```
INTEGER NMANY,NFEW
REAL e(NMANY),d(NFEW),c(NMANY),a,b
   Economize NMANY power series coefficients e(1:NMANY) in the range (a,b) into NFEW
   coefficients d(1:NFEW).
call pcshft((-2.-b-a)/(b-a),(2.-b-a)/(b-a),e,NMANY)
call pccheb(e,c,NMANY)
...
   Here one would normally examine the Chebyshev coefficients c(1:NMANY) to decide how
   small NFEW can be.
call chebpc(c,d,NFEW)
call pcshft(a,b,d,NFEW)
```

In our example, by the way, the 8th through 10th Chebyshev coefficients turn out to be on the order of -7×10^{-6}, 3×10^{-7}, and -9×10^{-9}, so reasonable truncations (for single precision calculations) are somewhere in this range, yielding a polynomial with 8 – 10 terms instead of the original 13.

Replacing a 13-term polynomial with a (say) 10-term polynomial without any loss of accuracy — that does seem to be getting something for nothing. Is there some magic in this technique? Not really. The 13-term polynomial defined a function $f(x)$. Equivalent to economizing the series, we could instead have evaluated $f(x)$ at enough points to construct its Chebyshev approximation in the interval of interest, by the methods of §5.8. We would have obtained just the same lower-order polynomial. The principal lesson is that the rate of convergence of Chebyshev coefficients has nothing to do with the rate of convergence of power series coefficients; and it is the *former* that dictates the number of terms needed in a polynomial approximation. A function might have a *divergent* power series in some region of interest, but if the function itself is well-behaved, it will have perfectly good polynomial approximations. These can be found by the methods of §5.8, but *not* by economization of series. There is slightly less to economization of series than meets the eye.

CITED REFERENCES AND FURTHER READING:

Acton, F.S. 1970, *Numerical Methods That Work*; 1990, corrected edition (Washington: Mathematical Association of America), Chapter 12.

Arfken, G. 1970, *Mathematical Methods for Physicists*, 2nd ed. (New York: Academic Press), p. 631. [1]

5.12 Padé Approximants

A *Padé approximant*, so called, is that rational function (of a specified order) whose power series expansion agrees with a given power series to the highest possible order. If the rational function is

$$R(x) \equiv \frac{\sum_{k=0}^{M} a_k x^k}{1 + \sum_{k=1}^{N} b_k x^k} \tag{5.12.1}$$

then $R(x)$ is said to be a Padé approximant to the series

$$f(x) \equiv \sum_{k=0}^{\infty} c_k x^k \tag{5.12.2}$$

if

$$R(0) = f(0) \tag{5.12.3}$$

and also

$$\frac{d^k}{dx^k}R(x)\bigg|_{x=0} = \frac{d^k}{dx^k}f(x)\bigg|_{x=0}, \qquad k = 1, 2, \dots, M+N \tag{5.12.4}$$

Equations (5.12.3) and (5.12.4) furnish $M + N + 1$ equations for the unknowns $a_0, \dots, a_M$ and $b_1, \dots, b_N$. The easiest way to see what these equations are is to equate (5.12.1) and (5.12.2), multiply both by the denominator of equation (5.12.1), and equate all powers of x that have either a's or b's in their coefficients. If we consider only the special case of a diagonal rational approximation, $M = N$ (cf. §3.2), then we have $a_0 = c_0$, with the remaining a's and b's satisfying

$$\sum_{m=1}^{N} b_m c_{N-m+k} = -c_{N+k}, \qquad k = 1, \dots, N \tag{5.12.5}$$

$$\sum_{m=0}^{k} b_m c_{k-m} = a_k, \qquad k = 1, \dots, N \tag{5.12.6}$$

(note, in equation 5.12.1, that $b_0 = 1$). To solve these, start with equations (5.12.5), which are a set of linear equations for all the unknown b's. Although the set is in the form of a Toeplitz matrix (compare equation 2.8.8), experience shows that the equations are frequently close to singular, so that one should not solve them by the methods of §2.8, but rather by full LU decomposition. Additionally, it is a good idea to refine the solution by iterative improvement (routine `mprove` in §2.5) [1].

Once the b's are known, then equation (5.12.6) gives an explicit formula for the unknown a's, completing the solution.

