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Uniform approximations for transcendental functions

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Abstract

A heuristic method to construct uniform approximations to analytic transcendental functions is developed as a generalization of the Hermite-Padé interpolation to infinite intervals. The resulting uniform approximants are built from elementary functions using known series and asymptotic expansions of the given transcendental function. In one case (Lambert's W function) we obtained a uniform approximation valid in the entire complex plane. Several examples of the application of this method to selected transcendental functions are given.

0.1 Introduction

Transcendental functions are usually solutions of analytic differential equations. In most cases a few terms of the series expansion of the transcendental function are easily obtained at certain points, e.g. x=0 and $x=\infty$. However, these expansions only give approximations at very small or very large x. It would be useful to evaluate the function approximately at intermediate points $0 < x < +\infty$. Common methods such as Lagrange interpolation, splines, or Chebyshev polynomials do not provide a uniform approximation valid for all $x \in (0, +\infty)$.

The purpose of this article is to introduce a simple heuristic method for finding uniform approximations to transcendental functions across an infinite range of the argument. The approximants which we call the "global Padé approximants" are combinations of elementary functions. The method is in a certain sense a generalization of Hermite-Padé approximation and requires the knowledge of series expansions of f(x) at several points, including infinity. We obtained uniform approximations for the elliptic function dn(x,m), the error function of real and imaginary arguments, the Bessel functions $J_0(x)$ and $Y_0(x)$, and the Airy function. The simplest approximants are often easily found by hand and give a relative precision of a few percent, throughout an infinite range of the argument. Finally, we give one example (Lambert's W function) of a uniform approximation valid throughout the entire complex plane.

0.2 Global approximations of nonsingular functions

Here we consider the problem of approximating a function f(x) uniformly on the real interval $(0, +\infty)$ when the function is regular within this interval. As a first example, take the function f(x) defined for $x \ge 0$ by the convergent integral

$$f(x) \equiv \int_0^\infty \frac{e^{-xt}dt}{t^5 + 2t + 1}.$$
 (1)

For $x \approx 0$ the integrand is dominated by its growing denominator, while the numerator remains close to 1. Therefore the first terms of the series expansion of f(x) at x = 0 are obtained by expanding $\exp(-xt)$ near x = 0,

$$f(x) = f_0 + f_1 x + \frac{f_2}{2!} x^2 + O(x^3),$$
 (2)

where the constants f_k are found as

$$f_k \equiv (-1)^k \int_0^\infty \frac{t^k dt}{t^5 + 2t + 1}, \quad 0 \le k \le 3.$$
 (3)

[Note that higher-order asymptotics at x=0 require terms of the form $x^n \ln x$ and cannot be obtained in this naive way.] The asymptotic expansion at $x \to \infty$

 $+\infty$ is obtained by expanding the denominator in t:

$$f(x) = x^{-1} - 2x^{-2} + 8x^{-3} + O(x^{-4}). (4)$$

Neither this expansion nor the series at x = 0 provide a uniform approximation for f(x). However, we may look for a rational function

$$r(x) = \frac{p_0 + p_1 x + x^2}{q_0 + q_1 x + q_2 x^2 + x^3}$$
 (5)

where the constants p_i , q_i must be such that the expansions of r(x) at x=0 and at $x=+\infty$ coincide with Eqs. (2)-(4). We find that the constants should be $p_0 \approx 24.4$, $p_1 \approx 4.49$, $q_0 \approx 37.7$, $q_1 \approx 29.4$, $q_2 \approx 6.49$. Numerical calculations show that r(x) approximates f(x) with relative error $< 10^{-2}$ for any $x \geq 0$ (see Fig. 1). Thus we are able to obtain a good plot of f(x) using only a few terms of the series at both ends of the interval.

Figure 1: A global Padé approximant of degree 3 (dashed line) for the function of Eq. (1) (solid line).

