Numerical Evaluation of Generalized Hypergeometric Functions for Degenerated Values of Parameters

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Introduction

In this paper, we give an algorithm to generate connection formulas of generalized hypergeometric functions \( _pF_{p-1} \) for degenerated values of parameters. We also show that these connection formulas give a fast method for numerical evaluation of generalized hypergeometric functions near \( \infty \).

Several methods to evaluate generalized hypergeometric functions are known; see, e.g., the famous text book “Numerical Recipes” [5]. As Van Der Hoeven proved, evaluating series gives a fast method when the precision is big. Since we need high precision values of generalized hypergeometric functions, we will use series expansions of generalized hypergeometric functions near \( \infty \) for numerical evaluation. We call the series expansion of \( _pF_{p-1}(z) \) at \( z = \infty \) a connection formula. Several methods to obtain connection formulas in degenerate cases are known among experts, but an algorithmic method which is fast and relevant for numerical evaluation is not known. Van Der Hoeven gave a method to construct series solutions around regular singular points by introducing an order among logarithmic monomials \( x^m (\log x)^n \) [3]. Note that Saito, Sturmfels and Takayama found an analogous method which is generalized to several variable case [4, Chapter 2]. By utilizing these methods, we will give a new method to obtain connection formulas in degenerate cases.

Methods discussed in this paper are used in our numerical checker for
1 Hypergeometric Function

The function defined by the following series is called the Gauss hypergeometric function.

\[ F(\alpha, \beta, \gamma; z) = \sum_{k=0}^{\infty} \frac{(\alpha)_k(\beta)_k}{(\gamma)_k(1)_k} z^k \]

\( (a)_k = (a)(a+1) \cdots (a+k-1) \)

The analytic continuation of this function is also called the Gauss hypergeometric function. This function satisfies the following differential equation.

\[ \{\delta_z(\delta_z + \gamma - 1) - z(\delta_z + \alpha)(\delta_z + \beta)\} F(\alpha, \beta, \gamma; z) = 0 \]

\( \delta_z = z \frac{\partial}{\partial z} \)

This differential equation is called the Gauss hypergeometric differential equation. By expanding the products \( \delta_z \) in terms of \( z \) and \( z \frac{\partial}{\partial z} \), we obtain

\[ \{z(z-1)\frac{\partial^2}{\partial z^2} + (\gamma - (\alpha + \beta + 1)z) \frac{\partial}{\partial z} - \alpha \beta\} F(\alpha, \beta, \gamma; z) = 0 \]

Hence, the Gauss hypergeometric function has singularities at \( z = 0, 1, \infty \).

It is known that the hypergeometric function have the following integral representation (Euler integral representation)

\[ F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma - \alpha)} \int_0^1 t^{\alpha-1}(1 - t)^{\gamma-\alpha-1}(1 - tz)^{-\beta} dt \]

Our goal is numerical evaluation of the generalized hypergeometric function defined by the following series

\[ _pF_{p-1}(\alpha_1, \cdots, \alpha_p, \beta_1, \cdots, \beta; z) = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k \cdots (\alpha_p)_k}{(\beta_1)_k \cdots (\beta_{p-1})_k(1)_k} z^k \]
The famous book “Numerical recipes”\textsuperscript{[5]} says that “a fast, general routine for the complex hypergeometric function \(2F1(a, b, c; z)\), is difficult or impossible”. One difficulty is that the generalized hypergeometric series converges only in \(|z| < 1\), then the method of evaluating series can be used only when \(|z| < 1\). However, in case of the generalized hypergeometric functions, there are connection formulas, by which we can express the hypergeometric series \(pF_{p-1}\) in terms of a set of series which converges at \(z = \infty\). For example, in case of \(2F1\), the connection formula is as follows.

Proposition 1 (connection formula, see, e.g., \[1\]) Assume \(\alpha - \beta, \beta - \alpha, \gamma \notin \mathbb{Z}_{\leq 0}\). Then, we have

\[
F(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)\Gamma(\beta - \alpha)}{\Gamma(\gamma - \alpha)\Gamma(\beta)} F(\alpha, \alpha - \gamma + 1, \alpha - \beta + 1)(-z)^{-\alpha} \\
+ \frac{\Gamma(\gamma)\Gamma(\alpha - \beta)}{\Gamma(\gamma - \beta)\Gamma(\alpha)} F(\beta, \beta - \gamma + 1, \beta - \alpha + 1)(-z)^{-\beta}
\]

The condition \(\alpha - \beta, \beta - \alpha, \gamma \notin \mathbb{Z}_{\leq 0}\) means that \(\alpha - \beta, \beta - \alpha, \gamma\) are not in the set \(\{0, -1, -2, -3, \ldots\}\). When the condition is satisfied, we say that the parameters are generic and when the condition is not satisfied, we say that the parameters are non-generic or degenerated.

