1

Introduction and definitions

1.1 Introduction and notational conventions

Suppose that we are given a power series $\sum_{i=0}^{\infty} c_i z^i$, representing a function $f(z)$, so that

$$f(z) = \sum_{i=0}^{\infty} c_i z^i. \tag{1.1}$$

This expansion is the fundamental starting point of any analysis using Padé approximants. Throughout this work we reserve the notation $c_i = 0, 1, 2, \ldots$, for the given set of coefficients, and $f(z)$ is the associated function. A Padé approximant is a rational fraction

$$[L/M] = \frac{a_0 + a_1 z + \cdots + a_L z^L}{b_0 + b_1 z + \cdots + b_M z^M} \tag{1.2}$$

which has a Maclaurin expansion which agrees with (1.1) as far as possible. We give a more complete and precise definition of Padé approximants in Section 1.4. Notice that in (1.2) there are $L+1$ numerator coefficients and $M+1$ denominator coefficients. There is a more or less irrelevant common factor between them, and for definiteness we take $b_0 = 1$. This choice turns out to be an essential part of the precise definition, and (1.2) is our conventional notation with this choice for b_0. So there are $L+1$ independent numerator coefficients and M independent denominator coefficients, making $L+M+1$ unknown coefficients in all. This number suggests that normally the $[L/M]$ ought to fit the power series (1.1) through the orders $1, z, z^2, \ldots, z^{L+M}$. In the notation of formal power series,

$$\sum_{i=0}^{\infty} c_i z^i = \frac{a_0 + a_1 z + \cdots + a_L z^L}{b_0 + b_1 z + \cdots + b_M z^M} + O(z^{L+M+1}). \tag{1.3}$$

Example

$$f(z) = 1 - \tfrac{1}{2}z + \tfrac{1}{3}z^2 + \cdots.$$

$$[1/0] = 1 - \tfrac{1}{2}z = f(z) + O(z^2),$$

$$[0/1] = \frac{1}{1 + \frac{1}{2}z} = f(z) + O(z^2),$$

$$[1/1] = \frac{1 + \frac{1}{6}z}{1 + \frac{2}{3}z} = f(z) + O(z^3).$$

Returning to (1.3) and cross-multiplying, we find that

$$(b_0 + b_1 z + \cdots + b_M z^M)(c_0 + c_1 z + \cdots) = a_0 + a_1 z + \cdots + a_L z^L + O(z^{L+M+1}) \qquad (1.4)$$

Equating the coefficients of $z^{L+1}, z^{L+2}, \ldots, z^{L+M}$, we find

$$\begin{aligned} b_M c_{L-M+1} + b_{M-1} c_{L-M+2} + \cdots + b_0 c_{L+1} &= 0, \\ b_M c_{L-M+2} + b_{M-1} c_{L-M+3} + \cdots + b_0 c_{L+2} &= 0, \\ &\ \vdots \\ b_M c_L \quad + b_{M-1} c_{L+1} \quad + \cdots + b_0 c_{L+M} &= 0. \end{aligned} \qquad (1.5)$$

If $j < 0$, we define $c_j = 0$ for consistency. Since $b_0 = 1$, Equations (1.5) become a set of M linear equations for the M unknown denominator coefficients:

$$\begin{bmatrix} c_{L-M+1} & c_{L-M+2} & c_{L-M+3} & \cdots & c_L \\ c_{L-M+2} & c_{L-M+3} & c_{L-M+4} & \cdots & c_{L+1} \\ c_{L-M+3} & c_{L-M+4} & c_{L-M+5} & \cdots & c_{L+2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_L & c_{L+1} & c_{L+2} & \cdots & c_{L+M-1} \end{bmatrix} \begin{bmatrix} b_M \\ b_{M-1} \\ b_{M-2} \\ \vdots \\ b_1 \end{bmatrix} = -\begin{bmatrix} c_{L+1} \\ c_{L+2} \\ c_{L+3} \\ \vdots \\ c_{L+M} \end{bmatrix}, \qquad (1.6)$$

from which the b_i may be found. The numerator coefficients, $a_0, a_1, \ldots, a_L$, follow immediately from (1.4) by equating the coefficients $1, z, z^2, \ldots, z^L$:

$$
\begin{aligned}
a_0 &= c_0, \\
a_1 &= c_1 + b_1 c_0, \\
a_2 &= c_2 + b_1 c_1 + b_2 c_0, \\
&\ \vdots \\
a_L &= c_L + \sum_{i=1}^{\min(L,M)} b_i c_{L-i}.
\end{aligned} \tag{1.7}
$$

