数理解析研究所講究録
1166巻 2000年 59-66

Symbolic computation of Appell systems on the Schrödinger algebra

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Abstract. The Schrödinger algebra arises as the symmetry algebra of the Schrödinger operator in mathematical physics. Here we consider a generalized heat equation on the Schrödinger algebra itself. We present an effective algorithmic method for finding polynomial solutions to this evolution equation using symbolic computation. Such systems of solutions are known as Appell systems. Specifically, a Maple worksheet is provided showing the steps and the output. Of interest is the fact that this method does not require solving any systems of linear equations in order to get the representation of the Lie algebra needed.

First we recall our general approach using symbolic computations to compute representations of a Lie algebra on its universal enveloping algebra. Given commutation relations for a Lie algebra, if the Lie algebra has a flag of subalgebras, one can efficiently compute a realization of the algebra acting on a space of functions. This is the method of the double dual. This can then be used to solve evolution equations, such as generalized heat equations, with polynomial initial conditions.

Keywords: Lie algebras, Schrödinger algebra, Schrödinger operator, symbolic computation, Appell systems

AMS classification: 17B81, 68W30, 81R05

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1 Introduction

Computing with Lie algebras and Lie groups has by now a firm place in applications. These range from control theory/filtering ([6, 7]), and robotics ([9]) to formal languages ([2, 10]).
We have developed methods using symbolic computation to realize a Lie algebra (1) as vector fields and (2) acting on its universal enveloping algebra. Such realizations are then used for solving various problems involving the given algebra.
The main goal in this work is to show how our computational approach to representations of a Lie algebra (and the corresponding Lie group arising via exponentiation) can be used to calculate solutions to certain evolution equations related to the Lie algebra. In particular, for natural analogs of the heat equation, one can find solutions with polynomial initial conditions. By 'natural analogs' of the heat equation, we mean that the generator is a sum of squares of (some of the) basis elements for the given Lie algebra. Here we illustrate with the heat equation on the Schrödinger algebra.

2 Background

Basic to the approach is to consider the Poincaré-Birkhoff-Witt (PBW) basis for the universal enveloping algebra and to recognize the generating function for this basis as a typical group element factored into one-parameter subgroups. Take a finite-dimensional Lie algebra $\mathcal{G}$ with basis $\{\xi_1, \ldots, \xi_d\}$, $d = \dim \mathcal{G}$, and ordered monomials

$$\xi^n = \xi_1^{n_1} \cdots \xi_d^{n_d}$$

all $n_i \geq 0$, comprising a PBW basis for its universal enveloping algebra $\mathcal{U}(\mathcal{G})$.

Form the exponential generating function with commuting variables $A = (A_1, \ldots, A_d)$:

$$g(A, \xi) = \sum \frac{A^n}{n!} \xi^n = e^{A_1\xi_1} e^{A_2\xi_2} \cdots e^{A_d\xi_d}$$

under the usual conventions $A^n = A_1^{n_1} \cdots A_d^{n_d}$, $n! = n_1! \cdots n_d!$. $g(A, \xi)$ is a group element in a neighborhood of the identity given in terms of the variables $(A_1, \ldots, A_d)$, which are *coordinates of the second kind.*

The action of left and right multiplication by basis elements ξ_i of the Lie algebra on the group element yields vector fields: ξ_i^* for right multiplication, $\xi_i^\ddagger$ for left multiplication:

$$\xi_i^* = \sum_k \pi_{ik}^*(A)\partial_k\,, \qquad \xi_i^\ddagger = \sum_k \pi_{ik}^\ddagger(A)\partial_k$$

where partials refer to differentiating with respect to A-variables, $\partial_k = \partial/\partial A_k$. The coefficients of the vector fields form matrices of functions, the *pi-matrices.*
Now, take a typical element $X \in \mathcal{G}$, $X = \sum_j \alpha_j \xi_j$. The α_i are *coordinates of the first kind.* Corresponding vector fields are $X^* = \sum_j \alpha_j \xi_j^*$ and $X^\ddagger = \sum_j \alpha_j \xi_j^\ddagger$.