We can use the connection formula to evaluate numerically the hypergeometric function near \(z = \infty\) in generic case. Degenerated cases will be discussed in the rest of this paper. We note that the evaluating hypergeometric series can be accelerated by the binary splitting algorithm\textsuperscript{[2], [3]}.

2 Connection Formulas of \(pF_{p-1}\)

In this section, we study connection formulas of \(pF_{p-1}\) between 0 and \(\infty\) and numerical evaluation by using the formula. In the case that parameters are generic, these formulas are well-known. They can be obtained by using the Barns integral representation (see, e.g., \[1\] Chapter2 4.6). When parameters are non-generic, there is no complete list of connection formulas nor an algorithm to obtain connection formulas in the literatures. We will give an algorithm to derive connection formulas when parameters are non-generic. The Algorithms 1 and 2 seem to be implicitly used among experts to study global behaviors of generalized hypergeometric functions, but Algorithm 3 will be new and it gives a fast routine.
Let us review the connection formula in the generic case. It will be the starting data to generate connection formulas in non-generic case.

**Proposition 2 (connection formulas of** $pF_{p-1}$, **see, e.g., [1])** Assume $\alpha_i - \alpha_j (i \neq j) \not\in \mathbb{Z}, \beta_i \not\in \mathbb{Z}_{\leq 0}$. Then, we have

$$pF_{p-1}(\alpha_1, \ldots, \alpha_p, \beta_1, \ldots, \beta_{p-1}; z) = \sum_{i=1}^{p} \Pi_{j=1, i \neq j}^{p-1} \Gamma(\beta_j) \Pi_{j=1}^{p} \Pi_{j=1, i \neq j}^{p} \Gamma(\alpha_j - \alpha_i) \Gamma(\beta_j - \alpha_i) pF_{p-1}(\alpha_i - \beta_1 + 1, \ldots, \alpha_i - \beta_{p-1} + 1, \alpha_i - \alpha_1 + 1, \ldots, \alpha_i - \alpha_{i-1} + 1, \ldots, \alpha_i - \alpha_p + 1; 1/z)(-z)^{-\alpha_i}$$

**Algorithm 1** The case of $\alpha_1 - \alpha_2 \in \mathbb{Z}$:

1. Use contiguity relations to make $\alpha_1 = \alpha_2$.
2. Multiply $(\alpha_2 - \alpha_1)$ to the both sides of the connection formula in the generic case.
3. Replace $(\alpha_2 - \alpha_1)\Gamma(-\alpha_1 + \alpha_2)$ by $\Gamma(-\alpha_1 + \alpha_2 + 1)$ and $(\alpha_2 - \alpha_1)\Gamma(\alpha_1 - \alpha_2)$ by $-\Gamma(\alpha_1 - \alpha_2 + 1)$.
4. Apply $\frac{\partial}{\partial \alpha_2}$ for the both sides and take the limit $\alpha_2 \to \alpha_1$.

This method can be generalized to more degenerated case.

**Algorithm 2** We assume $\alpha_1 = \alpha_2 = \cdots = \alpha_q (q \leq p)$ and $\forall i, j, \forall i - \alpha_j \not\in \mathbb{Z}$ ($q < i, j \leq p, i \neq j$):

1. Multiply $\Pi_{i=1}^{q-1} \Pi_{j=i+1}^{q} (\alpha_j - \alpha_i)$ to the both sides of the connection formula in the generic case.
2. Replace $(\alpha_j - \alpha_i)\Gamma(-\alpha_i + \alpha_j)$ by $\Gamma(-\alpha_i + \alpha_j + 1)$ and $(\alpha_j - \alpha_i)\Gamma(-\alpha_j + \alpha_i)$ by $-\Gamma(-\alpha_j + \alpha_i + 1)$.
3. Apply $\frac{\partial^{(q-1)}}{\Pi_{i=1}^{q} \partial \alpha_i}$ for the both sides and take the limit $\alpha_2 \to \alpha_1, \cdots, \alpha_q \to \alpha_1$.

Note that the left hand side of the output of the algorithm is

$$\left(\Pi_{i=1}^{q-1} i!\right) pF_{p-1}(\alpha_1, \ldots, \alpha_1, \alpha_{q+1}, \ldots, \alpha_p, \beta_1, \ldots, \beta_{p-1}; z)$$

and hence the right hand side of the output gives a series expansion of this function around $z = \infty$. 

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We conjecture that a repetition of applying the Algorithm 2 and of applying contiguity relations yields a connection formula for any degenerated case.

This method requires a complicated symbolic differentiation, but computer algebra systems are good at it. One can say that our method of using connection formula of $pF_{p-1}$ to evaluate numerical values around $z = \infty$ is a hybrid computation of symbolic computation and numerical computation.

