Calculating ${}_pF_q$

Daniel Schultz

For $\mathbf{a} = a_1, \dots, a_p$ and $\mathbf{b} = b_1, \dots, b_q$

$$ {}_pF_q\left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| z \right) := \sum_{n=0}^{\infty} \frac{(\mathbf{a})_n}{(\mathbf{b})_n} \frac{z^n}{n!} \tag{1} $$

The function is undefined when any b_i is $0, -1, -2, \dots$, i.e. $1/\Gamma(\mathbf{b}) = 0$. Also, $\hat{\mathbf{a}}_i$ denotes the length $p-1$ vector with the i^{th} entry omitted.

1 The case $p < q + 1$ [not implemented]

Just sum the series for any argument.

2 The case $p > q + 1$ [not implemented]

The formal series is divergent except for zero argument or terminating parameters. For nonzero arguments it can defined via Borel summation, leading to

$$ {}_pF_q\left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| z \right) = \sum_{i=1}^{p} \frac{\Gamma(\mathbf{b})\Gamma(\hat{\mathbf{a}}_i - a_i)}{\Gamma(\mathbf{b} - a_i)\Gamma(\hat{\mathbf{a}}_i)} (-z)^{-a_i} {}_{q+1}F_{p-1}\left(\begin{matrix} a_i, 1 + a_i - \mathbf{b} \\ 1 + a_i - \hat{\mathbf{a}}_i \end{matrix} \middle| \frac{(-1)^{p-q-1}}{z} \right) $$

Integer differences among the $\mathbf{a}$ can be handled via limiting cases, and the series on the right are convergent. The only difficulty here is when z is a ball containing 0 *but not identically* 0. [Just take few terms of the divergent series and use an asymptotic formula for the error?]

3 The case $p = q + 1$

3.1 inside unit circle

For arguments sufficiently inside the unit circle, just sum the series.

3.2 outside unit circle

For $z \notin [0, 1]$ (?),

$$ {}_pF_{p-1}\left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| z \right) = \sum_{i=1}^{p} \frac{\Gamma(\mathbf{b})\Gamma(\hat{\mathbf{a}}_i - a_i)}{\Gamma(\mathbf{b} - a_i)\Gamma(\hat{\mathbf{a}}_i)} (-z)^{-a_i} {}_pF_{p-1}\left(\begin{matrix} a_i, 1 + a_i - \mathbf{b} \\ 1 + a_i - \hat{\mathbf{a}}_i \end{matrix} \middle| \frac{1}{z} \right) $$

and for arguments sufficiently outside the unit circle we can just sum the series on the right. As before, integer differences among the $\mathbf{a}$ can be handled via limiting cases.

3.3 near unit circle, away from one

Theoretically for any argument outside the branch cut $[1, \infty]$, the series on the right hand side of

$$ (1+z)^{-2a_p} {}_pF_{p-1}\left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| \frac{4z}{(1+z)^2} \right) = \sum_{n=0}^{\infty} u_n z^n, \quad |z| < 1 $$

can be summed. However, since computation of the u_n's is a bit expensive, it should only be used when absolutely neccessary. There is a good reason for the prefactor $(1+z)^{-2a_p}$: is present in many quadratic transformation formulas in special cases and has the effect of lowering the order of the recurrence relation for u_n by one.

It is also possible to use Padé approximants here, but do we have useful error bounds?

3.4 near one

This is the most interesting case as the function can fail to be defined at one. The existence of $F(1)$ is governed by $\sigma = \Sigma(\mathbf{b}) - \Sigma(\mathbf{a})$. If σ is not an integer we have

$$F(1-z) = z^{\sigma} \sum_{n=0}^{\infty} u_n z^n + \sum_{n=0}^{\infty} v_n z^n \tag{2}$$

with the $u_1, u_2, \ldots$ determined from recurrences by $u_0 = \Gamma(-\sigma)\Gamma(\mathbf{b})/\Gamma(\mathbf{a})$ and the $v_{p-1}, v_p, \ldots$ are determined from recurrences by $v_0, \ldots, v_{p-2}$. Thus the difficulty is computing these $v_0, \ldots, v_{p-2}$.

If σ is an integer, then at most one $\log(z)$ enters into the series.

3.4.1 near one: generic approach

We simply evaluate Equation 2 and its derivatives up to and including order $p-1$ at $z = 1/4$ to solve for the $u_0, v_0, \ldots, v_{p-2}$. The explicit formula for u_0 is surprisingly useless in this approach.

