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A Study on Hypergeometric Polynomials and Their Implementation

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Abstract

In this course we will study multivariate hyper-geometric functions in the sense of Gel'fand, Kapranov, and Zelevinsky (GKZ systems). These functions generalize the classical hyper-geometric functions of Gauss, Horn, Appell, and Lauricella. We will emphasize the algebraic methods of Saito, Sturmfels, and Takayama to construct hyper-geometric series and the connection with deformation techniques in commutative algebra. We end with a brief discussion of the classification problem for rational hyper-geometric functions.

Keywords: Hypergeometric Polynomials, Implementation,

1. Introduction

The study of one-variable hyper-geometric functions is more than 200 years old. They appear in the work of Euler, Gauss, Riemann, and Kummer. Their integral representations were studied by Barnes and Mellin, and special properties of them by Schwarz and Goursat. The famous Gauss hyper-geometric equation is ubiquitous in mathematical physics as many well-known partial differential equations may be reduced to Gauss' equation via separation of variables.

There are three possible ways in which one can characterize hyper-geometric functions: as functions represented by series whose coefficients satisfy certain recursion properties; as solutions to a system of differential equations which is, in an appropriate sense, holonomic and has mild singularities; as functions defined by integrals such as the Mellin-Barnes integral. For one-variable hyper-geometric functions this interplay has been well understood for several decades.

In the several variables case, on the other hand, it is possible to extend each one of these approaches but one may get slightly different results. Thus, there is no agreed upon definition of a multivariate hyper-geometric function. For example, there is a notion due to Horn of multivariate hyper-geometric series in terms of the coefficients of the series.

The recursions they satisfy gives rise to a system of partial differential equations. It turns out that for more than two variables this system need not be holonomic, i.e. the space of local solutions may be infinite dimensional. On the other hand, there is a natural way to enlarge this system of PDE's into a holonomic system.

The relation between these two systems is only well understood in the two variable case. Even in the case of the classical Horn, Appell, Pochhammer, and Lauricella, multivariate hyper-geometric functions it is only in 2000's and 80's that an attempt was made by W. Miller Jr. and his collaborators to study the Lie algebra of differential equations satisfied by these functions and their relationship with the differential equations arising in mathematical physics.

There has been a great revival of interest in the study of hyper-geometric functions in the last two decades. Indeed, a search for the title word hyper-geometric in the MathSciNet database yields 3181 articles of which 1530 have been published since 2000! This newfound interest comes from the connections between hyper-geometric functions and many areas of mathematics such as representation theory, algebraic geometry and Hodge theory, combinatorics, D-modules, number theory, mirror symmetry, etc.

Review of Related Literature

A key new development is the work of Gel'fand, Graev, Kapranov, and Zelevinsky in the late 80's and early 90's which provided a unifying foundation for the theory of multivariate hypergeometric series. More recently, through the work of Oaku, Saito, Sturmfels, and Takayama, the algorithmic aspects of the theory of hypergeometric functions have been

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developed and the connections with the theory and techniques of computational algebra have been made apparent. It is this aspect of the theory which will be emphasized in this course.

The book of Saito, Sturmfels, and Takayama serves as the backbone for these lectures and we refer to it for many of the proofs. It would be impossible to give even an introduction to this theory in just three lectures. That is the reason why these notes are called what they are, rather than “An Introduction to Hypergeometric Functions” or some other similar title.

This emphasizes the fact that I have chosen to highlight a number of topics which I hope will make the reader interested in further study of this beautiful subject, but I have made no attempt to give a comprehensive view of the field. The purpose of the first lecture will be to motivate the notion of GKZ system. This will be done through the work of Miller and his collaborators.

Also, there is Frobenius’ method for obtaining series solutions of an ODE around a regular singular point and the extension to systems of PDEs by Saito, Sturmfels, and Takayama. In the last lecture we will discuss the construction of series solutions without logarithmic terms and we will end with a brief discussion of rational hyper-geometric functions and their connection with residue integrals.

There is no claim of originality in these notes; indeed, most of the non-classical material may be found in other sources. Moreover, these lectures are very much influenced by those given by Mutsumi Saito at last year’s “Workshop on D-modules and Hyper-geometric Functions” held in Lisbon. In fact, it was from Saito that I first learned about Miller’s work on bi-variate hyper-geometric functions and how it motivates the definition of GKZ systems.