Notation For convenience, write $\tilde{\xi}_i$, $\tilde{\pi}$, $\tilde{X}$ to denote either the left or right vector fields when the distinction is not essential.

First, let us look at the evolution equation linear in the basis

$$\frac{\partial u}{\partial t} = \tilde{X}\, u$$

with $u(0) = f(A)$, with polynomial f. Going back to $\mathcal{G}$ and the exponential group, we will factor the exponential $\exp(tX)$ into one-parameter subgroups, emphasizing the dependence on t,

$$g(t) = e^{tX} = e^{A_1(t)\xi_1} e^{A_2(t)\xi_2} \cdots e^{A_d(t)\xi_d}$$

the implicit dependence of A on α being in fact a change-of-coordinates map. Differentiating with respect to t yields

$$\dot{g} = Xg(t) = X^{\ddagger}g(t) = g(t)X = X^* g(t)$$

while, multiplication by ξ_i in each factor given by differentiating with respect to A_i,

$$\dot{g} = \left(\sum_k \dot{A}_k \partial_k\right) g$$

Summarizing,

Proposition 2.1 *The characteristics for the flow generated by a vector field $\tilde{X}$,*

$$\frac{\partial u}{\partial t} = \tilde{X}\, u \tag{1}$$

are given by

$$\dot{A}_k = \sum_j \alpha_j \tilde{\pi}_{jk}(A) \tag{2}$$

which in fact yield the coordinates of the second kind for the one-parameter subgroup generated by $\tilde{X}$.

Remark 2.2 The factorization into one-parameter subgroups was considered in Wei-Norman [11, 12].

The importance of equation (1) with X^* for polynomial initial conditions is illustrated by the **principal formula for the matrix elements** of the group acting on $\mathcal{U}(\mathcal{G})$ (see [4, p. 38]) . Namely, define

$$g(A;\xi)\,\xi^n = \sum_m \left\langle {m \atop n} \right\rangle \xi^m \tag{3}$$

Then the right dual representation yields

$$\left\langle {m \atop n} \right\rangle = (\xi_1^*)^{n_1} \cdots (\xi_d^*)^{n_d}\, A^m/m! \tag{4}$$

Another way to look at this is to consider the group law in coordinates of the second kind,

$$g(B;\xi)\, g(A;\xi) = g(B \odot A;\xi) \tag{5}$$

With $g(A;\xi) = \exp(tX)$, $X = \sum \alpha_k \xi_k$ as above, we have

$$g(B \odot A;\xi) = e^{tX^*}\, g(B;\xi) \tag{6}$$

with $X^* = \sum_{j,k} \alpha_j \pi^*_{jk}(B)\partial/\partial B_k$. Comparing coefficients of ξ^m yields $e^{tX^*}\, B^m = (B \odot A)^m$, i.e., $e^{tX^*}\, f(B) = f(B \odot A)$ for polynomials f.

2.1 Lie algebras with the flag property

Definition 2.3 A Lie algebra has the *flag property* if there is an increasing chain of subalgebras $\mathcal{B}_i$

$$\{0\} = \mathcal{B}_0 \subset \mathcal{B}_1 \subset \mathcal{B}_2 \subset \cdots \subset \mathcal{B}_d = \mathcal{G} \tag{7}$$