3.4.2 near one: Buehring [not implemented - this section might even be wrong]

Here we sum the first m terms of Equation 1 and use a formula derived by Buehring to sum the remaining terms. Since we will generically be dealing with logarithmically convergent series (when $z = 1$) in both sums, it is important to balance the choice of m between the two to ensure a sub-exponential algorithm. We have (Equations 2.7 and 2.9 in "analytic continuation of the generalized hypergeoemtric sereis near unit argument with emphasis on the zero-balanced series" by Buehring and Srivastava)

$$\begin{aligned}\sum_{n=m}^{\infty} \frac{(\mathbf{a})_n}{(\mathbf{b})_n} \frac{z^n}{n!} &= \frac{\Gamma(\mathbf{b})}{\Gamma(\mathbf{a})} z^m \sum_{k=0}^{\infty} \frac{\Gamma(\mathbf{a}+m+k)}{\Gamma(\mathbf{b}+m+k)} \frac{z^k}{\Gamma(1+m+k)} \\ &= \frac{\Gamma(\mathbf{b})(a_p)_m}{\Gamma(\hat{\mathbf{a}}_p)} z^m \sum_{k=0}^{\infty} A_k \left(\begin{array}{c} \hat{\mathbf{a}}_p \\ \mathbf{b} \end{array} \right) {}_2\tilde{F}_1 \left(\begin{array}{c} 1, a_p+m \\ 1+\sigma+a_p+m+k \end{array} \middle| z \right)\end{aligned}$$

where the A_k are independent of m and are polynomials in $a_1, \ldots, a_{p-1}, b_1, \ldots, b_{p-1}$. They can be defined in the base case $p = 2$ as

$$A_k \left(\begin{array}{c} a_1 \\ b_1 \end{array} \right) = \frac{(1-a_1)_k (b_1 - a_1)_k}{k!}$$

and inductively for larger p by Hadamard and Cauchy products. After all is said and done, the A_k satisfy an order $p-1$ recurrence with asymptotic

$$\frac{A_k}{k!} \ll \sum_{i<p} k^{\sigma + a_p - 1 - a_i} \tag{3}$$

Now set

$$F_k = {}_2\tilde{F}_1 \left(\begin{array}{c} 1, a_p+m \\ 1+\sigma+a_p+m+k \end{array} \middle| z \right)$$

We have

$$F_k = \frac{(k+\sigma-1-(1-z)(a_p+2k+m+2\sigma-2)) F_{k-1} + (1-z) F_{k-2}}{z(k+\sigma)(a_p+k+m+\sigma-1)}$$

and therefore the asymptotic

$$k! F_k \ll k^{-\sigma} |1-1/z|^k + k^{-m-\sigma-a_p}$$

To ensure convergence of the tail series, we should have $|1-1/z| < 1$ and $m + \mathrm{Re}(a_i) > 0$ for all $i < p$.

In reality the majorant method will probably produce a much worse bound $|A_k/k!| \leq ck^{\mu}$ so we are balancing the sum of the first m terms of a sum whose terms are like $n^{-1-\sigma}$ with another series that we can only prove has terms like $k^{\mu-m-\sigma-a_p}$. Any reasonable overestimation of μ can be compensated by a larger m. Finally, in order to sum in total no more than $O(d)$ terms for d digit accuracy, it probably suffices to take $m \approx d$ for reasonable parameter ranges.

4 old stuff

4.1 Tight ${}_2F_1$ bounds everywhere

The analysis is for real parameters $a, b, c \in \mathbb{R}$, but it should be possible to do something for complex parameters too.

With

$$f(w) = (1+w)^{-2a}\,{}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \,\middle|\, \frac{4w}{(1+w)^2}\right) = \sum_{n=0}^{\infty} r_n w^n, \quad |w| < 1 \tag{4}$$

we have $r_0 = 1$, $r_1 = \frac{4ab}{c} - 2a$, and $r_{n+1} = \lambda_0(n) r_n + (1 - \lambda_1(n)) r_{n-1}$, where

$$\lambda_0(n) = \frac{2(2b-c)(n+a)}{(n+1)(n+c)}$$
$$\lambda_1(n) = \frac{2(1-2a+c)(n+a)}{(n+1)(n+c)}$$