Research Study

The computation of the hyper-geometric function ${}_pF_q$, a special function encountered in a variety of applications, is frequently sought. However, aside from the most basic hyper-geometric functions, this is an extremely difficult task in practice. The reason for this is that the non-trivial structure of the series that defines the function creates many numerical issues such as cancellation and round-off error, which become especially significant for certain ranges of the parameters and the variable.

This results in many methods of numerical computation being ineffective for all but the simplest parameter and variable ranges. We focus in this dissertation on computing the two most commonly used hyper-geometric functions, the confluent hyper-geometric function ${}_1F_1(a; b; z)$ and the Gauss hyper-geometric function ${}_2F_1(a, b; c; z)$, which both suffer from these problems.

The program which will be used to compute these functions will be MATLAB, which employs double precision arithmetic, so it is especially important for effective methods to be found to overcome the numerical issues involved. The goal of this project is to carry out a comprehensive survey of methods for computing ${}_1F_1$ and ${}_2F_1$, and to determine how to choose appropriate methods for different parameter and variable ranges, resulting in reliable and fast computation for as large a range of the parameters (a, b for ${}_1F_1$ and a, b, c for ${}_2F_1$) and variable z as possible.

The algorithms used are required to be accurate, fast and robust for specific parameter and variable regions for which they have been selected.

In this research, we will test a large variety of approaches, such as a

range of series methods, ways of numerically solving the differential equations that the hyper-geometric functions satisfy and quadrature methods, as well as employing recurrence relations to attempt to use computations of relatively simple cases to obtain computations for extreme parameter cases.

We will also test asymptotic series for ${}_1F_1$. For ${}_2F_1$, we also explore the use of transformation formulae and expansions for special parameter cases. We aim to combine techniques that work for specific parameter regimes in order to compile a package of methods that is effective for as large a part of the complex plane for each parameter and variable as possible.

An important property that we will need to use is the convergence criteria of the hyper-geometric functions depending on the values of p and q . The radius of convergence of a series of a variable z is defined as a value r_c such that the series converges if $|z - d_c| < r_c$ and diverges if $|z - d_c| > r_c$, where d_c , in this case 0, is the centre of the disc of convergence.

For the hyper-geometric function, provided a_j and b_j are not non-positive integers for any j , the relevant convergence criteria stated below can be derived using the ratio test, which determines the absolute convergence of the series using the limit of the ratio of two consecutive terms.

- If $p \leq q$, then the ratio of coefficients of z^k in the Taylor series of the hyper-geometric function ${}_pF_q$ tends to 0 as $k \rightarrow \infty$; so the radius of convergence is ∞ , so that the series converges for all values of $|z|$.

Hence, ${}_pF_q$ is entire. In particular, the radius of convergence for ${}_0F_1$ and ${}_1F_1$ is ∞ .

- If $p = q + 1$, the ratio of coefficients of z^k tends to 1 as $k \rightarrow \infty$, so the radius of convergence is 1, so that the series converges only if $|z| < 1$.

In particular the radius of convergence of ${}_2F_1$ is 1.

- If $p > q + 1$, the ratio of coefficients of z^k tends to ∞ as $k \rightarrow \infty$, so the radius of convergence is 0, so that the series does not converge for any value of $|z|$.

We will seek approximations to the relevant hyper-geometric functions for $|z|$ within the radii of convergence, and then apply analytic continuation to compute them in the rest of the complex plane where appropriate.

For $p = q + 1$, there is a further restriction for convergence on the unit disc; the series only converges absolutely at $|z| = 1$ if $\text{Re}(\sum_{j=1}^p b_j - \sum_{j=1}^p a_j) > 0$, so the selection of values for a_j and b_j must reflect that.

Computation of Hyper-Geometric Functions

The computation of the hyper-geometric function is frequently sought due to the wide range of practical problems in which it appears. It arises, for example, in photon scattering from atoms, networks, Coulomb wave functions, binary stars, finance and many others. Due to this wide range of applications, it is useful to provide a survey of work carried out on computing hyper-geometric functions, and to discuss which methods are likely to work well for particular parameter regimes, as well as to supply information on how to test the reliability of a routine, test cases that a routine might have difficulty computing and how to evaluate other special functions required for computation of hyper-geometric functions.

