Approximating a zero of a function via the zero of its 1/p Pade' Approximant

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Abstract

z* is said to be a zero of a function f(z) if f(z*) = 0. The problem of finding such a z* for given functions has raised due concern and received considerable attention. Numerous attempts have been put forward leading to quite a number of formulae. Nonetheless a lot more is sought and is still being considered. In this paper we give a simple – yet neat and elegant – procedure arising from approximating the function in question by its 1/p Pade' approximant. The theme and essence of the method build on the zero of the 1/p Pade' approximant – effectively on the zero of the linear expression in the numerator. This zero - provides the basis for a zero of the function in question - thus endorsing the beauty and neatness of the method.

Keywords: analytic; analytic function; zero; zero of a function; matrix; determinant; determinant of a matrix; Padé approximant; continuity; continuity of a function; iteration; iteration function; iteration formula

Introduction

A Pade' Approximant is the "best" approximation of a function by a "rational function" of given order. e.g. R(z) = P(z) / Q(z), where P(z) and Q(z) are polynomials of degrees m and n –say

Under this technique the approximant's power series - R(z) in this case- is set to agree with the power series expansion of the function in hand up to and including the power m+ n – (m, n - as just defined).

The technique is attributed to Henri Pade'(1890), though it is claimed to have been discovered earlier by Georg Frobenius- who introduced the idea and investigated the features of rational approximants and power series.

Background and Derivation of the Method

Let us consider the problem of finding a zero – assumed simple – of a function f – assumed analytic.

Let w be a point in the neighborhood of the zero. Then

$$f(z) = f(w+t) = g(t) = \sum_{r=0}^{\infty} c_r \cdot t^r \tag{1}$$

Where

$$t = z - w \tag{2}$$

and

$$r!\,c_r = r!\,c_r(w) = \left(\frac{d^f g(t)}{dt^f}\right)_{t=0} = \left(\frac{d^f f(z)}{dz^f}\right)_{z=w} \tag{3}$$

We now look for the 1/p Pade' approximant to g(t) in the form:

$$P(t) = \frac{(a_0 + a_1 t)}{(1 + b_1 t + b_2 t^2 + \cdots + b_p t^p)} \tag{4}$$

The coefficients: a_0, a_1, b_1, b_2 , ..., b_p are to be determined so that the power series expansion of P(t) agrees with that of g(t) up to and including the term in t^{p+1}.

We thus get:-

$$\begin{aligned} a_0 &= c_0 \\ a_1 &= c_1 + c_0 b_1 \\ 0 &= c_m + \sum_{k=1}^{m} c_{m-k} \cdot b_k \ , m = 2(1)p \\ 0 &= c_m + \sum_{k=1}^{m} c_{m-k} \cdot b_k \ , m = p+1 \end{aligned} \tag{5}$$

We are particularly interested in $(-a_0 / a_1)$ the zero of P(t).

Since P(t) is a good approximant to g(t) (≡f(z)), it is expected that the zero of P(t) will provide a "reasonable" approximation to a zero of g(t).

Now the zero of P(t) is given by :-

$$t^* = z^* - w = -\frac{a_0}{a_1} \tag{6}$$

But,

$a_0 = c_0$ and $a_1 = c_1 + c_0 b_1$ and $b_1 = -\frac{H'_p}{H_p}$ where $H'_p = |U'_p|$, $H_p = |U_p|$, where U_p, U_p' are the matrices given below (7)

$$U'_p = \begin{pmatrix} c_2 & c_0 & 0 & 0 & \dots & 0 \\ c_3 & c_1 & c_0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ c_p & c_{p-2} & \dots & \dots & \dots & c_0 \\ c_{p+1} & c_{p-1} & \dots & \dots & \dots & c_1 \end{pmatrix} \tag{8}$$

$$U_p = \begin{pmatrix} c_1 & c_0 & 0 & 0 & \dots & 0 \\ c_2 & c_1 & c_0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ c_{p+1} & c_{p-1} & \dots & \dots & \dots & c_1 \end{pmatrix} \tag{9}$$