**Example 1** The following is a connection formula in a degenerated case which is obtained by the Algorithm 2

\[
2F1(\alpha_1, \alpha_1, \beta_1; z) = \frac{\Gamma(\beta_1)(-z)^{-\alpha_1}}{\Gamma(\alpha_1)\Gamma(-\alpha_1 + \beta_1)} \lim_{\alpha_2 \to \alpha_1} \frac{\partial}{\partial \alpha_2} 2F1(\alpha_2, 1 + \alpha_1 - \beta_1, 1 - \alpha_1 + \alpha_2, 1/2) 
\]

\[
- \frac{\Gamma(\beta_1)(-z)^{-\alpha_1}}{\Gamma(\alpha_1)\Gamma(-\alpha_1 + \beta_1)} \lim_{\alpha_2 \to \alpha_1} \frac{\partial}{\partial \alpha_2} 2F1(\alpha_2, 1 + \alpha_1 - \beta_1, 1 - \alpha_1 + \alpha_2, 1/2) 
\]

\[
- \gamma \Gamma(\beta_1) + \Gamma(\beta_1) \psi(\alpha_1) 
\]

\[
\frac{\Gamma(\beta_1) - \Gamma(\beta_1) \log(-z) + \Gamma(\beta_1) \psi(-\alpha_1 + \beta_1)}{\Gamma(\alpha_1)\Gamma(-\alpha_1 + \beta_1)} (-z)^{-\alpha_1} 2F1(\alpha_1, 1 + \alpha_1 - \beta_1, 1, 1/2). 
\]

Here, $\psi(z)$ is the derivative of $\log(\Gamma(z))$ and $\gamma$ is $-\psi(1)$.

Our computer experiments show that Algorithm 2 is not efficient. The next algorithm is an efficient version of deriving connection formulas in the degenerate case. Algorithm 2 is used only to get $c_0^0$’s in the following algorithm.

**Algorithm 3** In the case of $\alpha_1 = \alpha_2 = \cdots = \alpha_q$ (where $q = p$), series solutions at $z = \infty$ can be written as

\[
pF_{p-1} = (-z)^{-\alpha_1} \sum_{i=1}^{\infty} \{ c_0^i + c_1^i \log(-z) + \cdots + c_{q-1}^i \log^{q-1}(-z) \} z^{-i} 
\]

1. Derive recurrence relations for $c_j^i$ with respect to $i$ by a generalized hypergeometric differential equation (see, e.g., [3], [4]). $c_j^i$ ($i > 0$) are determined by $c_j^0$’s.

2. Obtain $c_j^0$ by applying a part of Algorithm 2.

3. Get other coefficients $c_j^i$ by using the recurrence relations for $c_j^i$ with respect to $i$. 

3 Examples of Using Connection Formulas in Degenerate Cases

Mathematica implementation for numerical evaluations of generalized hypergeometric functions is known to be very nice. Here we compare numerical evaluation by our formula (derived by our Algorithm 3), evaluation by Mathematica and evaluation by numerical integration.

Example 2 We try to evaluate the value of $\, _2F_1(10/3, 10/3, 7/2, 13 + 13\sqrt{-1}).$

We will present timing data of evaluation by the series expansion derived by Algorithm 3 and Mathematica. We present timing data on Mathematica only for reader’s convinience; it is nonsense to compare our timing data by our algorithms and those by Mathematica, because an algorithm used by Mathematica is not known and implementations are done on different languages.

| terms | time       | value                                                                 |
|-------|------------|-----------------------------------------------------------------------|
| 5     | 0.0013sec  | 0.00004646545068442618485 $+ 0.0000988864768356428440\sqrt{-1}$       |
| 10    | 0.0027sec  | 0.00004646545068442618485 $+ 0.0000988864768356428440\sqrt{-1}$       |
| 20    | 0.004117sec| 0.00004646545068442618485 $+ 0.0000988864768356428440\sqrt{-1}$       |
| 40    | 0.008538sec| 0.00004646545068442618485 $+ 0.0000988864768356428440\sqrt{-1}$       |
| 80    | 0.01779sec | 0.00004646545068442618485 $+ 0.0000988864768356428440\sqrt{-1}$       |

Here, terms mean the truncation degree of hypergeometric series. The precision is set to terms + 10. This timing data includes time to set $c_j$ in Algorithm 3. As we see in the table, the computation is done in less than 0.03 second.