each of codimension one in the next. Such a flag is an *increasing Lie flag.*

Note that this is a flag in the usual sense of $\mathcal{G}$ as a vector space, but is rather stringent as each $\mathcal{B}_i$ must be closed under Lie brackets. Suppose that $\{\xi_1, \ldots, \xi_d\}$ is a corresponding adapted basis for (7), i.e., for $1 \leq i \leq d$, $\{\xi_1, \ldots, \xi_i\}$ is a basis for $\mathcal{B}_i$. Then, reversing the order of the basis gives a *decreasing Lie flag.*
Every solvable, in particular every nilpotent, algebra has an increasing Lie flag. The Lie-Engel Theorem guarantees the existence of a flag of ideals. (See Humphreys [8] for background and proofs.)
There are Lie algebras that are not solvable yet which have the flag property. The simple Lie algebra, sl(2), with basis E_-, E_+, H and commutation relations $[E_-, E_+] = H$, $[H, E_\pm] = \pm E_\pm$ admits the Lie flag with adapted basis $\{E_+, H, E_-\}$. Direct sums of sl(2) thus have the flag property. The main example of this paper, the Schrödinger algebra, is another example of this phenomenon.

2.2 Commutation relations: the Kirillov matrix

Once a basis has been chosen, one way to define the Lie algebra is in terms of commutation relations. In other words, in terms of *structure constants*, c_{ij}^k, determined by

$$[\xi_i, \xi_j] = \sum_k c_{ij}^k \, \xi_k \tag{8}$$

It is convenient to summarize the commutation relations in the form of a *Kirillov matrix.* The commutation relations, eq. (8), yield matrix entries

$$K_{ij} = \sum_k c_{ij}^k x_k$$

linear forms in the variables $\{x_k\}$.

(**Warning:** these are purely formal and have nothing to do with the x-variables used below for representations on functions.)

We can interpret eq. (8) as giving the action of a linear map $\operatorname{ad}(\xi_i)$ on ξ_j, i.e.,

$$\operatorname{ad}(\xi_i)(\xi_j) = \sum_k c_{ij}^k \, \xi_k$$

The matrices, $\check{\xi}_i$, of the linear maps $\operatorname{ad}(\xi_i)$, $1 \leq i \leq d$, are the *adjoint representation* of $\mathcal{G}$. Thus,

$$(\check{\xi}_i)_{jk} = c_{ik}^j$$

2.3 Dual representations and flags

Given an increasing flag, with adapted basis $\{\xi_1, \ldots, \xi_d\}$, denote by $\check{\xi}_i^*$ the transpose of the matrix of ξ_i in the adjoint representation restricted to the subalgebra $\mathcal{B}_i$. I.e., columns $i+1$ through d of $\check{\xi}_i$ are zero'd out and then the matrix is transposed. In terms of the structure constants the entries of $\check{\xi}_i^*$ are

$$(\check{\xi}_i^*)_{jk} = c_{ij}^k \tag{9}$$

with the condition that $j, k \leq i$, otherwise null. Dually, for a decreasing flag, we denote by $\check{\xi}_i^\dagger$ the transposed matrix of the restriction of the adjoint action of ξ_i to the subalgebra $\mathcal{B}_i^d = \text{span}\{\xi_i, \ldots, \xi_d\}$, i.e., the first i columns are zero'd out, then the matrix transposed. So the entries of $\check{\xi}_i^\dagger$ are c_{ij}^k as in equation (9) except with the condition $j, k \geq i$ otherwise null.
We recall the main theorem from [4, p. 33] (see there for the proof)

Theorem A *For the dual representations we have:*

1. *Given an increasing flag, the pi-matrix for the right dual is given by*

$$\pi^*(A) = \exp(A_d\check{\xi}_d^*)\exp(A_{d-1}\check{\xi}_{d-1}^*)\cdots\exp(A_1\check{\xi}_1^*)$$

2. *Given a decreasing flag, the pi-matrix for the left dual is given by*

$$\pi^\dagger(A) = \exp(-A_1\check{\xi}_1^\dagger)\exp(-A_2\check{\xi}_2^\dagger)\cdots\exp(-A_d\check{\xi}_d^\dagger)$$

Remark 2.4 In [5] we explain the technique of using matrices to find the dual representations avoiding use of the adjoint action. This is efficient if the Lie algebra is given in matrix terms. In the present paper, we are interested primarily in the case where the commutation relations are the basic data.