Thus (1.6) and (1.7) normally determine the Padé numerator and denominator and are called the Padé equations; we have constructed an $[L/M]$ Padé approximant which agrees with $\sum_{i=0}^{\infty} c_i z^i$ through order z^{L+M}. Because the starting point of these manipulations is the given power series, we do not ever need to know about the existence of any function $f(z)$ with $\sum_{i=0}^{\infty} c_i z^i$ as its Maclaurin series, as in (1.1). Of course, we expect that a well-chosen sequence of Padé approximants will normally approximate a function $f(z)$ with the Maclaurin expansion $\sum_{i=0}^{\infty} c_i z^i$, but it is important to distinguish between problems of convergence of Padé approximants and problems of construction of Padé approximants. Given the power series, (1.6) and (1.7) show how the Padé approximants are constructed.

Every power series has a circle of convergence $|z| = R$. If $|z| < R$, the series converges, and if $|z| > R$, it does not. If $R = \infty$, the power series represents an analytic function (functions analytic everywhere we often call *entire*) and the series may be summed directly for any value of z to yield the function $f(z)$. If $R = 0$, the power series is undoubtedly formal. It contains information about $f(z)$, but just how this information is to be used is not immediately clear. However, if a sequence of Padé approximants of the formal power series converges to a function of $g(z)$ for $z \in \mathfrak{D}$, then we may reasonably conclude that $g(z)$ is a function with the given power series. In certain circumstances (see Chapter 5) we make such statements precise and prove them. Nevertheless, in this book we will not be hampered by a lack of rigorous justification of any technique, and empirical convergence is regarded as entirely satisfactory within its limitations. If the given power series converges to the same function for $|z| < R$ with $0 < R < \infty$, then a sequence of Padé approximants may converge for $z \in \mathfrak{D}$ where $\mathfrak{D}$ is a domain larger than $|z| < R$. We will then have extended our domain of convergence. This is frequently a practical approach to what amounts to analytic continuation. The method of expansion and reexpansion due to Weierstrass is more suited to principle than practice. As an example of how well Padé approximants may work in their natural context, we consider an example.

Example

$$f(z) = \sqrt{\frac{1+\frac{1}{2}z}{1+2z}} = 1 - \tfrac{3}{4}z + \tfrac{39}{32}z^2 - \cdots.$$

To calculate [1/1], Equation (1.6) becomes

$$(-\tfrac{3}{4})b_1 = -\tfrac{39}{32},$$

and so $b_1 = \frac{13}{8}$. Equation (1.7) gives $a_0 = 1$ and $a_1 = \frac{7}{8}$, with the check

$$(1 + \tfrac{13}{8}z)(1 - \tfrac{3}{4}z + \tfrac{39}{32}z^2) = 1 + \tfrac{7}{8}z + O(z^3).$$

Hence

$$[1/1] = \frac{1+\frac{7}{8}z}{1+\frac{13}{8}z},$$

and in Figure 1.1.1 we compare this with $f(z)$ for $z \geqslant 0$. In particular, $f(\infty) = 0.5$ and $[1/1](\infty) = \frac{7}{13} = 0.54 \ldots$, giving 8% accuracy at infinity. This example shows remarkable accuracy for a function with a radius of convergence of $\frac{1}{2}$, using just three terms of the series.

There is one feature of the calculation of Padé approximations to be emphasized at the start—these calculations require more numerical accuracy than one might at first expect. The Padé approximant exploits the differences of the coefficients to do its long-range extrapolation, and so the differences must all be accurate. We consider the problem of deciding how much numerical accuracy is needed to calculate an $[L/M]$ Padé approximant in Section 2.1.

Thus far, we have assumed that Padé approximants are calculated directly from (1.6) and (1.7) without implying any particular method. If Cramer's rule is used, we may calculate $b_0{:}b_1{:}\cdots{:}b_M$ from (1.6) and hence the denominator of (1.2). Aside from a common factor, the result is

$$Q^{[L/M]}(z) = \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_L & c_{L+1} \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+1} & c_{L+2} \\ \vdots & \vdots & & \vdots & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-2} & c_{L+M-1} \\ c_L & c_{L+1} & \cdots & c_{L+M-1} & c_{L+M} \\ z^M & z^{M-1} & \cdots & z & 1 \end{vmatrix}. \tag{1.8}$$

We take (1.8) to define $Q^{[L/M]}(z)$ and use this convention throughout. Again, recall that $c_j = 0$ if $j < 0$. Now consider