0.2.1 Global Padé approximants

Let us consider the above approximation problem more formally. We need to approximate a function f(x) which is finite everywhere in the interval $(0, +\infty)$. Suppose that f(x) has certain series expansions at x = 0 and at $x = +\infty$,

$$f(x) = \sum_{k=0}^{m-1} a_k x^k + O(x^m) \equiv a(x) + O(x^m),$$
 (6)

$$f(x) = \sum_{k=0}^{n-1} b_k x^{-k} + O(x^{-n}) \equiv b(x^{-1}) + O(x^{-n}).$$
 (7)

Here a(x) and b(x) are known polynomials. We can assume that $b_0 = 1$ in Eq. (7). We can always reduce the problem to this case: we can divide f(x) by its limit $f(+\infty)$ at $x = +\infty$ if $f(+\infty \neq 0)$. If $f(+\infty) = 0$, the series at $x = +\infty$ starts with a higher power of x^{-1} and we can multiply f(x) by the appropriate power of x and by a nonzero constant to make $b_0 = 1$.

We now look for a rational approximation of the form

$$f(x) \approx \frac{p(x)}{q(x)} \equiv \frac{p_0 + p_1 x + \dots + p_{\nu} x^{\nu}}{q_0 + q_1 x + \dots + q_{\nu} x^{\nu}},$$
 (8)

where ν is an appropriately chosen integer. The problem now is to find the coefficients p_i , q_i such that Eq. (8) has the correct expansions at x = 0 and at

 $x=+\infty$. Since the leading term of the expansion of Eq. (8) at $x=+\infty$ is p_{ν}/q_{ν} , we can set $p_{\nu}=q_{\nu}=1$.

This formulation is similar to the problem of Hermite-Padé interpolation with two anchor points [1], except that one of the points is at infinity where we need to use an expansion in x^{-1} . We call a "global Padé approximant" an ansatz of the form of Eq. (8). The unknown coefficients p_i , q_i are found from a system of linear equations written compactly as

$$p(x) - q(x) a(x) = O(x^{m}) \text{ at } x = 0,$$
 (9)

$$\frac{p(x)}{x^{\nu}} - \frac{q(x)}{x^{\nu}}b(x^{-1}) = O(x^{-n}) \text{ at } x = +\infty.$$
 (10)

Here it is implied that the surviving polynomial coefficients in x or x^{-1} are equated. This assumes that p(x) and q(x) have no common polynomial factors.

After the choice $p_{\nu}=q_{\nu}=1$, Eqs. (9)-(10) are an inhomogeneous linear system of (m+n-1) equations for 2ν unknowns $p_i, q_i, 0 \leq i < \nu$. Therefore a solution with lowest degree ν (when it exists) is unique if m+n is an odd number. For small degrees ν it is easy to solve this system of equations by hand. Heuristically, the approximation in Eq. (8) is the best when the orders m, n of expansion are close to each other, $m \approx n$.

It is important to note that the solution of Eqs. (9)-(10) with the lowest degree ν does not always exist, and when it exists, q(x) sometimes has zeros within the interval $(0, +\infty)$. In these cases one has to choose a higher degree ν .

One can show that the construction of "global Padé approximants" is equivalent to Hermite-Padé interpolation after a projective transformation of the form

$$x \to \frac{ax+b}{cx+d}.\tag{11}$$

Our procedure is however more direct and easier to follow in hand calculations.

0.2.2 Global approximations via identities

The function $f(x) = \arctan x$ satisfies the identity $\frac{\pi}{2} = \arctan \frac{1}{x} + \arctan x$. We may look for a rational function r(x) that satisfies the same identity. The simplest such function,

$$r_0\left(x\right) = \frac{\pi}{2} \frac{x}{x+1},\tag{12}$$

approximates $\arctan x$ with absolute error < 0.06 for all $x \ge 0$.

As another example, consider the elliptic function dn(x, m) defined by

$$x = \int_{\mathrm{dn}(x,m)}^{1} \frac{dy}{\sqrt{(1-y^2)(y^2 - 1 + m)}}.$$
 (13)

Here m is a parameter, 0 < m < 1 (we follow the conventions of Ref. [2], Chapter 16). The function $\operatorname{dn}(x,m)$ is a periodic function of x (on the real line) with the period 2K, where $K \equiv K(m)$ is the complete elliptic integral. The function $\operatorname{dn}(x,m)$ oscillates between the minimum and the maximum values at the end

points of the half-period interval. The values of the extrema are dn(0, m) = 1; $dn(K, m) = \sqrt{1 - m} < 1$. There is a Taylor series expansion

$$dn(x,m) = 1 - \frac{m^2 x^2}{2!} + \frac{m(m+4)x^4}{4!} + O(x^6)$$
(14)

and an identity

$$dn(x,m) dn(K-x,m) = \sqrt{1-m}.$$
 (15)