Padé approximants are typically used when there is some unknown underlying function $f(x)$. We suppose that you are able somehow to compute, perhaps by laborious analytic expansions, the values of $f(x)$ and a few of its derivatives at $x = 0$: $f(0)$, $f'(0)$, $f''(0)$, and so on. These are of course the first few coefficients in the power series expansion of $f(x)$; but they are not necessarily getting small, and you have no idea where (or whether) the power series is convergent.

By contrast with techniques like Chebyshev approximation (§5.8) or economization of power series (§5.11) that only condense the information that you already know about a function, Padé approximants can give you genuinely new information about your function's values. It is sometimes quite mysterious how well this can work. (Like other mysteries in mathematics, it relates to *analyticity*.) An example will illustrate.

Imagine that, by extraordinary labors, you have ground out the first five terms in the power series expansion of an unknown function $f(x)$,

$$f(x) \approx 2 + \frac{1}{9}x + \frac{1}{81}x^2 - \frac{49}{8748}x^3 + \frac{175}{78732}x^4 + \cdots \tag{5.12.7}$$

(It is not really necessary that you know the coefficients in exact rational form — numerical values are just as good. We here write them as rationals to give you the impression that they derive from some side analytic calculation.) Equation (5.12.7) is plotted as the curve labeled "power series" in Figure 5.12.1. One sees that for $x \gtrsim 4$ it is dominated by its largest, quartic, term.

We now take the five coefficients in equation (5.12.7) and run them through the routine `pade` listed below. It returns five rational coefficients, three a's and two b's, for use in equation (5.12.1) with $M = N = 2$. The curve in the figure labeled "Padé" plots the resulting rational function. Note that both solid curves derive from the *same* five original coefficient values.

To evaluate the results, we need *Deus ex machina* (a useful fellow, when he is available) to tell us that equation (5.12.7) is in fact the power series expansion of the function

$$f(x) = [7 + (1+x)^{4/3}]^{1/3} \tag{5.12.8}$$

which is plotted as the dotted curve in the figure. This function has a branch point at $x = -1$, so its power series is convergent only in the range $-1 < x < 1$. In most of the range shown in the figure, the series is divergent, and the value of its truncation to five terms is

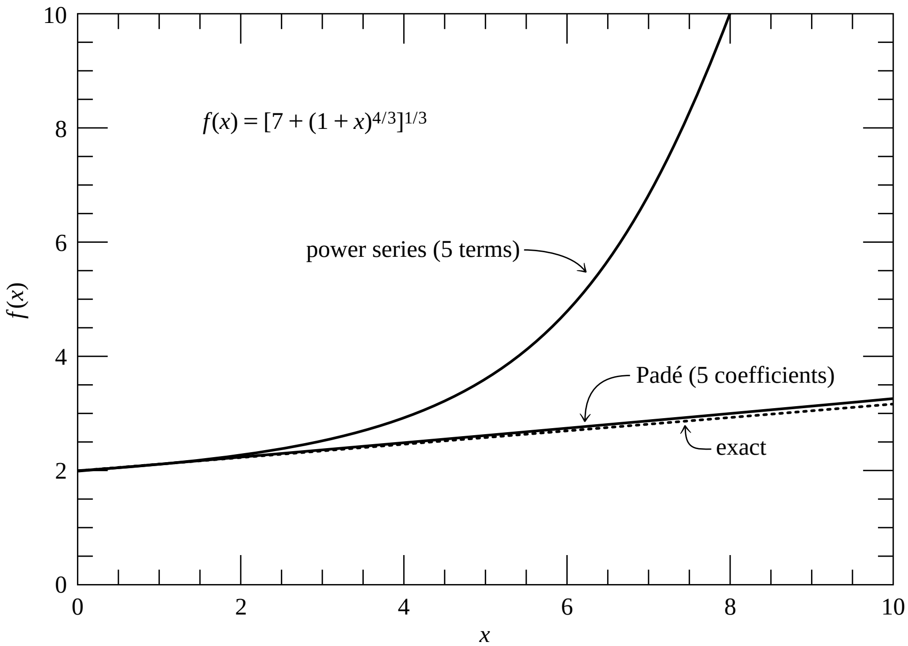

Figure 5.12.1. The five-term power series expansion and the derived five-coefficient Padé approximant for a sample function $f(x)$. The full power series converges only for $x < 1$. Note that the Padé approximant maintains accuracy far outside the radius of convergence of the series.

rather meaningless. Nevertheless, those five terms, converted to a Padé approximant, give a remarkably good representation of the function up to at least $x \sim 10$.