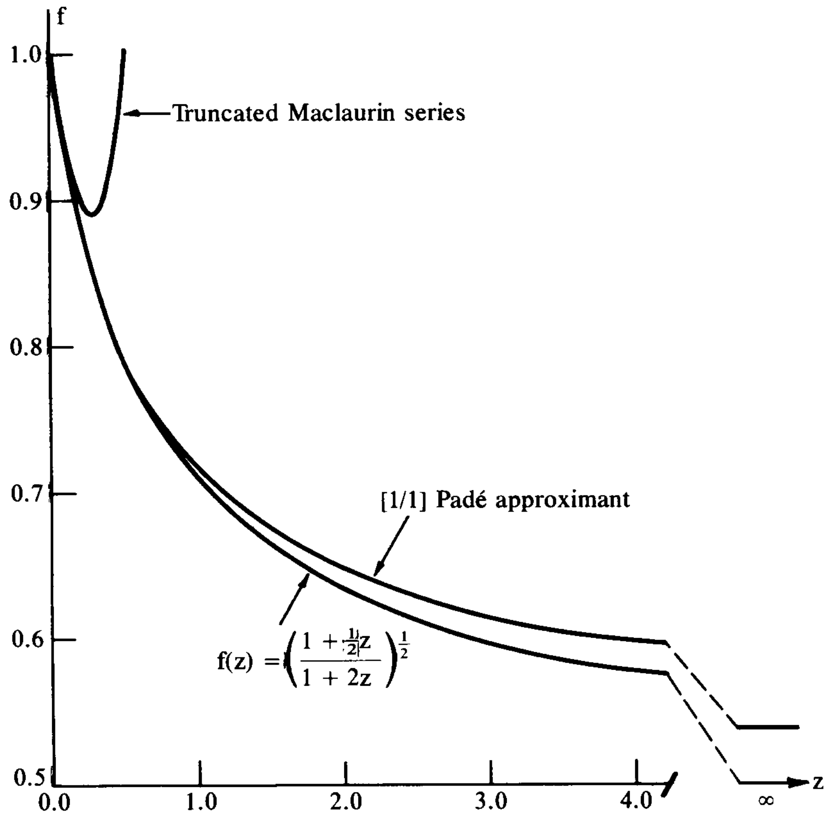

Figure 1.1.1. Values of $f(z) = \sqrt{(1+z/2)/(1+2z)}$, its [1/1] Padé approximant, and its truncated Maclaurin series, $1 - 3z/4 + 39z^2/32$.

$$Q^{[L/M]}(z)\sum_{i=0}^{\infty} c_i z^i = \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_{L+1} \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+2} \\ \vdots & \vdots & & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-1} \\ c_L & c_{L+1} & \cdots & c_{L+M} \\ \sum_{i=0}^{\infty} c_i z^{M+i} & \sum_{i=0}^{\infty} c_i z^{M+i-1} & \cdots & \sum_{i=0}^{\infty} c_i z^i \end{vmatrix}.$$

By subtracting z^{L+1} times the first row from the last, z^{L+2} times the second row from the last, etc., up to z^{L+M} times the penultimate row from the last, we reduce the series in the last row. They become lacunary series, with a gap of M terms missing. Using the initial terms of these series, we define

$$P^{[L/M]}(z) = \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_{L+1} \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+2} \\ \vdots & \vdots & & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-1} \\ c_L & c_{L+1} & \cdots & c_{L+M} \\ \sum_{i=0}^{L-M} c_i z^{M+i} & \sum_{i=0}^{L-M+1} c_i z^{M+i-1} & \cdots & \sum_{i=0}^{L} c_i z^i \end{vmatrix}. \tag{1.9}$$

Again, (1.9) is our notational convention. We now prove our first theorem.

***Theorem* 1.1.1.** *With the definitions* (1.8) *and* (1.9),

$$Q^{[L/M]}(z)\sum_{i=0}^{\infty} c_i z^i - P^{[L/M]}(z) = O(z^{L+M+1}). \tag{1.10}$$

