Research Plan

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My main research interests are symbolic computation and its applications in combinatorics, knot theory, statistics, and cryptography. Symbolic computation aims to give algorithmic and constructive answers to various problems in mathematics and computer science, such as polynomial factorization, computing solutions of systems of polynomial equations, and quantifier elimination. Systems of algebraic differential equations and difference equations are important research subjects in mathematics, physics, and related areas. The algebraic study of such systems gives useful information about their applications in physics, statistics, and other areas. Much of my work is devoted to developing algorithms for computing solutions and illustrating algebraic structures of differential equations and difference equations by using constructive tools (such as Gröbner bases and resultant theory) in computer algebra and differential algebra. My work has found interesting applications in the certification of integer sequences, checking special cases of a conjecture of Krattenthaler, and verifying several instances of the colored Jones polynomial are Laurent polynomial sequences. The following sections describe my research plans in the future.

The algebraic-geometric method for solving algebraic difference equations

An algebraic ordinary difference equation (AOΔE) is a difference equation of the form

$$F(x, y(x), y(x+1), \cdots, y(x+m)) = 0, \tag{1}$$

where F is a nonzero polynomial in $y(x), y(x+1), \cdots, y(x+m)$ with coefficients in the field $\mathbb{K}(x)$ of rational functions over an algebraically closed field $\mathbb{K}$ of characteristic zero, and $m \in \mathbb{N}$. We call m the *order* of (1). AOΔEs naturally appear from various problems, such as symbolic summation [18, 11], factorization of linear difference operators [2], analysis of time or space complexity of computer programs with recursive calls [20]. We are interested in computing symbolic solutions (for instance, polynomials solutions, rational solutions) of AOΔEs. In particular, for a first-order AOΔE, the corresponding algebraic equation $F(x, y, z) = 0$ defines an algebraic curve in the two dimensional affine plane over the field $\overline{\mathbb{K}(x)}$. A solution in a certain class of functions, such a rational or algebraic functions, determines a parametrization of this algebraic curve. Thus, we may apply algebraic tools from parametrization theory of algebraic curves to study solutions of first-order AOΔEs. Based on this observation, we propose an algebraic-geometric approach to solve first-order AOΔEs:

1 Decide whether a given first-order AOΔE can be parametrized with functions form a given class, such as rational parametrization;

2 Solve the corresponding reduced AOΔE by using techniques from computer algebra and differential algebra.

This idea is inherited from the differential case and turns out to be successful for solving algebraic differential equations. For details, see [27]. Using this method, we give an complete algorithm [26] to compute rational solutions of first-order autonomous AOΔEs. Possible future work is as follows:

- Design algorithms to compute polynomial and rational solutions of high-order AOΔEs.
- Compute rational solutions of non-autonomous first-order AOΔEs.

The improved holonomic gradient method via gauge transformation

1 Contraction of Ore ideals with applications

1.1 Introduction

Let $\mathbb{K}$ be a field of characteristic 0. Consider the following linear recurrence equation:

$$a_0(n)f(n) + \cdots + a_r(n)f(n+r) = 0, \tag{2}$$

where $a_i \in \mathbb{K}[n]$ with $a_r \neq 0$, and $i = 0, \ldots, r$. The roots of $a_r(n)$ is called the singularities of (2). There is a strong connection between the roots of a_r and the singularities of a solution of (2) .

It is well know that every singularity of a solution of (2) must be a root of a_r. However, the converse is not true. Generally speaking, the leading coefficient a_r may have roots at a point where no solution is singular. Such points are called apparent singularities, and it is sometimes useful to identify them. The technique for doing so is called desingularization. For instance, consider the recurrence operator

$$L = (1 + 16n)^2\partial^2 - 32(7 + 16n)\partial - (1 + n)(17 + 16n)^2,$$

which comes from [1, Section 4.1]. In this, we use ∂ to denote the shift operator $f(n) \mapsto f(n + 1)$. For any choice of two initial values $u_0, u_1 \in \mathbb{Q}$, there is a unique sequence $u\colon \mathbb{N} \to \mathbb{Q}$ with $u(0) = u_0$, $u(1) = u_1$ and L applied to u gives the zero sequence. A priori, it is not obvious whether or not u is actually an integer sequence, if we choose u_0, u_1 from $\mathbb{Z}$, because the calculation of the $(n+2)$nd term from the earlier terms via the recurrence encoded by L requires a division by $(1+16n)^2$, which could introduce fractions. In order to show that this division never introduces a denominator, we note that every solution of L is also a solution of its left multiple

$$\begin{aligned} T \quad = \quad & \partial^3 + \left(128n^3 - 104n^2 - 11n - 3\right)\partial^2 + \\ & \left(-256n^2 + 127n + 94\right)\partial - \\ & (128n^2 + 24n - 131)(1 + n)^2, \end{aligned} \tag{3}$$