The obvious oscillatory approximation,

$$dn(x,m) \approx \frac{1+\sqrt{1-m}}{2} + \frac{1-\sqrt{1-m}}{2}\cos\frac{\pi x}{K},$$
 (16)

gives about 8% relative precision throughout the interval $x \in [0, K]$. We can significantly improve the precision if we take into account Eq. (15). The function

$$r_1(x,m) \equiv (1-m)^{1/4} \frac{1 + b\cos(\frac{\pi x}{K})}{1 - b\cos(\frac{\pi x}{K})}$$
 (17)

satisfies Eq. (15) for any b. The constant b is fixed by $r_1(0, m) = 1$. For testing, we chose m = 0.9 because the approximation is worst when m is close to 1. We found that the maximum relative error of Eq. (17) is less than 10^{-4} .

The precision can be improved by including more cosines. For instance, the approximant

$$r_2(x,m) = (1-m)^{1/4} \frac{1 + b_1 \cos\left(\frac{\pi x}{K}\right) + b_2 \cos\left(\frac{2\pi x}{K}\right)}{1 - b_1 \cos\left(\frac{\pi x}{K}\right) + b_2 \cos\left(\frac{2\pi x}{K}\right)}$$
(18)

satisfies Eq. (15), and the coefficients $b_{1,2}$ may be chosen to reproduce the first two terms of Eq. (14). Then the maximum relative error of $r_2(x, m)$ for m = 0.9 is less than 10^{-11} .

0.3 Global approximants for singular functions

In this section we consider the two-point approximation problem on the interval $(0, +\infty)$ when the function has singularities at one or both ends of the interval.

If the function f(x) has a pole at a finite $x = x_0$, then we could multiply f(x) by an appropriate power of $(x - x_0)$ and obtain a new function without poles. If f(x) has a pole at $x = +\infty$ with the asymptotic expansion of the form $f(x) = x^l (b_0 + b_1 x^{-1} + ...)$ at $x \to +\infty$ [here l > 0], we should select the degree of the polynomial q(x) in Eq. (8) to be l units less than the degree of p(x). Then essentially the same procedure as above will yield a global Padé approximant for the function f(x).

The presence of an essential singularity is usually clear from the asymptotic expansion of the function f(x): the expansion contains a fractional power, an exponential, or a logarithm of x. (Most often, the essential singularity is at

 $x=+\infty$.) It is impossible to reproduce an exponential, a logarithmic or a power law singularity with rational functions. Instead we should try to build a global approximant for f(x) by mixing polynomials with the elementary functions such as e^x or $\ln x$ in a suitable manner. A heuristic rule that works in many cases is to write the asymptotic at $x=+\infty$, find its other singularities, and replace x by a rational function with undetermined coefficients to remove these singularities.

0.3.1 Error function of real argument $\operatorname{erf} x$

The error function

$$\operatorname{erf} x \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2} dx \tag{19}$$

has well-known expansions at x = 0 and at $x = +\infty$:

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \left(x - \frac{x^3}{3} + \frac{x^5}{10} + O\left(x^7\right) \right), \tag{20}$$

$$\operatorname{erf} x = 1 - \frac{e^{-x^2}}{x\sqrt{\pi}} \left[1 - \frac{1}{2x^2} + \frac{3}{4x^4} + O\left(x^{-6}\right) \right]. \tag{21}$$

A heuristic approximation may be built using the approximate identity

$$(\operatorname{erf} x)^2 + \frac{\sqrt{\pi}e^{-x^2}}{2x}\operatorname{erf} x \approx 1 \implies \operatorname{erf} x \approx \frac{4x}{\sqrt{\pi}e^{-x^2} + \sqrt{\pi}e^{-2x^2} + 16x^2}$$
 (22)

(the author is grateful to Matthew Parry for bringing this to his attention). Equation (22) gives about 2% of relative precision for all real x. However, it is not immediately clear how to improve the precision of this approximation.

