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.

Desingularization of linear differential and difference operators

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 must 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 example, the solution space of the differential equation $xf'(x) - 4f(x) = 0$ is spanned by x^4 as a vector space, but none of those functions has singularity at the origin.

More specifically, for an ordinary equation $p_0(x)f(x)+\cdots+p_r(x)f^{(r)}(x) = 0$ with polynomial coefficients $p_0, \ldots, p_r$ and $p_r \neq 0$, the roots of p_r are called the singularities of the equation. A root α of p_r is called *an apparent singularity* 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 equation is apparent, then we can always construct a second linear 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*. There are similar techniques for the difference case. Our contributions in this area are as follows:

- Contraction of Ore ideals with applications [31]. Ore operators form a common algebraic abstraction of linear ordinary differential and recurrence equations. 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. We present an algorithm for computing a basis 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. This algorithm is based on recent work on desingularization for Ore operators by Chen, Jaroschek, Kauers, and Singer. Using a basis 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. Completely desingularized operators have interesting applications such as certifying integer sequences and checking special cases of a conjecture of Krattenthaler.

- Desingularization in the q-Weyl algebra [14]. We give an order bound for desingularized operators, and thus derive an algorithm for computing desingularized operators in the first q-Weyl algebra. Moreover, an algorithm is presented for computing a generating set of the first q-Weyl closure of a given q-difference operator. As an application, we certify that several instances of the colored Jones polynomial are Laurent polynomial sequences by computing the corresponding desingularized operator.

- Apparent singularities of D-finite systems [4]. We generalize the notions of ordinary points and singularities from linear ordinary differential equations to D-finite systems. Ordinary points and apparent singularities of a D-finite system are characterized in terms of its formal power series solutions. We also show that apparent singularities can be removed like in the univariate case by adding suitable additional solutions to the system at hand. Several algorithms are presented for removing and detecting apparent singularities. In addition, an algorithm is given for computing formal power series solutions of a D-finite system at apparent singularities.

I plan to work on the following problems in the near future:

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

- Develop the desingularization technique for linear Mahler equations.

- Study the desingularization problem for the multivariate linear difference equations with polynomial coefficients.

Computing symbolic solutions of algebraic differential and difference equations

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

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

where $m \in \mathbb{N}$ and 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. AOΔEs arise naturally in various kinds of problems, such as symbolic summation, factorization of linear difference operators, and the analysis of time or space complexity of computer programs with recursive calls. In these and other applications, the determination of the (closed form) solutions of a given AOΔE is a fundamental problem of general interest. We can define algebraic ordinary differential equations (AODEs) analogously. Our contributions in this area are as follows:

- Rational solutions of first-order AOΔEs [29]. We propose an algebraic geometric approach for studying rational solutions of first-order AOΔEs. For an autonomous first-order AOΔE, we give an upper bound for the degrees of its rational solutions, and thus derive a complete algorithm for computing corresponding rational solutions.

- Rational solutions of algebraic ordinary differential equations of arbitrary order [28]. We first prove a sufficient condition for the existence of a bound on the degree of the possible polynomial solutions to an AODE. An AODE satisfying this condition is called *noncritical*. Then we prove that some common classes of low-order AODEs are noncritical. For the rational solutions, we determine a class of AODEs, which are called *maximally comparable*, such that the possible poles of any rational solutions are recognizable from their coefficients. This generalizes the well-known fact that all the rational solutions to a given linear ODE are contained in the set of zeros of the leading coefficient. Finally, we develop an algorithm to compute all rational solutions of certain maximally comparable AODEs, which is applicable to 78.54% of the AODEs in Kamke's collection of standard differential equations.

I plan to work on the following problems in the near future:

- Design algorithms to compute polynomial and rational solutions of high-order AOΔEs.

- Compute rational solutions of non-autonomous first-order AOΔEs.

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

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 [17]. 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:

- 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.
- 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.
- 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 [5] 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. Our contributions in this area is as follows:

- Computations of the Expected Euler Characteristic for the Largest Eigenvalue of a Real non-central Wishart Matrix [24].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.

I plan to work on the following problems in the near future:

- 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.

- 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 [31], 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 [14]. In [4], 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.

- 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 [19], 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.

- 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 [5]. 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 [16, 2, 4] to compute its formal solutions. For instance, the author's recent work [4] 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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