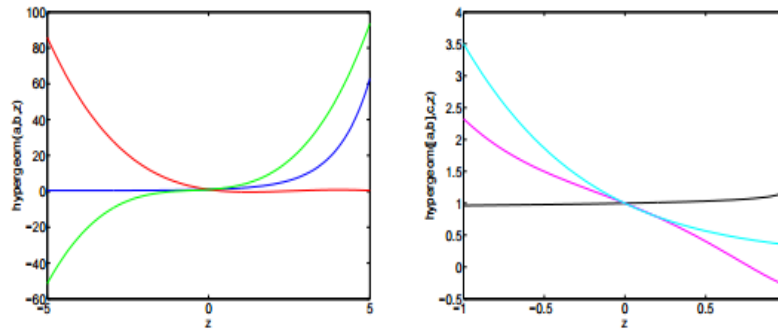


Figure 1: Graphs of ${}_1F_1(a; b; z)$, generated using MATLAB, for real $z \in [-5, 5]$ with $(a, b) = (0.1, 0.2)$ (dark blue), $(a, b) = (-3.8, 1.5)$ (red) and $(a, b) = (-3, -2.5)$ (green), and ${}_2F_1(a, b; c; z)$ for real $z \in [-1, 1]$ with $(a, b, c) = (0.1, 0.2, 0.4)$ (black), $(a, b, c) = (-3.6, -0.7, -2.5)$ (purple) and $(a, b, c) = (-5, 1.5, 6.2)$ (sky blue).

Research of this form will be useful in many ways. Firstly, the Numerical Algorithms Group who sponsored this project, will benefit from research on computing hyper-geometric functions being carried out, to help them achieve their goal of writing a package for the NAG Library.

Secondly, programmers working with software which does not have an built-in hyper-geometric function evaluator may be able to use the theory of computing these functions to write such a program for themselves.

Another important reason why research into this area is desirable is that the state-of-the-art software currently used for special functions has not yet been perfected. This is illustrated by a number of cases when MATLAB R2008b is asked to compute the function ${}_2F_1(a, b; c; z)$ for certain values of a, b, c and z . Firstly, although the MATLAB routine for computing hyper-geometric functions, 'hyper-geom', is generally slow but tolerable for all parameter and variable values (MATLAB usually took around 10–15 seconds to compute a confluent or Gauss hyper-geometric function the first time after loading the program on the processor used), the problem can sometimes be serious. For example, when the command `hypergeom([1,0.9],2,exp(1i*pi/3))` is used, over 5 minutes is taken for MATLAB to compute the solution on the processor used (an Intel(R) Atom(TM) CPU N270, with processor speed 1.60GHz).

Secondly, there is a major issue with the MATLAB routine in some cases where c is close to a negative integer. For example, when `hypergeom([-1,-1.5],-2.000000000000001,0.5)` is called, a set of parameters for which the Gauss hyper-geometric series has only 2 non-zero terms, the answer returned using 16 digit arithmetic is 0.621859216769114, giving only 2 digit accuracy on the correct answer of 0.625000000000000, which can be found by manual calculation.

This motivates the need for research into effective methods that will compute hyper-geometric functions accurately. There are also problems that arise when computing ${}_1F_1(a; b; z)$ in MATLAB. When `hypergeom(1, 200, 1)` is called, the answer obtained is 6.69×10^{299} to 3 significant figures.

By examination, we can see that each term of the power series of ${}_1F_1(1; 200; 1)$ is a smaller positive real number than each term of ${}_1F_1(1; 1; 1)$, for example, and so the value ${}_1F_1(1; 200; 1)$ is smaller than that of ${}_1F_1(1; 1; 1)$. ${}_1F_1(1; 1; 1) = e = 2.72$ to 3 significant figures, and hence MATLAB's evaluation of ${}_1F_1(1; 200; 1)$ is incorrect.

Furthermore, MATLAB will not generate an evaluation for ${}_1F_1(1; 200; 1)$ either. The methods used by MATLAB and

Mathematical are not publicly known, so it is important to devise a package of routines that do not suffer from these problems.

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