Bengt
06/19/24

A follow-up to my 05/16/24 handout – improving the accuracy of the modified Padé approach for ${}_2F_1$ near the $z = 1$ singularity

Figure 1 below is reproduced from my 05/16/24 handout.

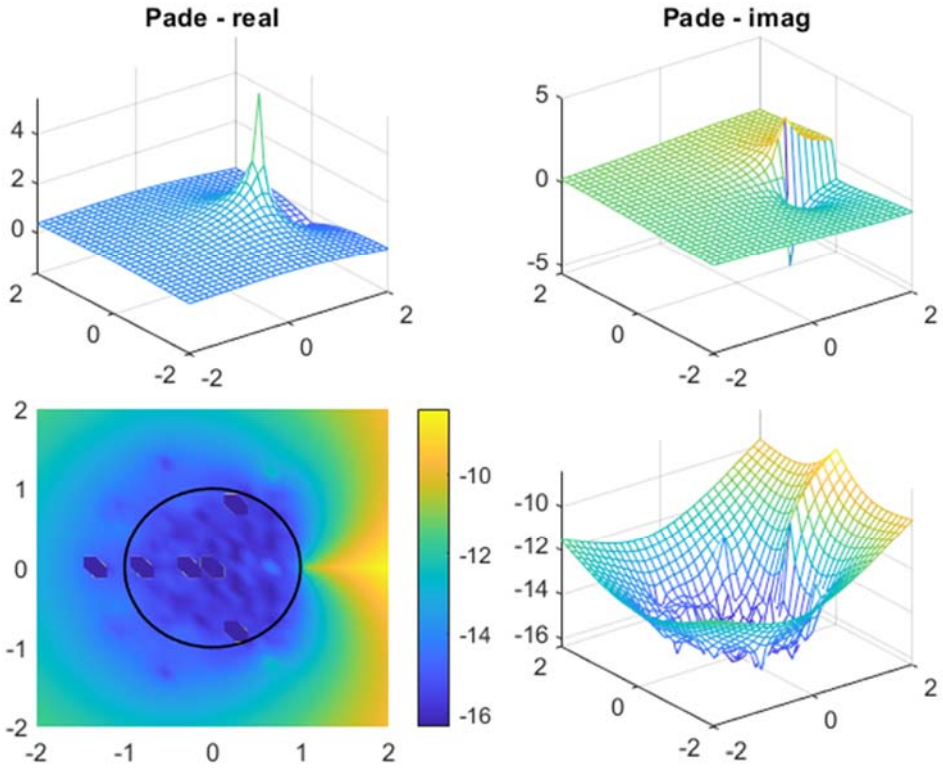

Figure 1. Results of a direct calculation (in double precision) using the modified Padé method. The bottom row of subplots shows the error compared to Matlab's hypergeom function. The unit circle is marked in the bottom left subplot.

It shows very good accuracy within the unit circle, however with a small loss near the singularity at $z = 1$. By use of the relation

$$
\begin{aligned}
{}_2F_1(a,b;c;z) \quad &= \frac{\Gamma(b-a)\Gamma(c)}{\Gamma(b)\Gamma(c-a)}(-z)^{-a}\,{}_2F_1(a,a-c+1;a-b+1;\frac{1}{z}) \\
&+ \frac{\Gamma(a-b)\Gamma(c)}{\Gamma(a)\Gamma(c-b)}(-z)^{-b}\,{}_2F_1(b,b-c+1;-a+b+1;\frac{1}{z})
\end{aligned}
\quad , \tag{1}
$$

each evaluation outside the unit circle can be replaced by two inside it, giving much improved results for $|z|>1$, as shown in this previous handout's Figure 2. The peak error became then quite small, and occurred at $z = 1$.