2.4 Double dual

The left dual representation $\{\xi_i^\dagger\}$ is itself dual to the action of the basis elements on the enveloping algebra $\mathcal{U}(\mathcal{G})$. Define formal raising and differentiation operators as follows

$$\begin{aligned} \mathcal{R}_i\,\xi^n &= \xi_1^{n_1}\cdots\xi_i^{n_i+1}\cdots\xi_d^{n_d} \\ \mathcal{V}_i\,\xi^n &= n_i\,\xi_1^{n_1}\cdots\xi_i^{n_i-1}\cdots\xi_d^{n_d} \end{aligned}$$

Then, defining

$$\hat{\xi}_i = \sum_k \mathcal{R}_k\pi_{ik}^\dagger(\mathcal{V})$$

for $1 \leq i \leq d$, we have $\xi_i\,\xi^n = \hat{\xi}_i\,\xi^n$ in the enveloping algebra. This is the *double dual.* From this, we have a representation of $\mathcal{G}$ on functions of $(x_1, \ldots, x_d)$ by replacing $\mathcal{R}_i \to x_i$ and $\mathcal{V}_i \to \partial/\partial x_i$.

3 Schrödinger algebra

Referring to [1] for details on the definition of the Schrödinger algebra, we now present the ($n = 1$, centrally-extended) Schrödinger algebra with basis $\{M, G, K, P_0, P_x, D\}$. Note that 'D' stands for 'dilation', not 'differentiation'.

Order the basis as follows:

$$\xi_1 = M\,, \qquad \xi_2 = K\,, \qquad \xi_3 = G\,, \qquad \xi_4 = D\,, \qquad \xi_5 = P_x\,, \qquad \xi_6 = P_0$$

For the Schrödinger algebra, with rows and columns labelled by the corresponding operators,

$$K_{ij} = \begin{array}{c} \\ M \\ K \\ G \\ D \\ P_x \\ P_0 \end{array} \begin{array}{c} \begin{array}{cccccc} M & K & G & D & P_x & P_0 \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\,x_2 & -x_3 & -x_4 \\ 0 & 0 & 0 & -x_3 & -x_1 & -x_5 \\ 0 & 2\,x_2 & x_3 & 0 & -x_5 & -2\,x_6 \\ 0 & x_3 & x_1 & x_5 & 0 & 0 \\ 0 & x_4 & x_5 & 2\,x_6 & 0 & 0 \end{pmatrix} \end{array}$$

Observe that the basis is adapted to an increasing Lie flag. Using Theorem A, we find

$$\pi^{\dagger} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 2A_2 & A_3 & 1 & 0 & 0 \\ A_3 & 0 & A_2 & 0 & e^{A_4} & 0 \\ A_3^2/2 & A_2^2 & A_2A_3 & A_2 & A_3e^{A_4} & e^{2A_4} \end{pmatrix}$$

with corresponding double dual,

$$\hat{m} = \mathcal{R}_1\,, \quad \hat{K} = \mathcal{R}_2\,, \quad \hat{G} = \mathcal{R}_3\,, \quad \hat{D} = \mathcal{R}_4 + 2\mathcal{R}_2\mathcal{V}_2 + \mathcal{R}_3\mathcal{V}_3$$

and

$$\begin{aligned} \hat{P}_x &= \mathcal{R}_1\mathcal{V}_3 + \mathcal{R}_3\mathcal{V}_2 + \mathcal{R}_5\exp(\mathcal{V}_4) \\ \hat{P}_0 &= \frac{1}{2}\mathcal{R}_1\mathcal{V}_3^2 + \mathcal{R}_2\mathcal{V}_2^2 + \mathcal{R}_3\mathcal{V}_2\mathcal{V}_3 + \mathcal{R}_4\mathcal{V}_2 + \mathcal{R}_5\mathcal{V}_3\exp(\mathcal{V}_4) + \mathcal{R}_6\exp(2\mathcal{V}_4) \end{aligned}$$