The unit disk $|w| < 1$ is mapped into the whole complex z-plane minus $[1, \infty)$ by $z = \frac{4w}{(1+w)^2}$, hence this provides a method for computing the usual branch of ${}_2F_1$ if we can bound the tails of the sum. Note that $\lambda_0, \lambda_1 \to 0$, and for the moment entertain the assumption that $|\lambda_0| \le \lambda_1 \le 1$ for all n:

$$\begin{aligned} |r_2| &= |\lambda_0 r_1 + (1-\lambda_1) r_0| \\ &\le |\lambda_0||r_1| + (1-\lambda_1)|r_0| \\ &\le (|\lambda_0| + 1 - \lambda_1)\max(|r_0|, |r_1|) \\ &\le \max(|r_0|, |r_1|). \end{aligned}$$

Hence $|r_n| \le \max(|r_0|, |r_1|)$ for all n by induction. For general real parameters a, b, c the inequality $|\lambda_0(n)| \le \lambda_1(n)$ is not possible for all n as singularities (either logarithmetic or algebraic) of the ${}_2F_1$ at $z = \infty$ and $z = 1$ mean that the r_n can grow like an arbitrarily large power of n.

To remedy this, consider $\tilde{r}_n := r_n n^{-\mu}$ for some arbitrary real μ. The transformed recurrence is $\tilde{r}_n = \tilde{\lambda}_0(n)\tilde{r}_{n-1} + (1 - \tilde{\lambda}_1(n))\tilde{r}_{n-2}$ where

$$\tilde{\lambda}_0(n) = \left(\frac{n}{n+1}\right)^{\mu} \lambda_0(n)$$
$$\tilde{\lambda}_1(n) = 1 - \left(\frac{n-1}{n+1}\right)^{\mu} (1 - \lambda_1(n))$$

If $|\tilde{\lambda}_0(n)| \le \tilde{\lambda}_1(n) \le 1$ for all $n \ge n_0$, then it follows as above that $r_n \le \max(|\tilde{r}_{n_0}|, |\tilde{r}_{n_0-1}|) n^{\mu}$ for all $n > n_0$. There are two ways to turn this into an algorithm for bounding the tails. Either choose an n_0 and compute a μ (not recommended), or since

$$\tilde{\lambda}_0(n) = 2(2b-c)n^{-1} + O\left(n^{-2}\right)$$
$$\tilde{\lambda}_1(n) = 2(1-2a+c+\mu)n^{-1} + O\left(n^{-2}\right)$$

we can choose any $\mu > -1 + 2a - c + |2b - c|$ and compute an n_0. This is an optimal bound on μ.

4.2 Tight ${}_3F_2$ bounds near 1

Series expansions of solutions around $z = 1$ can be constructed as

$$\sum_{n=0}^{\infty} r_n (1-z)^{n+\lambda}$$

where $\lambda = 0$ or $\lambda = b_1 + b_2 - a_1 - a_2 - a_3$ and $r_{n+2} + \kappa_1(n) r_{n+1} + \kappa_0(n) r_n = 0$ where

$$\begin{aligned} \kappa_0(n) &= \frac{(a_1+\lambda+n)(a_2+\lambda+n)(a_3+\lambda+n)}{(\lambda+n+1)(\lambda+n+2)(a_1+a_2+a_3-b_1-b_2+\lambda+n+2)} \\ &= 1 + (b_1+b_2-5)\,n^{-1} + O(n^{-2}) \\ \kappa_1(n) &= -2 - (b_1+b_2-5)\,n^{-1} + O(n^{-2}) \end{aligned}$$

For $\lambda = b_1 + b_2 - a_1 - a_2 - a_3$ the r_n are determined once r_0 is fixed, while for $\lambda = 0$, the r_n depend freely on r_0 and r_1. This gives 3 solutions.

By the substitution $r_n = \tilde{r}_n n^\mu$ where $\mu = -2 + \max(b_1, b_2)$, this equation can be brought to the form

$$\tilde{r}_{n+2} + \left(-2 + \frac{d_1}{n} + \frac{d_2}{n^2} + O(\frac{1}{n^3})\right)\tilde{r}_{n+1} + \left(1 - \frac{d_1}{n} - \frac{d_2}{n^2} + O(\frac{1}{n^3})\right)\tilde{r}_n = 0$$

where crutially $d_1 = 1 + |b_1 - b_2|$ is positive. This equation can be rewritten as

$$\tilde{r}_{n+2} - \tilde{r}_{n+1} = \left(1 - \frac{d_1}{n} - \frac{d_2}{n^2}\right)(\tilde{r}_{n+1} - \tilde{r}_n) + O(\frac{\max(|\tilde{r}_{n+1}|, |\tilde{r}_n|)}{n^3})$$

All constants hidden by the O notation are effective and depend only on the parameters b_i, a_i. We would like to show that $\tilde{r}_n = O(n^\epsilon)$ for every $\epsilon > 0$.

