Algorithms for the Padé approximants used in HEPA Computation, again

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In the next pages is given another explanation for the algorithms used in HEPAComp. Hopefully someone reads it this time.

1 Padé approximant

Let $n = m = 3$. Let $Q_3(z)f(z) - P_3(z) = \mathcal{O}(z^7)$, where $f(z) = c_0 + c_1 z + c_2 z^2 + \ldots + c_6 z^6$.

1. HEPAComp solves the following matrix equation:

$$\begin{pmatrix} c_1 & c_2 & c_3 \\ c_2 & c_3 & c_4 \\ c_3 & c_4 & c_5 \end{pmatrix} \begin{pmatrix} q_3 \\ q_2 \\ q_1 \end{pmatrix} = \begin{pmatrix} -c_4 \\ -c_5 \\ -c_6 \end{pmatrix}.$$

We set $q_0 = 1$ and we obtain all coefficients of $Q_3(z)$, the denominator. The numerator is computed by the coefficients of $Q_3(z)$.

2. Another method to obtain the coefficients:

$$Q_3^*(z) = \begin{vmatrix} c_1 & c_2 & c_3 & c_4 \\ c_2 & c_3 & c_4 & c_5 \\ c_3 & c_4 & c_5 & c_6 \\ z^3 & z^2 & z & 1 \end{vmatrix}.$$

We obtain $Q_3^*(z)$, and after normalization it is equal to $Q_3(z)$:

$$Q_3^*(z)/q_0^* = Q_3(z).$$

3. We can generalize both of the above approaches by Equation 5.4 of [1, §8.5 Hermite-Padé polynomials]:

$$Q_3^*(z) = \begin{vmatrix} 1 & 0 & 0 & 0 & c_0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & c_1 & c_0 & 0 & 0 \\ 0 & 0 & 1 & 0 & c_2 & c_1 & c_0 & 0 \\ 0 & 0 & 0 & 1 & c_3 & c_2 & c_1 & c_0 \\ 0 & 0 & 0 & 0 & \boxed{c_4} & \boxed{c_3} & \boxed{c_2} & \boxed{c_1} \\ 0 & 0 & 0 & 0 & \boxed{c_5} & \boxed{c_4} & \boxed{c_3} & \boxed{c_2} \\ 0 & 0 & 0 & 0 & \boxed{c_6} & \boxed{c_5} & \boxed{c_4} & \boxed{c_3} \\ 0 & 0 & 0 & 0 & \boxed{1} & \boxed{z} & \boxed{z^2} & \boxed{z^3} \end{vmatrix}.$$

The matrix equation that HEPAComp solves is much smaller than the full determinant, while the result is the same. Computing the numerator:

$$P_3^*(z) = \begin{vmatrix} 1 & 0 & 0 & 0 & c_0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & c_1 & c_0 & 0 & 0 \\ 0 & 0 & 1 & 0 & c_2 & c_1 & c_0 & 0 \\ 0 & 0 & 0 & 1 & c_3 & c_2 & c_1 & c_0 \\ 0 & 0 & 0 & 0 & c_4 & c_3 & c_2 & c_1 \\ 0 & 0 & 0 & 0 & c_5 & c_4 & c_3 & c_2 \\ 0 & 0 & 0 & 0 & c_6 & c_5 & c_4 & c_3 \\ 1 & z & z^2 & z^3 & 0 & 0 & 0 & 0 \end{vmatrix}.$$

Normalization: $P_3^*(z)/p_0^* = P_3(z)/p_0$ ($p_0 = c_0$, but might not be equal to 1).