The operator T has the interesting property that the factor $(1+16n)^2$ has been "removed" from the leading coefficient, which immediately certifies the integrality of its solutions. The process of obtaining the operator T from L is called desingularization, because there is a polynomial factor in the leading coefficient of L which does not appear in the leading coefficient of T.

In more algebraic terms, we consider the following problem. Given an operator $L \in \mathbb{Z}[x][\partial]$, where $\mathbb{Z}[x][\partial]$ is an Ore algebra, we consider the left ideal $\langle L\rangle = \mathbb{Q}(x)[\partial]L$ generated by L in the extended algebra $\mathbb{Q}(x)[\partial]$. The contraction of $\langle L\rangle$ to $\mathbb{Z}[x][\partial]$ is defined as $\mathrm{Cont}(L) := \langle L\rangle \cap \mathbb{Z}[x][\partial]$. This is a left ideal of $\mathbb{Z}[x][\partial]$ which contains $\mathbb{Z}[x][\partial]L$, but in general more operators. Our goal is to compute a $\mathbb{Z}[x][\partial]$-generating set of $\mathrm{Cont}(L)$. In the example above, such a generating set is given by $\{L, T\}$. The traditional desingularization problem corresponds to computing a generating set of the $\mathbb{Q}[x][\partial]$-left ideal $\langle L\rangle \cap \mathbb{Q}[x][\partial]$.

1.2 Main results

Given an Ore operator L with polynomial coefficients in x, it generates a left ideal I in the Ore algebra over the field $\mathbb{K}(x)$ of rational functions.

(1) We present an algorithm for computing a generating set of the contraction ideal of I in the Ore algebra over the ring $R[x]$ of polynomials, where R may be either $\mathbb{K}$ or a domain with $\mathbb{K}$ as its fraction field.

(2) Using a generating set of the contraction ideal, we compute a completely desingularized operator for L whose leading coefficient not only has minimal degree in x but also has minimal content.

(3) Using completely desingularized operators, we study how to certify the integrality of a sequence and check special cases of a conjecture of Krattenthaler.

This work is published in ISSAC'16 [28].

1.3 Future work

(1) Our algorithms rely heavily on the computation of Gröbner bases over a principal ideal domain R. At present, the computation of Gröbner bases over R is not fully available in a computer algebra system. So the algorithms are not yet implemented. We would like to implement our algorithm in Maple or Mathematica by using linear algebra over R as much as possible.

(2) Design algorithms for determining a generating set of a contraction ideal in the multivariate Ore algebra.

2 Apparent singularities of D-finite systems

2.1 Introduction

A D-finite function is specified by a linear ordinary differential equation with polynomial coefficients and finitely many initial values. Each singularity of a

D-finite function will be a root of the coefficient of the highest order derivative appearing in the corresponding differential equation. For instance, x^{-1} is a solution of the equation $xf'(x) + f(x) = 0$, and the singularity at the origin is also the root of the polynomial x. However, the converse is not true. For instance, the solution space of the differential equation $xf'(x) - 3f(x) = 0$ is spanned by x^3 as a vector space, but none of those functions has singularity at the origin.

More specifically, we consider the following ordinary differential equation

$$p_0(x)f(x) + \cdots + p_r(x)f^{(r)}(x) = 0, ,$$

where $p_i \in \mathbb{K}[x]$ with $p_r \neq 0$, and $\mathbb{K}$ is a field of characteristic 0. The roots of p_r are called the singularities of the equation. A root α of p_r is call *apparent* if the differential equation admits r linearly independent formal power series solutions in $x - \alpha$. Deciding whether a singularity is apparent is therefore the same as checking whether the equation admits a fundamental system of formal power series solutions at this point. This can be done by inspecting the so-called *indicial polynomial* of the equation at α and solving a system of finitely many linear equations. If a singularity α of an ordinary differential is apparent, then we can always construct a second ordinary differential equation whose solution space contains all the solutions of the first equation, and which does not have α as a singularity any more. This process is called *desingularization.* The purpose of our work is to generalize the facts sketched above to the multivariate setting.