We may transform the function $\operatorname{erf} x$ by the ansatz

$$\operatorname{erf} x \equiv 1 - \frac{e^{-x^2}}{x\sqrt{\pi}}g(x) \tag{23}$$

and obtain the expansions of g(x) at x=0 and at $x=+\infty$,

$$g(x) = \sqrt{\pi}x - 2x^2 + \sqrt{\pi}x^3 - \frac{4}{3}x^4 + O(x^5),$$
 (24)

$$g(x) = 1 - \frac{1}{2x^2} + \frac{3}{4x^4} + O(x^{-6}).$$
 (25)

The problem to approximate g(x) is now in the form of Sec. 0.2.1. We may obtain, for instance, the following global Padé approximant of degree 2,

$$g(x) \approx \frac{x\sqrt{\pi} + (\pi - 2)x^2}{1 + x\sqrt{\pi} + (\pi - 2)x^2}.$$
 (26)

This provides a uniform approximation to $\operatorname{erf} x$ with an error less than 2%.

0.3.2 Error function of imaginary argument erfi x

The error function of imaginary argument erfi x is defined as $\operatorname{erf}(ix) \equiv i \operatorname{erfi} x$. The function $\operatorname{erfi} x$ has global approximants valid for all $x \in (-\infty, +\infty)$, e.g.

$$r(x) = \frac{e^{x^2}}{x\sqrt{\pi}} \frac{p(x)}{q(x)}, \quad \frac{p(x)}{q(x)} \equiv \frac{\frac{105}{8}x^2 + \frac{25}{4}x^4 + \frac{5}{8}x^6 + x^8}{\frac{105}{16} + \frac{15}{16}x^2 + \frac{9}{2}x^4 + 2x^6 + x^8}.$$
 (27)

This approximates $\operatorname{erfi} x$ to within 6% of relative accuracy for all real x. Higher-order approximants may be found explicitly:

$$q_n(x) = \sum_{k=0}^n \frac{(2k-1)!!}{2^k} \binom{n}{k} x^{2n-2k},$$
 (28)

$$p_n(x) = \sum_{l=1}^{n} x^{2l} \sum_{k=1}^{l} \frac{(-1)^{k-1}}{2^{n-l}} \frac{(2n-2l+2k-1)!!}{(2k-1)!!} {n \choose l-k}.$$
 (29)

A numerical calculation suggests that the relative error can be estimated as

$$\left| \frac{p_n(x)}{q_n(x)} - \operatorname{erfi} x \right| < 2^{-n} \sqrt{\frac{n}{2}} \left| \operatorname{erfi} x \right|. \tag{30}$$

0.3.3 The Bessel functions $J_0(x)$ and $Y_0(x)$

A more complicated example is provided by the Bessel functions $J_0(x)$ and $Y_0(x)$. The series at x = 0 are

$$J_0(x) = 1 - \frac{x^2}{4} + \frac{x^4}{64} + O(x^6)$$

$$Y_0(x) = \frac{2\gamma}{\pi} + \frac{2}{\pi} \ln \frac{x}{2} + \frac{x^2}{2\pi} \left[\gamma - 1 + \ln \frac{x}{2} \right] + O(x^4 \ln x),$$

where $\gamma \approx 0.5772$ is Euler's constant. The asymptotics at $x = +\infty$ are

$$J_{0}(x) = \sqrt{\frac{2}{\pi x}} \left(1 - \frac{9x^{-2}}{128} \right) \sin\left(x + \frac{\pi}{4}\right)$$

$$+ \sqrt{\frac{2}{\pi x}} \left(-\frac{x^{-1}}{8} + \frac{75x^{-3}}{1024} \right) \cos\left(x + \frac{\pi}{4}\right) + O\left(x^{-4}\right),$$

$$Y_{0}(x) = -\sqrt{\frac{2}{\pi x}} \left(1 - \frac{9x^{-2}}{128} \right) \cos\left(x + \frac{\pi}{4}\right)$$

$$+ \sqrt{\frac{2}{\pi x}} \left(-\frac{x^{-1}}{8} + \frac{75x^{-3}}{1024} \right) \sin\left(x + \frac{\pi}{4}\right) + O\left(x^{-4}\right).$$