2 Hermite-Padé approximant

Let $n = m = l = 3$. Let $P_3(z) + Q_3(z)f(z) + R_3(z)g(z) = \mathcal{O}(z^{11})$, where:

$$f(z) = c_0 + c_1 z + c_2 z^2 + \ldots + c_{10} z^{10}, \quad g(z) = d_0 + d_1 z + d_2 z^2 + \ldots + d_{10} z^{10}.$$

1. HEPAComp solves the following matrix equation:

$$\begin{pmatrix} c_1 & c_2 & c_3 & c_4 & d_1 & d_2 & d_3 \\ c_2 & c_3 & c_4 & c_5 & d_2 & d_3 & d_4 \\ c_3 & c_4 & c_5 & c_6 & d_3 & d_4 & d_5 \\ c_4 & c_5 & c_6 & c_7 & d_4 & d_5 & d_6 \\ c_5 & c_6 & c_7 & c_8 & d_5 & d_6 & d_7 \\ c_6 & c_7 & c_8 & c_9 & d_6 & d_7 & d_8 \\ c_7 & c_8 & c_9 & c_{10} & d_7 & d_8 & d_9 \end{pmatrix} \begin{pmatrix} q_3 \\ q_2 \\ q_1 \\ q_0 \\ r_3 \\ r_2 \\ r_1 \end{pmatrix} = \begin{pmatrix} -d_4 \\ -d_5 \\ -d_6 \\ -d_7 \\ -d_8 \\ -d_9 \\ -d_{10} \end{pmatrix}.$$

We set $r_0 = 1$ and we obtain all coefficients of $Q_3(z)$ and $R_3(z)$. The coefficients of $P_3(z)$ are computed by the former ones.

2. Another method to obtain the coefficients:

$$R_3^*(z) = \begin{vmatrix} c_1 & c_2 & c_3 & c_4 & d_1 & d_2 & d_3 & d_4 \\ c_2 & c_3 & c_4 & c_5 & d_2 & d_3 & d_4 & d_5 \\ c_3 & c_4 & c_5 & c_6 & d_3 & d_4 & d_5 & d_6 \\ c_4 & c_5 & c_6 & c_7 & d_4 & d_5 & d_6 & d_7 \\ c_5 & c_6 & c_7 & c_8 & d_5 & d_6 & d_7 & d_8 \\ c_6 & c_7 & c_8 & c_9 & d_6 & d_7 & d_8 & d_9 \\ c_7 & c_8 & c_9 & c_{10} & d_7 & d_8 & d_9 & d_{10} \\ 0 & 0 & 0 & 0 & z^3 & z^2 & z & 1 \end{vmatrix}, \; Q_3^*(z) = \begin{vmatrix} c_1 & c_2 & c_3 & c_4 & d_1 & d_2 & d_3 & d_4 \\ c_2 & c_3 & c_4 & c_5 & d_2 & d_3 & d_4 & d_5 \\ c_3 & c_4 & c_5 & c_6 & d_3 & d_4 & d_5 & d_6 \\ c_4 & c_5 & c_6 & c_7 & d_4 & d_5 & d_6 & d_7 \\ c_5 & c_6 & c_7 & c_8 & d_5 & d_6 & d_7 & d_8 \\ c_6 & c_7 & c_8 & c_9 & d_6 & d_7 & d_8 & d_9 \\ c_7 & c_8 & c_9 & c_{10} & d_7 & d_8 & d_9 & d_{10} \\ z^3 & z^2 & z & 1 & 0 & 0 & 0 & 0 \end{vmatrix}.$$

After normalization we obatin the following formulas (we have $r_0 = 1$ and $q_0 \neq 1$):

$$R_3^*(z)/r_0^* = R_3(z), \quad Q_3^*(z)/q_0^* = Q_3(z)/q_0.$$

The coefficients of both polynomials can be obtained at once:

$$\Omega_7(z) = \begin{vmatrix} c_1 & c_2 & c_3 & c_4 & d_1 & d_2 & d_3 & d_4 \\ c_2 & c_3 & c_4 & c_5 & d_2 & d_3 & d_4 & d_5 \\ c_3 & c_4 & c_5 & c_6 & d_3 & d_4 & d_5 & d_6 \\ c_4 & c_5 & c_6 & c_7 & d_4 & d_5 & d_6 & d_7 \\ c_5 & c_6 & c_7 & c_8 & d_5 & d_6 & d_7 & d_8 \\ c_6 & c_7 & c_8 & c_9 & d_6 & d_7 & d_8 & d_9 \\ c_7 & c_8 & c_9 & c_{10} & d_7 & d_8 & d_9 & d_{10} \\ z^7 & z^6 & z^5 & z^4 & z^3 & z^2 & z & 1 \end{vmatrix}.$$

The result is:

$$\Omega_7(z) = q_3 z^7 + q_2 z^6 + q_1 z^5 + q_0 z^4 + r_3 z^3 + r_2 z^2 + r_1 z + r_0.$$

Then the coefficients are split and assigned their proper polynomials. This is analogous to the matrix equation. All these formulas have been verified by a computer program.