Proof. We note that $\deg\{P^{[L/M]}\} \leqslant L$, $\deg\{Q^{[L/M]}\} \leqslant M$ and that the remainder is

$$Q^{[L/M]}(z)\sum_{i=0}^{\infty} c_i z^i - P^{[L/M]}(z)$$

$$= \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_{L+1} \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+2} \\ \vdots & \vdots & & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-1} \\ c_L & c_{L+1} & \cdots & c_{L+M} \\ \sum_{i=L+1}^{\infty} c_i z^{M+i} & \sum_{i=L+2}^{\infty} c_i z^{M+i-1} & \cdots & \sum_{i=L+M+1}^{\infty} c_i z^i \end{vmatrix}$$

$$= \sum_{i=1}^{\infty} z^{L+M+i} \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_{L+1} \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+2} \\ \vdots & \vdots & & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-1} \\ c_L & c_{L+1} & \cdots & c_{L+M} \\ c_{L+i} & c_{L+i+1} & \cdots & c_{L+M+i} \end{vmatrix}. \tag{1.11}$$

Equation (1.11) is occasionally a useful form for the error using Padé approximation. Equation (1.10) goes a long way towards satisfying (1.3). To this end, consider

$$Q^{[L/M]}(0) = \begin{vmatrix} c_{L-M+1} & c_{L-M+2} & \cdots & c_L \\ c_{L-M+2} & c_{L-M+3} & \cdots & c_{L+1} \\ \vdots & \vdots & & \vdots \\ c_{L-1} & c_L & \cdots & c_{L+M-2} \\ c_L & c_{L+1} & \cdots & c_{L+M-1} \end{vmatrix}.$$

This is called a Hankel determinant, because of the systematic way in which its rows are formed from the given coefficients c_j. Notice that if $Q^{[L/M]}(0) \neq 0$, then the linear equations (1.6) are nonsingular and the solution given by (1.8) is unambiguous. Furthermore, we may divide (1.10) by $Q^{[L/M]}(z)$, yielding

$$\sum_{i=0}^{\infty} c_i z^i - \frac{P^{[L/M]}(z)}{Q^{[L/M]}(z)} = O(z^{L+M+1}).$$

This result has proved our second theorem:

***Theorem* 1.1.2 [Jacobi, 1846].** *With the definitions* (1.8) *and* (1.9), *the* $[L/M]$ *Padé approximant of* $\sum_{i=0}^{\infty} c_i z^i$ *is given by*

$$[L/M] = \frac{P^{[L/M]}(z)}{Q^{[L/M]}(z)} \tag{1.12}$$

provided $Q^{[L/M]}(0) \neq 0$.

The only difficulties, which we defer to Section 1.4, are those occurring when $Q^{[L/M]}(0) = 0$. We extend the notation $[L/M]$ of (1.12) as $[L/M]_f$ to emphasize approximation of $f(z)$, and as $[L/M](z)$ to emphasize the z-dependence. We will thus have the various forms

$$[L/M] = [L/M]_f = [L/M](z) = [L/M]_f(z)$$

available for convenience. It is common practice to display the approximants in a table, called the Padé table, shown as Table 1.1.1. Among other things, we prove in Section 1.2 that part of the Padé table of $\exp(z)$ is given by the entries in Table 1.1.2.

Table 1.1.1. *The Padé table.*

M \ L	0	1	2	$\cdots$
0	[0/0]	[1/0]	[2/0]	$\cdots$
1	[0/1]	[1/1]	[2/1]	$\cdots$
2	[0/2]	[1/2]	[2/2]	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

Table 1.1.2. *Part of the Padé table of* exp(z) *[Padé, 1892].*

$M \backslash L$	0	1	2
0	$\dfrac{1}{1}$	$\dfrac{1+z}{1}$	$\dfrac{2+2z+z^2}{2}$
1	$\dfrac{1}{1-z}$	$\dfrac{2+z}{2-z}$	$\dfrac{6+4z+z^2}{6-2z}$
2	$\dfrac{2}{2-2z+z^2}$	$\dfrac{6+2z}{6-4z+z^2}$	$\dfrac{12+6z+z^2}{12-6z+z^2}$

1.2 Padé approximants to the exponential function

The coefficients c_i of the Maclaurin expansion of the exponential function are sufficiently simple that explicit forms of the numerator and denominator of the Padé approximants can be found. In this section we will calculate the denominator $Q^{[L/M]}(z)$. The numerator follows by an extremely simple and elegant trick, based on the identity $\exp(-z) = 1/\exp(z)$, and this derivation is discussed in Section 1.5. Padé, in his thesis, elaborated the properties of his approximants with special emphasis on the example of the exponential function: it is a beautiful example of how the approximants work in an ideal situation. Further properties of Padé approximants of $\exp(z)$ are to be found in Section 4.6, Section 5.7, and Sections 10.3–10.4.