Why does this work? Are there not other functions with the same first five terms in their power series, but completely different behavior in the range (say) $2 < x < 10$? Indeed there are. Padé approximation has the uncanny knack of picking the function *you had in mind* from among all the possibilities. *Except when it doesn't!* That is the downside of Padé approximation: it is uncontrolled. There is, in general, no way to tell how accurate it is, or how far out in x it can usefully be extended. It is a powerful, but in the end still mysterious, technique.

Here is the routine that gets a's and b's from your c's. Note that the routine is specialized to the case $M = N$, and also that, on output, the rational coefficients are arranged in a format for use with the evaluation routine `ratval` (§5.3). (Also for consistency with that routine, the array of c's is passed in double precision.)

```
      SUBROUTINE pade(cof,n,resid)
      INTEGER n,NMAX
      REAL resid,BIG
      DOUBLE PRECISION cof(2*n+1)       For consistency with ratval.
      PARAMETER (NMAX=20,BIG=1.E30)     Max expected value of n, and a big number.
C     USES lubksb,ludcmp,mprove
         Given cof(1:2*n+1), the leading terms in the power series expansion of a function, solve
         the linear Padé equations to return the coefficients of a diagonal rational function approx-
         imation to the same function, namely (cof(1) + cof(2)x + ··· + cof(n+1)x^N)/(1 +
         cof(n+2)x + ··· + cof(2*n+1)x^N). The value resid is the norm of the residual vector;
         a small value indicates a well-converged solution.
      INTEGER j,k,indx(NMAX)
      REAL d,rr,rrold,sum,q(NMAX,NMAX),qlu(NMAX,NMAX),x(NMAX),
     *     y(NMAX),z(NMAX)
      do 12 j=1,n                       Set up matrix for solving.
         x(j)=cof(n+j+1)
```

```
        y(j)=x(j)
        do 11 k=1,n
            q(j,k)=cof(j-k+n+1)
            qlu(j,k)=q(j,k)
        enddo 11
    enddo 12
    call ludcmp(qlu,n,NMAX,indx,d)      Solve by LU decomposition and backsubstitution.
    call lubksb(qlu,n,NMAX,indx,x)
    rr=BIG
1   continue                            Important to use iterative improvement, since the
        rrold=rr                            Padé equations tend to be ill-conditioned.
        do 13 j=1,n
            z(j)=x(j)
        enddo 13
        call mprove(q,qlu,n,NMAX,indx,y,x)
        rr=0.
        do 14 j=1,n                     Calculate residual.
            rr=rr+(z(j)-x(j))**2
        enddo 14
    if(rr.lt.rrold)goto 1               If it is no longer improving, call it quits.
    resid=sqrt(rr)
    do 16 k=1,n                         Calculate the remaining coefficients.
        sum=cof(k+1)
        do 15 j=1,k
            sum=sum-x(j)*cof(k-j+1)
        enddo 15
        y(k)=sum
    enddo 16                            Copy answers to output.
    do 17 j=1,n
        cof(j+1)=y(j)
        cof(j+n+1)=-x(j)
    enddo 17
    return
    END
```

CITED REFERENCES AND FURTHER READING:

Ralston, A. and Wilf, H.S. 1960, *Mathematical Methods for Digital Computers* (New York: Wiley), p. 14.

Cuyt, A., and Wuytack, L. 1987, *Nonlinear Methods in Numerical Analysis* (Amsterdam: North-Holland), Chapter 2.

Graves-Morris, P.R. 1979, in *Padé Approximation and Its Applications*, Lecture Notes in Mathematics, vol. 765, L. Wuytack, ed. (Berlin: Springer-Verlag). [1]

5.13 Rational Chebyshev Approximation

In §5.8 and §5.10 we learned how to find good polynomial approximations to a given function $f(x)$ in a given interval $a \le x \le b$. Here, we want to generalize the task to find good approximations that are rational functions (see §5.3). The reason for doing so is that, for some functions and some intervals, the optimal rational function approximation is able to achieve substantially higher accuracy than the optimal polynomial approximation with the same number of coefficients. This must be weighed against the fact that finding a rational function approximation is not as straightforward as finding a polynomial approximation, which, as we saw, could be done elegantly via Chebyshev polynomials.