This leads to a representation on functions of two variables x_1, x_2 as follows. Since M is central, map it to the scalar m. Then take $x_1 = \mathcal{R}_2$, $x_2 = \mathcal{R}_3$. We want P_x and P_0 to act on functions of x_1, x_2, so set $\mathcal{R}_5$ and $\mathcal{R}_6$ to zero. Finally, noting that there will be no more $\mathcal{V}_4$'s, we can map $\mathcal{R}_4$ to a scalar c. This gives the following representation of the Schrödinger algebra: $M = m$, $K = x_1$, $G = x_2$, $D = c + 2x_1\frac{\partial}{\partial x_1} + x_2\frac{\partial}{\partial x_2}$ and

$$P_x = m\frac{\partial}{\partial x_2} + x_2\frac{\partial}{\partial x_1}\,, \quad P_0 = c\frac{\partial}{\partial x_1} + \frac{m}{2}\frac{\partial^2}{\partial x_2^2} + x_1\frac{\partial^2}{\partial x_1^2} + x_2\frac{\partial^2}{\partial x_1 \partial x_2}$$

It is worth remarking that the heat operator (Schrödinger operaror in imaginary time) in this representation is

$$P_0 - \frac{1}{2m}P_x^2 = (x_1 - \frac{x_2^2}{2m})\frac{\partial^2}{\partial x_1^2} + (c - \frac{1}{2})\frac{\partial}{\partial x_1}$$

3.1 Heat equation on the Schrödinger algebra

Now consider the evolution equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\,(P_0^2 + P_x^2)u$$

with initial condition $u(0) = x_1^k x_2^l$, for $k, l \geq 0$. Denote the solution by $h_{k,l}$.

The idea is that (the angle brackets denoting expected value)

$$\exp\left(t(P_0^2 + P_x^2)/2\right) = \langle \exp(w_1 P_0 + w_2 P_x) \rangle$$

where w_1, w_2 are independent Gaussian each with mean 0 and variance t. I.e., we combine the group action (linear generator) with averaging over random variables. This is a main feature of Appell systems (see [3]).

The general setting we are considering here and implementation in Maple goes as follows.

We are given a commuting family of differential operators $\{Y_i\}_{1\leq i\leq r}$ in the variables $(x_1, \ldots, x_d)$ with the property that for each i, there exists a positive integer q_i such that $Y_i^{q_i}\, x^n = 0$ on all monomials $x^n = x_1^{n_1} \cdots x_d^{n_d}$. Each Y_i is said to *act nilpotently on polynomials.* In this setting, we wish to solve

$$\frac{\partial u}{\partial t} = \frac{1}{2}\,(Y_1^2 + \cdots + Y_r^2)u$$

with polynomial initial conditions.
The implementation in Maple is given in three steps.
(The worksheet and output is given on the next page.)

1. Define each Y_i as an operator, i.e., as a mapping on an expression, f, say.
   See worksheet: lines starting with `PX` *and* `PO`.

2. Compute $\exp(w_1 Y_1 + \cdots + w_r Y_r)x^n$.
   See worksheet: procedure `expop`.

3. Interpreting w_i as independent Gaussian random variables with mean 0 and variance t, compute the expected value. This is conveniently done by integrating with respect to the appropriate density.
   See worksheet: the mapping `Gauss`.

4 Conclusion

The approach discussed here is useful when the Lie algebra is described by giving commutation relations for elements of a basis, as is usual in mathematical physics. In this context, the method of calculating representations using flags is efficient as it does not require solving any systems of linear equations. In combination with averaging with respect to random variables, only computation of the group action is needed. That is, evolution equations linear in the basis elements is sufficient. In combination with the double dual, this gives solutions on spaces for polynomial initial conditions.

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