4.3 majorant method

This is a terse summary of Messarobba. We would like to study the various functions

$$F(z), \quad F\left(\frac{1}{z}\right), \quad F(1-z), \quad (1+z)^{-2a_1} F\left(\frac{4z}{(1+z)^2}\right), \quad \dots$$

as convergent power series for $|z| < 1$ as this allows for the computation of F everywhere. In order to evaluate these power series, we need bounds on the coefficients, and tight bounds are already difficult to prove for ${}_2F_1$ and ${}_3F_2$. If we are not near the radius of convergence of these series, an overestimation of the coefficients is acceptable if it allows us to actually get proven bounds.

Each of these functions $f(z)$ satisfies a homogeneous linear differential equation $P(f(z)) = 0$ which will we write in terms of $\theta = z\frac{d}{dz}$. Since $z\theta = \theta z - z$, we can write the operator P with θ *on the left*. When θ is on the left and z is on the right, it is easy to transform the differential equation to a recurrsion on the coefficients. For example, for $F(z) = {}_2F_1\left(\begin{matrix} a_1, a_2 \\ b_1 \end{matrix} \middle| z\right) = \sum_{n=0}^{\infty} u_n z^n$, we have

$$P = (\theta + b_1 - 1)(\theta) - (\theta + a_1 - 1)(\theta + a_2 - 1)z \Leftrightarrow \frac{u_n}{u_{n-1}} = \frac{(n + a_1 - 1)(n + a_2 - 1)}{(n + b_1 - 1)(n)}$$

4.3.1 coefficient recursions

Write the differential operator as $P(z,\theta) = \theta^r p_r(z) + \cdots + \theta p_1(z) + p_0(z) = P_s(\theta)z^s + \cdots + P_1(\theta)z + P_0(\theta) \in \mathbb{F}[z,\theta]$ with θ on the left and assume that $P_0(0) \neq 0$. Define the operator $L(z,\theta) = P(z,\theta)p_r(z)^{-1} = \sum_{j=0}^{\infty} Q_j(\theta)z^j$ and note that $\deg(Q_0(\theta)) = r$ and $\deg(Q_j(\theta)) < r$ for $j > 0$. Let $\lambda \in \overline{\mathbb{F}}$ denote a fixed root of Q_0 such that none of $\lambda - 1, \lambda - 2, \dots$ is a root of Q_0. Let $\mu(\nu)$ denote the multiplicity of ν as a root of Q_0 (or as a root of P_0). For a double sequence $\{u_{\lambda+n,k}\}_{n,k\geq 0}$, let

$$u(z) = \sum_{\substack{n=0 \\ \nu=\lambda+n}}^{\infty} \sum_{k=0}^{\infty} u_{\nu,k} z^\nu \frac{\log^k z}{k!},$$

be a solution to $P(z,\theta)(u(z)) = 0$. This is actually a polynomial in $\log z$, so let $\tau(n)$ be a nondecreasing integer-valued function of n satisfying $u_{\lambda+n,k} = 0$ for $k \geq \tau(n)$. We will see shortly that we can take $\tau(0) \leq \mu(\lambda + 0)$ and $\tau(n) \leq \tau(n-1) + \mu(\lambda + n)$. In terms of the operator S_k, which shifts a sequence $\{a_k\}_{k\geq 0}$ to $\{a_{k+1}\}_{k\geq 0}$, the differential equation says that

$$P_0(\nu + S_k)u_\nu = -\sum_{j=1}^{s} P_j(\nu + S_k)u_{\nu-j}$$

Since $P_0(\nu + S_k) = S_k^{\mu(\nu)}(c_0 + c_1 S_k + \cdots)$, this equation allows us to determine all $u_{\lambda+n,k}$ with $k \geq \mu(\lambda+n)$ once the initial values $E_\lambda = \{u_{\lambda+n,k} \,|\, 0 \leq k < \mu(\lambda+n)\}$ are determined. Considering all possible λ gives r linearly independent solutions to $P = 0$.