One new test just carried out was to use as comparison a quad precision code for hypergeom (from the Advanpix extended precision toolbox) rather than MATLAB's double precision version (from its symbolic toolbox). Apart from the former being much faster (in spite of its higher accuracy), it made no visually noticeable difference to the bottom two subplots of the previous handout's Figure 2, i.e., the peak error that was seen near $z = 1$ came from the

modified Padé calculation. The purpose of the present handout is to describe an improvement near this singularity point, based on the formula

$$
\begin{aligned}
{}_2F_1(a,b;c;z) \quad &= \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}\, z^{-a}\, {}_2F_1(a,a-c+1;a+b-c+1;1-\frac{1}{z}) \\
&+ \frac{\Gamma(c)\Gamma(a-b-c)}{\Gamma(a)\Gamma(b)} (1-z)^{c-a-b}\; z^{a-c}\, {}_2F_1(c-a,1-a;c-a-b+1;1-\frac{1}{z})
\end{aligned}
\tag{2}
$$

For z near to $z = 1$, this requires two evaluations of ${}_2F_1$ near the origin, i.e., where the modified Padé method has its highest accuracy. Figure 2 details the mapping $z \to 1-\frac{1}{z}$, showing in Part (a) in red a circle of radius 0.4 centered at $z = 1$ and in Part (b) the region surrounding the origin that this circle maps to – well inside the unit circle. Combining the mappings provided by (1) and (2), a z-value anywhere in the complex plane can be therefore evaluated by either one or two ${}_2F_1$ evaluations within the region shown in Figure 3. As seen in the bottom left subplot in Figure 1 of the 05/16/24 handout, the Padé method features excellent accuracy within this region.

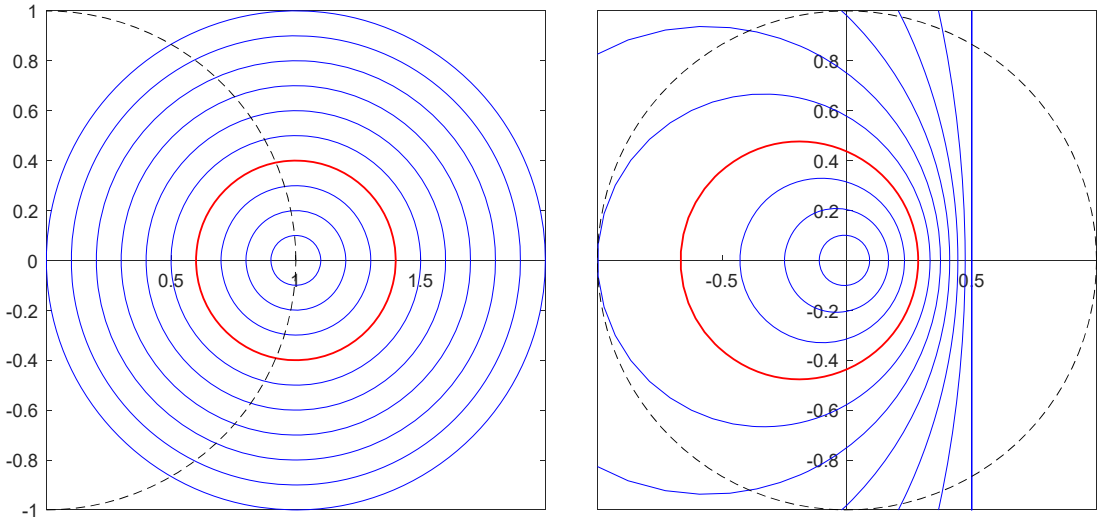

Figure 2. Left: The z-plane with circles of radii 0.1, 0.2, … , 1.0 centered at $z = 1$. Right: The images of these circles after the mapping $z \to 1-\frac{1}{z}$. In both subplots, the unit circle is shown dashed.

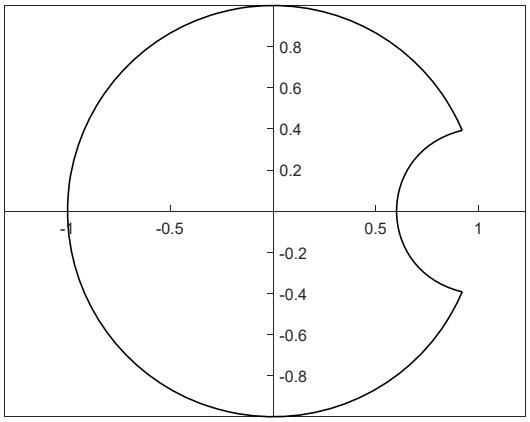

Figure 3. The inside of the displayed region shows all locations at which ${}_2F_1$ evaluations are needed in order to evaluate this function at any complex plane location.