Timing data by Mathematica 4.0:

| precision | time     | value                                                                 |
|-----------|----------|-----------------------------------------------------------------------|
| 10        | 0.04 Sec | 0.0000464654 $+ 0.0000988864\sqrt{-1}$                               |
| 25        | 0.04 Sec | 0.0000464654 $+ 0.0000988864\sqrt{-1}$                               |
| 50        | 0.09 Sec | 0.0000464654 $+ 0.0000988864\sqrt{-1}$                               |

We also try to evaluate the same value by using Barns integral representation and adaptive rule.

Timing Data:

| precision | time     | value                                                                 |
|-----------|----------|-----------------------------------------------------------------------|
| 4         | 0.3885sec| 0.0000450918 $+ 0.000093032899722079852\sqrt{-1}$                   |
| 5         | 0.466sec | 0.0000450918 $+ 0.000093032899722079852\sqrt{-1}$                   |
| 6         | 0.702sec | 0.0000450918 $+ 0.000093032899722079852\sqrt{-1}$                   |
Example 3 We try to evaluate the value of \( _2F_1(7/2, 7/2, 31/5, 1.3+1.8\sqrt{-1}) \), which will be more difficult than the previous example for series expansion, since \( 1.3 + 1.8\sqrt{-1} \) is closer to the boundary of the domain of convergence.

The precision is set to terms + 10. The convergence is slower than the case of \( z = 13 + 13\sqrt{-1} \). We also try to evaluate the same value by using Euler’s integral representation and trapezoidal rule.
Figure 2: a timing comparison of different algorithms
“data2r” : Algorithm 3
“data2m” : Mathematica
“data2b” : Euler’s integral representation and trapezoidal rule

| sample size | time   | value                                                        |
|-------------|--------|--------------------------------------------------------------|
| 2000        | 13.11sec | -0.376954276724114820-0.2822864217813210745√−1             |
| 4000        | 85.41sec | -0.376954276222648211-0.2822864217919839264√−1             |
| 8000        | 346.4sec | -0.376954276144992000-0.2822864217936281214√−1             |

The precision is set to 19. The numerical integration requires more CPU time, but the accuracy seems to be better than the series expansion. This data tell us that series expansion at \( z = \infty \) should not be used around \(|z| = 1\).

Timing data by Mathematica 4.0:

| precision | time   | value                                                        |
|-----------|--------|--------------------------------------------------------------|
| 10        | 0.01 Second | -0.376954 - 0.282286√−1                                      |
| 25        | 0.01 Second | -0.37695427613081226577499361663051762042942548627034        |
| 50        | 0.01 Second | -0.376954276149275024157349298314398979724012538853√−T       |
The Figure below is a visualization of the difference $|r_{20} - r_{10}|$. Here, $r_{20}$ is the truncation of our connection formula of $\binom{7}{2}F_1\left(\frac{7}{2}, \frac{7}{2}, \frac{31}{5}, x + y\sqrt{-1}\right)$ at the degree 20 and $r_{10}$ is that at the degree 10.

The difference is close to zero in $|z| >> 1$, but it is larger in the neighborhood of $|z| = 1$. Developing a method for high-precision evaluation around $|z| = 1$ will be a future problem.

**Example 4** We will evaluate values of $\binom{3}{2}F_2\left(\frac{7}{2}, \frac{7}{2}, \frac{7}{2}, \frac{31}{5}, \frac{36}{7}; z\right)$. We compare the adaptive integration method of the Barns integral and numerical evaluation of our degenerated connection formulas derived by Algorithm 3.

**Numerical integration (precision is set to 19):**

| $z$ | time   | value                                      |
|-----|--------|--------------------------------------------|
| $z = 130 + 130\sqrt{-1}$ | 0.2219sec | 0.000001881452796232078012 0.000006893851655427774880$\sqrt{-1}$ |
| $z = 13 + 13\sqrt{-1}$ | 0.1605sec | 0.007312359138710618527 -0.006400306129230969169$\sqrt{-1}$ |
| $z = 1.3 + 1.3\sqrt{-1}$ | 0.112sec | -1.097506492885595820 +0.6369234717153367928$\sqrt{-1}$ |

**Series expansion (terms are set to 20, and precision is set to 19):**
Timing data by Mathematica 4.0 (precision is set to 10):

|         | time       | value                          |
|---------|------------|-------------------------------|
| $z = 130 + 130\sqrt{-1}$ | 0.01571sec | $0.00001345106300346753915 + 0.00000679609941828839164\sqrt{-1}$ |
| $z = 13 + 13\sqrt{-1}$    | 0.01404sec | $0.007350815068974895610 - 0.006282360701607166085\sqrt{-1}$ |
| $z = 1.3 + 1.3\sqrt{-1}$  | 0.004741sec | $-1.097992622097576377 + 0.636475978799937697\sqrt{-1}$ |

We conclude that our formulas derived by algorithm 3 give a fast method to evaluate generalized hypergeometric functions around $\infty$.

References

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