{a}{\alpha e^{\epsilon}}\delta e^{\epsilon_2} u_z \\
\tilde{u}_{\tilde{z}\tilde{z}} &= \frac{1}{\alpha^2 e^{2\epsilon}}\delta e^{\epsilon_2} u_{zz}.
\end{aligned}$$

The symmetry condition is given by

$$\begin{aligned}
\tilde{u}_{\tilde{x}\tilde{x}} + \tilde{u}_{\tilde{y}\tilde{y}} + \tilde{u}_{\tilde{z}\tilde{z}} &= 0 \\
\frac{\delta e^{\epsilon_2}}{\alpha^2 e^{2\epsilon}}(u_{xx} + u_{yy} + u_{zz}) &= 0.
\end{aligned}$$

The symmetry condition always can be expressed in terms of the original Laplace equation unless $\alpha = 0$. Thus there are no further constraints on a, b or α, δ.

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