The counterpart to Figure 1 now becomes as shown in Figure 4 (using here $n = 10$ terms in each Taylor expansion within the Padé method).

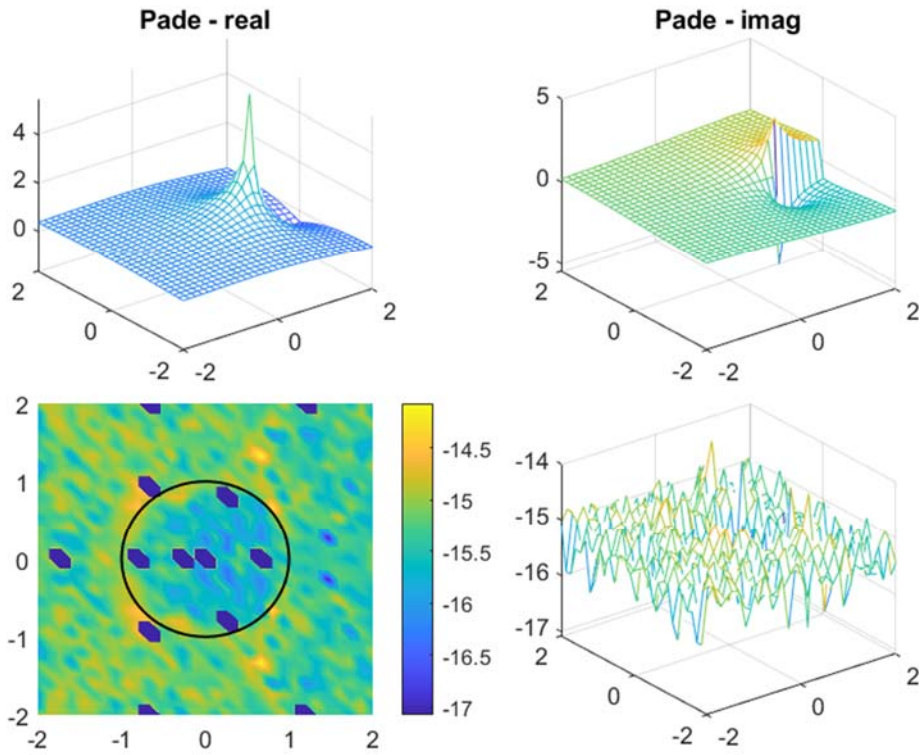

Figure 4. Results of a calculation (in double precision) using the modified Padé method in conjunction with equations (1), (2), as described in the text. There is now no visible hint of any accuracy irregularity surrounding $z = 1$.

Discussion:

I am starting to think that maybe two papers might be suitable relating to the Padé method:

1. The specific case of the Gauss hypergeometric function ${}_2F_1$, and
2. The general ${}_{p+1}F_p$ case.

One reason for separating in two cases is that, while (1) generalizes to all ${}_{p+1}F_p$ cases, I believe (2) is derived via the Pfaff transformation, which is specific to the $p = 1$ case. Accurate treatment of the $z = 1$ singularity might be considerably more involved in the case of general p. Also, the Gauss case is of great interest in its own.

The promising result in the bottom two subplots of Figure 4 needs to be verified for a wide range of parameter values. Of some concern is that the linear system that arises within the Padé algorithm typically is very ill conditioned. In the present test, MATLAB shows condition numbers around 10^{+20}, which easily could have destroyed all significant digits. It apparently hasn't, so there is something that needs to be understood here.

Comparisons need to be made against existing methods.

There is still the issue of Froissart doublets, which are poles with extremely small residue. In the present test case, several of these are located inside the unit circle, and would show up in the error plots if one would have happened to do an evaluation right at such a location. A possible (but not very elegant) remedy could be to test for these and, in the unlikely case of evaluating extremely close to one, instead using the average value from a few evaluation points for ex. on a small circle around that point. Another possible remedy would be to change the number of terms in each internal Taylor expansion (from, say, $n = 10$ to $n = 11$). That ought to have minimal effect on the overall accuracy, but these rare exceptional points would end up in completely different locations.