4.3.2 tail bounds

Let $K < \tau(\infty)$ denote the higest power of $\log z$ occuring in $u(z)$, and consider the truncation

$$\tilde{u}(z) = \sum_{n=0}^{N-1} \sum_{k=0}^{K} u_{\lambda+n,k} z^{\lambda+n} \frac{\log^k z}{k!},$$

and the normalized residual $q(z)$ defined by $P(z,\theta)(\tilde{u}(z)) = Q_0(\theta) q(z)$. This has the form

$$q(z) = \sum_{j=0}^{s-1} \sum_{k=0}^{K} q_{\lambda+N+j,k} z^{\lambda+N+j} \frac{\log^k z}{k!}$$

where the $q_{\lambda+N}, \ldots, q_{\lambda+N+s-1}$ can be computed from $P(z,\theta)$ and $u_{\lambda+N-1}, \ldots, u_{\lambda+N-s}$.

Consider $y(z) = p_r(z)(\tilde{u}(z) - u(z))$ as a solution of $L(z,\theta)(y(z)) = Q_0(\theta)(q(z))$. Suppose that for some $n_0 > 0$ we have constructed power series $\hat{a}(z) = \sum_{j>0} \hat{a}_j z^j$, $\hat{q}(z) = \sum_{n>0} \hat{q}_n z^n$, and $\hat{y}(z) = \sum_{n\geq 0} \hat{y}_n z^n$ with nonnegative coefficients satisfying

1. For all $j > 0$ and $n \geq n_0$,

$$n \sum_{t=0}^{\tau(n)-1} \left| [X^t] \frac{Q_j(\lambda+n+X)}{X^{-\mu(\lambda+n)} Q_0(\lambda+n+X)} \right| \leq \hat{a}_j.$$

2. For all $n \geq n_0$ and $k \geq 0$, $|q_{\lambda+n,k}| \leq \hat{q}_n$.
3. $|y_{\lambda+n,k}| \leq \hat{y}_n$ for all $n < n_0$ and $k \geq 0$.
4. $|y_{\lambda+n,k}| \leq \hat{y}_n$ for all $n \geq n_0$ and $k < \mu(\lambda+n)$.
5. $\hat{y}(z)$ satsifies

$$z\hat{y}'(z) = \hat{a}(z)\hat{y}(z) + \hat{q}(z).$$

If all of these are true, we have $|z^{-\lambda} y(z)| \leq \hat{y}(z)$. The reason for dividing the differential equation by $p_r(z)$ on the right is that $\deg Q_j < \deg Q_0$, so we can expect finite values for the $\hat{a}_j$.

Now, we have

$$\sum_{j=1}^{\infty} Q_j(\theta) z^j = \frac{P(z,\theta)}{p_r(z)} - Q_0(\theta) = \frac{P(z,\theta)}{p_r(z)} - \frac{P(0,\theta)}{p_r(0)}.$$

For all differential equations arising from hypergeometric functions considered here, $\sum_{j=1}^{\infty} Q_j(\theta) z^j$ will be a finite linear combination of functions of the form $(i, k \geq 0)$

$$z\frac{\partial}{\partial z} \frac{z^i}{(1-z)^k}, \quad z\frac{\partial}{\partial z} \log\left(\frac{1}{1-z}\right),$$

or

$$z\frac{\partial}{\partial z} \frac{z^i}{(1-z^2)^k}, \quad z\frac{\partial}{\partial z} \frac{1}{2} \log\left(\frac{1}{1-z^2}\right), \quad z\frac{\partial}{\partial z} \frac{1}{2} \log\left(\frac{1+z}{1-z}\right),$$

all with nonnegative coefficients as power series in z. The coefficients of the linear combination, say $f_j(\theta)$, will be polynomials in θ. Bounding the combinations

$$n \sum_{t=0}^{\tau(n)-1} \left| [X^t] \frac{f_j(\lambda+n+X)}{X^{-\mu(\lambda+n)} Q_0(\lambda+n+X)} \right|$$

for each j and for all $n \geq n_0$ will give a valid $\hat{a}(z)$ and a nice formula for $\hat{h}(z) = \exp \int_0^z \hat{a}(z)/z dz$. It now suffices to choose a $\hat{q}(z)$ so that

$$\hat{y}(z) = \hat{h}(z) \int_0^z \frac{\hat{q}(z)/z}{\hat{h}(z)} dz$$

satisfies conditions 2 and 4.