There are several ways to build a global ansatz that matches these expansions. It is clear that the oscillating functions and the square roots must be present in

the ansatz. We obtained the expressions

$$J_{0}(x) \approx \sqrt{\frac{2}{\pi (0.123 + x)}} \left[\sin \left(x + \frac{\pi}{4} \right) - \frac{x}{2.64 + 8x^{2}} \cos \left(x + \frac{\pi}{4} \right) \right],$$

$$Y_{0}(x) \approx -\sqrt{\frac{2}{\pi (\frac{1}{4} + x)}} \left[\cos \left(x + \frac{\pi}{4} \right) + \frac{x \sin \left(x + \frac{\pi}{4} \right)}{\frac{1}{3} + 8x^{2}} \right] \left(1 + \frac{\ln \left(1 + \frac{0.0364}{x^{2}} \right)}{2\sqrt{\pi}} \right).$$

[The constant in the argument of the logarithm is $4\exp{(-2\gamma-2\sqrt{\pi})}\approx 0.0364$.] These are perhaps the simplest, lowest-order global approximants accurate away from zeros to about 2% for $J_0\left(x\right)$ and to about 5% for $Y_0\left(x\right)$ for all $x\geq 0$ (see Fig. 2). Although global approximants of this kind can be found for arbitrary orders, the (numerical) solution of the required nonlinear equations becomes more difficult for higher orders.

Figure 2: Global approximants (dashed lines) for $J_0(x)$ and $Y_0(x)$ (solid lines).

0.3.4 The Airy function Ai(x)

The Airy function Ai(x) has two different asymptotic expansions at infinity,

$$\operatorname{Ai}\left(x\right) \sim \begin{cases} \frac{1}{2\sqrt{\pi}} x^{-1/4} \exp\left(-\frac{2}{3} x^{3/2}\right) \left[1 + O\left(x^{-3/2}\right)\right], & x \to +\infty\\ \frac{1}{\sqrt{\pi}} x^{-1/4} \cos\left(\frac{2}{3} \left|x\right|^{3/2} - \frac{\pi}{4}\right) \left[1 + O\left(x^{-3/2}\right)\right], & x \to -\infty \end{cases}, (31)$$

whereas the Taylor expansion at x = 0 is

$$Ai(x) = \frac{1}{3^{2/3}\Gamma(\frac{2}{3})} - \frac{3^{1/6}\Gamma(\frac{2}{3})}{2\pi}x + O(x^3).$$
 (32)

It is difficult to build a single analytic ansatz for the whole real line, and for practical purposes it is easier to approximate the Airy function separately in the x>0 and x<0 domains. The simplest ansatz is

$$\operatorname{Ai}(x) \approx \begin{cases} \frac{1}{2\sqrt{\pi}} (x + a_1)^{-1/4} \exp\left(-\frac{2}{3}x^{3/2}\right), & x > 0\\ \frac{1}{\sqrt{\pi}} (|x| + a_2)^{-1/4} \cos\left(\frac{2}{3}|x|^{3/2} - \frac{\pi}{4}\right), & x < 0 \end{cases}$$
(33)

The constants a_1 and a_2 are chosen so that the value of the ansatz at x=0 is correct. With the numerical values $a_1 \approx 0.40$, $a_2 = 4a_1 \approx 1.60$ the ansatz of Eq. (33) approximates the Airy function to about 20% for x < 0 and to about 2% for x > 0 (see Fig. 3).

The ansatz of Eq. (33) is simple but gives a function with a discontinuous derivative. This can be avoided with a more complicated ansatz, for instance, replacing $(x + a)^{-1/4}$ in Eq. (33) by a more complicated function. In practice, Eq. (33) serves sufficiently well as a qualitative visualization of the Airy function.

Figure 3: Approximation of the Airy function Ai(x) by the ansatz of Eq. (33).