3. As above, we can generalize both approaches by Equation 5.4 of [1, §8.5 Hermite-Padé polynomials]:

$$R_3^*(z) = \begin{vmatrix} 1 & 0 & 0 & 0 & c_0 & 0 & 0 & 0 & d_0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & c_1 & c_0 & 0 & 0 & d_1 & d_0 & 0 & 0 \\ 0 & 0 & 1 & 0 & c_2 & c_1 & c_0 & 0 & d_2 & d_1 & d_0 & 0 \\ 0 & 0 & 0 & 1 & c_3 & c_2 & c_1 & c_0 & d_3 & d_2 & d_1 & d_0 \\ 0 & 0 & 0 & 0 & c_4 & c_3 & c_2 & c_1 & d_4 & d_3 & d_2 & d_1 \\ 0 & 0 & 0 & 0 & c_5 & c_4 & c_3 & c_2 & d_5 & d_4 & d_3 & d_2 \\ 0 & 0 & 0 & 0 & c_6 & c_5 & c_4 & c_3 & d_6 & d_5 & d_4 & d_3 \\ 0 & 0 & 0 & 0 & c_7 & c_6 & c_5 & c_4 & d_7 & d_6 & d_5 & d_4 \\ 0 & 0 & 0 & 0 & c_8 & c_7 & c_6 & c_5 & d_8 & d_7 & d_6 & d_5 \\ 0 & 0 & 0 & 0 & c_9 & c_8 & c_7 & c_6 & d_9 & d_8 & d_7 & d_6 \\ 0 & 0 & 0 & 0 & c_{10} & c_9 & c_8 & c_7 & d_{10} & d_9 & d_8 & d_7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & z & z^2 & z^3 \end{vmatrix}.$$

We have analogous formulas for $Q_3^*(z)$ and $\Omega_7(z)$. The matrix equation that HEPAComp solves is a lot smaller than the full determinant, of course the result is the same.

Finally:

$$P_3^*(z) = \begin{vmatrix} 1 & 0 & 0 & 0 & c_0 & 0 & 0 & 0 & d_0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & c_1 & c_0 & 0 & 0 & d_1 & d_0 & 0 & 0 \\ 0 & 0 & 1 & 0 & c_2 & c_1 & c_0 & 0 & d_2 & d_1 & d_0 & 0 \\ 0 & 0 & 0 & 1 & c_3 & c_2 & c_1 & c_0 & d_3 & d_2 & d_1 & d_0 \\ 0 & 0 & 0 & 0 & c_4 & c_3 & c_2 & c_1 & d_4 & d_3 & d_2 & d_1 \\ 0 & 0 & 0 & 0 & c_5 & c_4 & c_3 & c_2 & d_5 & d_4 & d_3 & d_2 \\ 0 & 0 & 0 & 0 & c_6 & c_5 & c_4 & c_3 & d_6 & d_5 & d_4 & d_3 \\ 0 & 0 & 0 & 0 & c_7 & c_6 & c_5 & c_4 & d_7 & d_6 & d_5 & d_4 \\ 0 & 0 & 0 & 0 & c_8 & c_7 & c_6 & c_5 & d_8 & d_7 & d_6 & d_5 \\ 0 & 0 & 0 & 0 & c_9 & c_8 & c_7 & c_6 & d_9 & d_8 & d_7 & d_6 \\ 0 & 0 & 0 & 0 & c_{10} & c_9 & c_8 & c_7 & d_{10} & d_9 & d_8 & d_7 \\ 1 & z & z^2 & z^3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}.$$

Normalization: $P_3^*(z)/p_0^* = P_3(z)/p_0$.

References

[1] George A. Baker, Jr., Peter Graves-Morris, *Padé approximants*, Second Edition, Cambridge University Press, New York, 1996.