Our task is to calculate

$$Q^{[L/M]}(z) = \begin{vmatrix} \dfrac{1}{(L-M+1)!} & \dfrac{1}{(L-M+2)!} & \cdots & \dfrac{1}{L!} & \dfrac{1}{(L+1)!} \\ \dfrac{1}{(L-M+2)!} & \dfrac{1}{(L-M+3)!} & \cdots & \dfrac{1}{(L+1)!} & \dfrac{1}{(L+2)!} \\ \vdots & \vdots & & \vdots & \vdots \\ \dfrac{1}{L!} & \dfrac{1}{(L+1)!} & \cdots & \dfrac{1}{(L+M-1)!} & \dfrac{1}{(L+M)!} \\ z^M & z^{M-1} & \cdots & z & 1 \end{vmatrix}. \tag{2.1}$$

It is easier to begin with the constant term in (2.1), and so we define $C(L/M) \equiv Q^{[L/M]}(0)$, which is the coefficient of the '1' in the lower right-hand corner of (2.1),

$$C(L/M) = \begin{vmatrix} \dfrac{1}{(L-M+1)!} & \dfrac{1}{(L-M+2)!} & \cdots & \dfrac{1}{L!} \\ \dfrac{1}{(L-M+2)!} & \dfrac{1}{(L-M+3)!} & \cdots & \dfrac{1}{(L+1)!} \\ \vdots & \vdots & & \vdots \\ \dfrac{1}{L!} & \dfrac{1}{(L+1)!} & \cdots & \dfrac{1}{(L+M-1)!} \end{vmatrix}. \tag{2.2}$$

We assume that $L \geqslant M-1$. If this condition does not hold, the factorial functions must be suitably reinterpreted as gamma functions for the analysis to be valid. We remove the denominators from each row, by defining

$$p = \prod_{i=1}^{M} \frac{1}{(L+i-1)!},$$

and then

$$C(L/M) = p \cdot \begin{vmatrix} \dfrac{L!}{(L-M+1)!} & \dfrac{L!}{(L-M+2)!} & \cdots & L & 1 \\ \dfrac{(L+1)!}{(L-M+2)!} & \dfrac{(L+1)!}{(L-M+3)!} & \cdots & L+1 & 1 \\ \vdots & \vdots & & \vdots & \vdots \\ \dfrac{(L+M-1)!}{L!} & \dfrac{(L+M-1)!}{(L+1)!} & \cdots & L+M-1 & 1 \end{vmatrix}. \tag{2.3}$$

In (2.3), the determinant has M rows. Subtract the $(M-1)$th row from the Mth, then the $(M-2)$th row from the $(M-1)$th, etc. The identity

$$\frac{r!}{s!} - \frac{(r-1)!}{(s-1)!} = (r-s)\frac{(r-1)!}{s!} \tag{2.4}$$

is used repeatedly. In column 1 of (2.3), $r-s=M-1$; in column 2, $r-s=M-2$; etc., and so one finds that

$$C(L/M)=p(M-1)!\begin{vmatrix} \frac{L!/(M-1)}{(L-M+1)!} & \frac{L!/(M-2)}{(L-M+2)!} & \cdots & L & 1 \\ \frac{L!}{(L-M+2)!} & \frac{L!}{(L-M+3)!} & \cdots & 1 & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ \frac{(L+M-2)!}{L!} & \frac{(L+M-2)!}{(L+1)!} & \cdots & 1 & 0 \end{vmatrix}$$

$$= p(-)^{M-1}(M-1)!\begin{vmatrix} \frac{L!}{(L-M+2)!} & \frac{L!}{(L-M+3)!} & \cdots & 1 \\ \frac{(L+1)!}{(L-M+3)!} & \frac{(L+1)!}{(L-M+4)!} & \cdots & 1 \\ \vdots & \vdots & & \vdots \\ \frac{(L+M-2)!}{L!} & \frac{(L+M-2)!}{(L+1)!} & \cdots & 1 \end{vmatrix}. \tag{2.5}$$

This is a $(M-1)\times(M-1)$ determinant with a form identical to (2.3) but with M replaced by $M-1$. Consequently, an obvious inductive argument shows that

$$\begin{aligned} C(L/M) &= p\cdot\prod_{i=1}^{M}(-1)^{i-1}(i-1)! \\ &= (-1)^{M(M-1)/2}\prod_{i=1}^{M}\frac{(i-1)!}{(L+i-1)!}. \end{aligned} \tag{2.6}$$

Thus, for the case $M=1$,

$$C(L/1)=\frac{1}{L!},$$

and for the case $M=2$,