2.2 Main results

(1) We generalize the notions of singularities and ordinary points from linear ordinary differential equations to D-finite systems. Ordinary points of a D-finite system are characterized in terms of its formal power series solutions.

(2) We show that apparent singularities can be removed like in the univariate case by adding suitable additional solutions to the system at hand.

(3) Several algorithms are presented for removing and detecting apparent singularities of D-finite systems.

(4) An algorithm is given for computing formal power series solutions of a D-finite system at apparent singularities.

This work is available in [3].

2.3 Future work

(1) Generalize our algorithms for removing and detecting apparent singularities of D-finite systems to other singularities.

(2) Study the desingularization problem for the multivariate linear difference equations with polynomial coefficients.

3 Laurent series solutions of algebraic ordinary differential equations

3.1 Introduction

An algebraic ordinary differential equation (AODE) is of the form

$$F(x, y, y', \ldots, y^{(n)}) = 0,$$

where F is a polynomial in $y, y', \ldots, y^{(n)}$ with coefficients in $\mathbb{K}(x)$, the field $\mathbb{K}$ is algebraically closed field of characteristic zero, and $n \in \mathbb{N}$. Many problems from applications (such as physics, combinatorics and statistics) can be characterized in terms of AODEs. Therefore, determining (closed form) solutions of an AODE is one of the central problems in mathematics and computer science.

Although linear ODEs [9] have been intensively studied, there are still many challenging problems for solving (nonlinear) AODEs. As far as we know, approaches for solving AODEs are only available for very specific subclasses. For example, Riccati equations, which have the form $y' = f_0(x) + f_1(x)y + f_2(x)y^2$ for some $f_0, f_1, f_2 \in \mathbb{K}(x)$, can be considered as the simplest form of nonlinear AODEs. In [14], Kovacic gives a complete algorithm for determining Liouvillian solutions of a Riccati equation with rational function coefficients.

Since the problem of solving an arbitrary AODE is very difficult, it is natural to ask whether a given AODE admits some special kinds of solutions, such as polynomials, rational functions, or formal power series. During the last two decades, an algebraic-geometric approach for finding symbolic solutions of AODEs has been developed. The work by Feng and Gao in [6, 7] for computing rational general solutions of first-order autonomous AODEs can be considered as the starting point. The authors of [16, 8, 24, 23] developed methods for finding different kinds of solutions of non-autonomous, higher-order AODEs. For formal power series solutions, we refer to [5, 21]. As far as we know, there is few results concerning Laurent series solutions of AODEs. Our main purpose is to give a method for determining such solutions.

3.2 Main results

(1) We present several approaches to compute formal power series solutions of a given AODE.

(2) Given an AODE, we determine a bound for the order of its Laurent series solutions. Using the order bound, one can transform a given AODE into a new one whose Laurent series solutions are only formal power series.

(3) As applications, new algorithms are presented for determining all particular polynomial and rational solutions of certain classes of AODEs.

This work is available in [25].

3.3 Future work

(1) Design algorithms for computing formal power series solutions of AODEs, which extends the classic Implicit Function Theorem of AODEs.

(2) Compute rational solutions of first-order algebraic difference equations by using the parametrization of algebraic curves.

4 Desingularization in the q-Weyl algebra

4.1 Introduction

Prof. Stavros Garoufalidis, who is an expert for knot theory, presented the following conjecture in an email with the author:

Conjecture 4.1. *(Garoufalidis): Let $J_{K,n}(q)$ denote the Jones polynomial of a knot colored by the n-dimensional irreducible representation of $\mathfrak{sl}_2$ and normalized by $J_{Unknot,n}(q) = 1$. Then, (a) $(1 - q^n) * J_{K,n}(q)$ satisfies a bimonic recursion relation. (b) $J_{K,n}(q)$ does not satisfy a monic recursion relation.*

Using q-holonomic summation methods (as implemented in the `qMultiSum` package [19] or `HolonomicFunctions` package [12]) or by guessing (as implemented in the `Guess` package [10]), we can always compute q-holonomic recurrence equations for $(1 - q^n) * J_{K,n}(q)$ and $J_{K,n}(q)$, respectively. However, the equation for $(1 - q^n) * J_{K,n}(q)$ usually does not satisfy the property in Conjecture 4.1. Furthermore, we can not see immediately that $J_{K,n}(q)$ does not satisfy a monic recursion relation.

In order to certify Conjecture 4.1 for some specific $J_{K,n}(q)$, we develop the desingularization technique in the q-Weyl algebra.