But from Eq. (3) we have,

$$c_r = \left(\frac{f^{(r)}(z)}{r!}\right) z = w \tag{10}$$

Now introducing $u=f/f'$ and combining Eqs.(2), (3) with Eqs.(6) and (7) we have:-

$$z^* = w - \frac{u(w)}{\left(1 - \frac{u(w)H'_p(w)}{H_p(w)}\right)}$$

$$= \left[z - u(z)/\left(1 - u(z)H'_p(w)/H_p(w)\right)\right]_{z=w}$$

assuming the continuity of the bracketed term and using the continuity of a determinant as a function of its elements.
Denoting z* by z_{k+1} and replacing w by z_k, we have the following iteration formula :-

$$z_{k+1} = F_p(z_k),$$

Where, $F_p(z)$ - the iteration function – is given by

$$F_p(z) = z - \frac{u(z)}{\left(1 - \frac{u(z)H'p(z)}{Hp(z)}\right)} \tag{11}$$

$$F_p(z) = z - \frac{c_0}{\left(c_1 - c_0\frac{H'p}{H_p}\right)} \tag{11-1}$$

A Compact Computational Procedure

For computational purposes let us define a matrix of order p+1–q as follows:-

$$A_{p+1-q} = \begin{pmatrix} c_1 & c_0 & 0 & 0 & \dots & 0 \\ c_2 & c_1 & c_0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ c_{p-q} & c_{p-q-1} & \dots & \dots & c_1 & c_0 \\ c_{p+1-q}{}^{(q)} & c_{p-q}{}^{(q)} & \dots & \dots & c_2{}^{(q)} & c_1{}^{(q)} \end{pmatrix} \tag{12}$$

$$c_k{}^{(0)} \equiv c_k \tag{13}$$

Let us now set out to compute the determinant $|A_{p+1-q}|$, abiding by the following steps: -
Multiplying the elements of the last row by $-c_0 / c_1^{(q)}$, adding to the penultimate row - the last but one - and expanding after the last column, we obtain the following recurrence relation :-

$$|A_{p+1-q}| = c_1^{(q)} |A_{p-q}|, (\equiv c_1^{(q)} |A_{p+1-(q+1)}|), \tag{14}$$

Where, $c_m^{(0)} = c_m$ - (as defined by Eq.(13)),

$$c_m^{(q)} = c_m - c_{m+1}^{(q-1)} c_0 / c_1^{(q-1)}, \tag{15}$$

$$m = 1\ (1)\ (p+1-q)\ ,\ q = 1\ (1)\ p$$

Using these relations for q = 0 (1) p, we get

$$|A_{p+1}| = \prod_{j=0}^{p} c_1{}^{(j)}\ ,\ |A_p| = \prod_{j=0}^{p-1} c_1{}^{(j)} \tag{16}$$

Hence we have,

$$|A_{p+1}| = |A_p| \cdot c_1{}^{(p)} \tag{17}$$

From Eqs (8),(9),(11-1) , together with Eqs (15) and (17) it follows that $F_p(z)$ takes the more compact form

$$F_p(z) = z - c_0(z) / c_1^{(p)}(z) \tag{18}$$

A NUMERICAL EXAMPLE

To illustrate the simplicity of the procedure it suffices to consider a simple example with p = 5 – say.
Consider the function cos(x).

$$\cos(x) = 1 - x^2/2 + x^4/24 - x^6/720 + \ldots \quad (19)$$

Let,

$$x^2 = y \quad (20)$$

Then

$$f(y) = \cos(y^{1/2}) = 1 - y/2 + y^2/24 - y^3/720 + y^4/40320 - y^5/3628800 + \ldots \quad (21)$$

For $y \neq 0$ we get $f(y) = \cos(y^{1/2})$; $f'(y) = -1/2 \sin(y^{1/2}) / y^{1/2}$; $f^{(r)}(y) = -1/4y\, f^{(r-2)}(y) + (4r-6)\, f^{(r-1)}(y)$, $r \geq 2$ (22)

r(C)k \ k	0	1	2	3	4	5
1	-5.00000(-1)	-4.16667(-1)	-4.0666667(-1)	-4.05445(-1)	-4.053028(1)	-4.05287(-1)
2	4.16667(-2)	3.88889 (-2)	3.845238(-2)	3.839448(-2)	3.838755(-2)	
3	-1.38889(-3)	-1.33929(-3)	-1.330688(-3)	-1.329503(3)		
4	2.48016(-5)	2.42504(-5)	2.4150232(-5)			
5	-2.75573(-7)	-2.71398(-7)				
6	2.08768(-9)					

$y^{(0)} = 0$, $x^{(0)} = (y^{(0)})^{1/2} = 0$, $c_0 = 1$
$y^{(1)} = y^{(0)} - c_0 / c_1^{(5)}$
$= 0 + 1/0.4052867$
$= 2.4673887$
Hence,
$x^{(1)} = (y^{(1)})^{1/2} = 1.57079$ - agreeing with $\pi/2$ up to 6 significant figures.
A further iteration with p = 0 (say) – Newton's Formula – gives
$x^{(2)} = (y^{(2)})^{1/2} = (2.4674011003)^{1/2}$
$= 1.570793268$ - ($\pi/2$ correct to the 10 significant figures quoted) !!

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