0.3.5 Lambert's W function

Another example is Lambert's W function defined by the algebraic equation

$$W(x) e^{W(x)} = x. (34)$$

This function has real values for $-e^{-1} \le x < +\infty$. We can use the series expansions of W(x) at $x = -e^{-1}$, x = 0 and $x = +\infty$ to build global approximants on the subintervals $\left[-e^{-1}, 0\right]$ and $(0, +\infty)$. The series at x = 0 and at $x = -e^{-1}$ are

$$W(x) = x - x^2 + \frac{3}{2}x^3 + O(x^4),$$
 (35)

$$W(x) = -1 + y - \frac{1}{3}y^3 + \frac{11}{72}y^4 + O(y^5), \qquad (36)$$

where we defined $y \equiv \sqrt{2ex + 2}$. The asymptotic expansion at large |x| is

$$W(x) \sim \ln x - \ln(\ln x) + \frac{\ln(\ln x)}{\ln x} + \frac{1}{2} \left(\frac{\ln(\ln x)}{\ln x}\right)^2 + \dots$$
 (37)

A uniform approximation for $x \in (0, +\infty)$ can be obtained by replacing x in the above asymptotic expansion by 1 + x or other suitable rational function. For instance, the ansatz inspired by the first three terms of Eq. (37),

$$W(x) \approx \ln(1+x) \left(1 - \frac{\ln(1+\ln(1+x))}{2 + \ln(1+x)}\right),$$
 (38)

approximates W(x) for real x > 0 with a relative error less than 10^{-2} , while

$$W(x) \approx \frac{ex}{1 + \left[(2ex + 2)^{-1/2} + \frac{1}{e-1} - \frac{1}{\sqrt{2}} \right]^{-1}}$$
(39)

is good for $-e^{-1} \le x \le 1$ and gives a relative error less than 10^{-3} .

0.4 An approximation to W(x) in the entire complex plane

Here we present an approximant for W(z) which is valid for all (complex) z. The practical significance of a global ansatz for W(z) is to provide a precise initial approximation W_0 for W(z), from which an efficient numerical computation of W(z) for complex z is possible using e.g. the Newton-Raphson iteration.

The idea is to reproduce the first few terms of the asymptotic expansion of W(z) at large |z| and of the series at z=0 and at $z=-e^{-1}$. Since the expansion at $z=-e^{-1}$ uses $y\equiv\sqrt{2ez+2}$ as the expansion variable while the asymptotic expansion uses $\ln z$, we need to combine terms of both kinds into one ansatz. We choose an ansatz of the form

$$W(z) \approx \frac{2\ln(1+By) - \ln(1+C\ln(1+Dy)) + E}{1 + [2\ln(1+By) + 2A]^{-1}}.$$
 (40)

Here the constants $A \approx 2.344$, $B \approx 0.8842$, $C \approx 0.9294$, $D \approx 0.5106$, and $E \approx -1.213$ are determined numerically to give approximately correct expansions at the three anchor points to 3 terms.

Numerical computations show that Eq. (40) gives the complex value of the principal branch of Lambert's W function in the entire complex plane with relative error less than 10^{-2} , with the standard choices of the branch cuts for \sqrt{z} and $\ln z$.

0.5 Conclusion

In this paper, we have presented a heuristic method for approximating transcendental functions f(x) using combinations of elementary functions. This method is a generalization of the Hermite-Padé interpolation to infinite intervals and non-rational functions. We showed several examples where the approximations are easy to construct by hand, given the first few terms of series expansions of f(x) at x=0 and $x=+\infty$. For functions with essential singularities, an ansatz can usually be found by replacing Laurent series and arguments of powers and logarithms by rational functions. The simplest approximants typically give a precision of a few percent. The numerous examples suggest that the ansatz resulting from this procedure will approximate the function across the entire range of the argument, $x \in (0, +\infty)$.

In one case (Lambert's W function) we were able to construct a global uniform approximant valid in the entire complex plane. This is a somewhat surprising result; it is probably due to the simple nature of the singularities of W(z). A similar construction will certainly be impossible for some functions such as $\Gamma(x)$ or Riemann's $\zeta(x)$ which are too ill-behaved for a full global approximation to succeed. (However, it has been shown that these functions allow global uniform approximants in the half-plane domains $\operatorname{Re} x > 0$ for $\Gamma(x)$ [4] and $\operatorname{Re} x > 1/2$ for $\zeta(x)$ [3]; these are the domains where these functions are free of zeros and poles, except for the singularity at $x = +\infty$).

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