As an example, consider the q-holonomic sequence

$$f(n) = [n]_q := \frac{q^n - 1}{q - 1}$$

that is a q-analog of the natural numbers. The minimal-order homogeneous q-recurrence satisfied by $f(n)$ is

$$(q^n - 1)f(n + 1) - (q^{n+1} - 1)f(n) = 0,$$

in operator notation:

$$\big((q^n - 1)\partial - q^{n+1} + 1\big) \cdot f(n) = 0. \tag{4}$$

When we multiply this operator by a suitable left factor, we obtain a monic (and hence: desingularized) operator of order 2:

$$\frac{1}{q^{n+1} - 1}\big(\partial - q\big)\big((q^n - 1)\partial - q^{n+1} + 1\big) = \partial^2 - (q + 1)\partial + q. \tag{5}$$

The process of deriving (5) from (4) to called desingularization in the q-Weyl algebra.

4.2 Main results

(1) We give an order bound for desingularized operators, and thus derive an algorithm for computing desingularized operators in the first q-Weyl algebra.

(2) An algorithm is presented for computing a generating set of the first q-Weyl closure of a given q-difference operator.

(3) As an application, we certify that several instances of $J_{K,n}(q)$ always satisfy the properties specified in Conjecture 4.1.

This work is available in [13].

4.3 Future work

(1) Study the desingularization problem in the multivariate q-Weyl algebra.

(2) Develop the desingularization technique for linear Mahler equations.

5 An enhanced holonomic gradient method with algebraic and numerical analysis of differential equations

5.1 Introduction

Studying problems in differential equations which arose in statistics will lead us a remarkable advances in the algebraic and algorithmic study of differential equations and the combination of algebraic algorithms and numerical algorithms for differential equations. An important approach in the algebraic analysis of differential equation is the holonomic gradient method.

Let us first recall the idea of the holonomic gradient method [15]. A holonomic function with n variables is a function which satisfies n linear ordinary differential equations with multivariate polynomial coefficients for each independent variable. Those differential equations satisfied by a holonomic function is called a holonomic system. The holonomic gradient method (HGM) is an approach to evaluate numerically normalizing constants and their derivatives of holonomic probability distributions. HGM consists of three steps:

(1) Finding a holonomic system satisfied by the normalizing constant. We may use the restriction algorithm from D-module theory and related methods to compute it.

(2) Finding an initial value vector for the holonomic system. It is equivalent to evaluating the normalizing constant and its derivatives at a point. This step is usually performed by numerical integration.

(3) Solving the holonomic system numerically. We can use classical methods in numerical analysis such as the Runge-Kutta method of solving ordinary differential equations and efficient solvers of systems of linear equations.

For the first step of HGM, there are efficient algorithms (such as the creative telescoping method) to derive a holonomic system for the target normalizing constant. The holonomic system can be translated into a linear ODE system (Pfaffian system) for the normalizing constant and its derivatives. However, if the normalizing constant is not the dominant [4] solution among all the solutions of the corresponding linear ODE system as the independent variable goes to infinity, then the usual methods involved in the third step of HGM only works for a small interval. Besides, the evaluation step relies on the precision of initial values of the target normalizing constant and its derivatives. The current methods for evaluating initial values with high-precision are also not satisfactory.

We want to design an enhanced HGM by combining theoretical study of ODEs, algebraic algorithms, and numerical algorithms for ODEs to give a more efficient numerical evaluator in the second and third step of HGM. Furthermore, we will apply the improved HGM to study problems in differential equations which arose in statistics, combinatorics and so on.

5.2 Main results

We give an approximate formula of the distribution of the largest eigenvalue of real Wishart matrices by the expected Euler characteristic method for the general dimension. The formula is expressed in terms of a definite integral with parameters. We derive a differential equation satisfied by the integral for the 2×2 matrix case and perform a numerical analysis of it.

This work is available in [22].

5.3 Future work

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We want to achieve our goals from the following aspects.

(1) Euler characteristic method to approximate the tail probability of the maximum of a bivariate Gaussian process.A Gaussian process is a stochastic process with important applications in probability theory and statistical modelling. We can show that the tail probability of the maximum of a bivariate Gauss process can be approximated by the expectation of products of two Euler characteristic numbers when two parameters involved are large. The expected Euler characteristic can be expressed as a sum of four definite integrals $F_i(a, b)$'s, where $F_i(a, b)$ is at most 4-fold with a holonomic integrand, and a, b are parameters. We will use our enhanced HGM (see below) to numerically evaluate those integrals, and

thus derive good approximations for the tail probability of the maximum of a bivariate Gaussian process.

(2) Use desingularization for numerical evaluation of Pfaffian systems. Given a single linear ODE, a root of the coefficient for its highest derivative is called a singularity of the differential equation. The singularities of solutions of a linear ODE must be that of the equation. However, the converse is not true. This phenomenon also happens for holonomic systems and the corresponding Pfaffian system. Given a Pfaffian system with a singularity at x_0, evaluation of its solutions at x_0 is a bottleneck for the numerical solving of differential equations. One strategy to overcome this difficulty is to utilizing the desingularization technique. Desingularization is a process to deriving consequences of a Pfaffian system such that the new one is also a Pfaffian system of the target function and certain singularities of the original system become ordinary points of the new one. The author's PhD and postdoctoral work mainly focus on the algebraic and algorithmic study of desingularization of holonomic systems. In [28], the applicant gives a complete algorithm for removing all the removable singularities of univariate linear ODEs. The difference analogue has interesting applications in combinatorics and knot theory [13]. In [3], the author and his collaborators give an algorithm for removing apparent singularities of holonomic systems. The desingularization technique has not been studied from the view point of numerical valuation. Given a Pfaffian system, we may use desingularization to construct a new Pfaffian system of the target function such that the singularities of the original system have been removed as much as possible. Afterwards, we may apply the enhanced HGM to evaluate the target function at those removed "singularities" of the original Pfaffian system.

(3) Theoretical study of connection formulas for numerical evaluation. Given a linear ODE, there exist well-known algorithms to compute its asymptotic solutions. However, the asymptotic approximations have the inevitable feature that the independent variable is always restricted to certain real intervals or complex regions. In practice, we may want to calculate approximation for the same solutions in other regions. One way to achieve this goal is to utilize an appropriate connection formula [17], which is an equation expressing one solution of the given ODE in terms of other solutions. The connection formulas can be obtained from parametric integral representation of solutions or derived directly from the differential equation without the usage of integral representation. It has been intensively studied for second-order linear ODEs in various circumstances (for instance, the associated Legendre equation). We would like to generalize the techniques for deriving connection formulas to general Pfaffian systems, combine HGM and those formulas to numerically evaluate normalizing constant in a more efficient and accurate way. In particular, Saiei-Jaeyeong Matsubara-Heo, who is a postdoctoral fellow at Kobe University, recently derived connection formulas for GKZ hypergeometric functions. This is a milestone result in the study of connection formulas. We want to utilize his formula for numerical evaluation of definite integrals with parameters, which will yield a remarkable progress in numerical evaluation problems of definite integrals with parameters.

(4) Use gauge transformations to construct a stabile Pfaffian system and compute its formal solutions for numerical evaluation. Let $f(x)$ be be a solution of a Pfaffian system. This system is stabile for $f(x)$ if $f(x)$ is dominant among solutions of the given system as x goes to infinity. A major problem for numerical evaluation in HGM is that if the ODE system is not stabile for the target function, then numerical solving of the ODE system only works locally. One way to overcome this difficulty is to make a gauge transformation of the dependent functions of the ODE system such that the corresponding new ODE system is stabile for the new target function. For a given Pfaffian system that is not stabile for a target function, one can always derive a lower-dimensional stabile Pfaffian system algorithmically by gauge transformations. This approach has been successfully used in the CDF evaluation for largest eigenvalue of a complex non-central Wishart matrix [4]. We want to do further study in this direction and design more efficient and reliable algorithms for evaluating normalizing constants by using gauge transformations. Given a Pfaffian system, there are algorithms (Moser 1960, Bakatou-Pfuegel 2007, Chen et al. 2019) to compute its formal solutions. For instance, the author's recent work [3] gives complete algorithms to compute formal power series of linear ODE systems at ordinary points or apparent singularities. However, these algorithms have not yet been studied in the view point of numerical evaluation of solutions of a Pfaffian system. In the third step of HGM, we need to solve a linear ODE system for the normalizing constant and its derivatives numerically. We may first compute a formal fundamental solution system of the given Pfaffian system by using algorithms from computer algebra. Afterwards, we may construct the extrapolation function by taking a linear combination of those formal solutions with unknown coefficients, which can be determined by solving linear equations. Finally, we use the corresponding extrapolation function to numerically evaluate the normalizing constant.

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