

# Numerics of Generalized Lambert $W$ Function

Tony C. Scott<sup>1</sup>, Greg Fee<sup>2</sup> and Johannes Grotendorst<sup>3</sup>

<sup>1</sup> Institut für Physikalische Chemie, RWTH Aachen University, 52056 Aachen, Germany  
email: tcscott@gmail.com

<sup>2</sup> Centre for Experimental and Constructive Mathematics (CECM), Simon-Fraser University, Burnaby, BC V5A 1S6 Canada  
email: gjfee@cecm.ca

<sup>3</sup> Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany  
email: j.grotendorst@fz-juelich.de

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## Abstract

Herein, we present another sequel to work on a generalization of the Lambert  $W$  function. We provide a fast and efficient computational scheme for getting *all* the roots of the transcendental-algebraic governing the generalized Lambert  $W$  function for a broad class of cases in the real plane.

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## 1 Introduction

In previous work [1], we focussed on asymptotic series expansions of solutions to:

$$e^{-cx} = a_o (x - r_1)(x - r_2) \quad (1)$$

This was a first generalization of the Lambert  $W$  function which appears in a number of applications [2–5]. The work of [1] presented series expansions, both Taylor type and asymptotic, for eq. (1). However, it is realized that eq. (1) can have as much as 3 roots in the real plane and the series expansions account for only 2 particular solutions (either real or complex) for a given range. For general implementation, in particular implementation in a computer algebra or symbolic manipulation system, it is necessary to fully work out the floating-point attributes of any given special function. There are many schemes like the Newton-Raphson scheme to find a numerical root for a given function in a given range. However, it becomes necessary to work out a fast and efficient scheme to obtain *all* the numerical roots of eq. (1) to ensure its implementation.

Subsequently, it was realized that eq. (1) could be further generalized to the case of a rational polynomial [9]:

$$e^{-cx} = \frac{P_N(x)}{Q_M(x)} \quad (2)$$

where  $c > 0$  is a constant as before and  $P_N(x)$  and  $Q_M(x)$  are polynomials in  $x$  of respectively orders  $N$  and  $M$  and we will keep this general form in mind when the scheme for obtaining solutions to eq. (1) is generalized.

This presentation is outlined as follows. Firstly, we focus on a 3-root example of eq. (1) and establish *bounds* for the roots and from these bounds, we zero in on the roots themselves in better than quadratic convergence using a Newton-Raphson scheme backed up with the *Kantorovich* theorem. We then discuss the generalizations of this approach for eq. (2) when the right side  $P_N$  is a cubic or quartic polynomial i.e. with  $N = 3, 4$  and  $M = 0$ . This approach is demonstrated with concrete examples.

## 2 Maximum Number of Roots

Firstly, it is important to establish the following

Proposition:

For a transcendental-algebraic equation corresponding to the case  $M = 0$  for eq. (2), and has the form:

$$e^{-cx} = P_N(x) \quad (3)$$

where  $P_N(x)$  is a polynomial of degree  $N$  with  $N$  *real* distinct roots, there is at most  $N + 1$  real roots to eq. (3).

This proposition can be demonstrated graphically with Maple [10] by the following exercise:

Let  $P_N(x)$  be a Chebyshev polynomial of order  $N$ . Then  $P_N(x)$  has  $N$  real roots. If we shift the polynomial by 1, i.e.  $x \rightarrow x - 1$ , then multiply the result by a scaling factor like  $-1$  for odd  $N$ , we can easily find a  $c > 0$  so that  $e^{-cx}$  and  $P_N(x)$  have  $N + 1$  intersections:  $N$  real roots are positive or zero and one root is negative. The exponential function  $e^{cx}$ ,  $c > 0$  is growing faster than any polynomial and  $e^{-cx}$  is less than 1 and decreasing.

In general for a polynomial of degree  $N$  with  $N$  distinct roots, the Gauss-Lucas theorem and specifically Rolle's theorem tells us that between any two successive real roots, the structure of  $P_N(x)$  is very simple allowing for one point in which the derivative of the polynomial  $P'_N(x)$  is zero. For the case when  $P_N(x)$  has less than  $N$  real roots, say  $n$  real roots where  $n < N$  because of multiplicity of the real roots, we expect  $n + 1$  real roots as an upper bound. Note that when the roots  $r_i$  are all equal to each other, then eq. (3) can be factored and the polynomial degree reduced.

### 3 Solutions to Quadratic Transcendental Equation in Eq. (1)

#### 3.1 Establishing the bounds of the roots

To illustrate the problem, let us start with a particular example of eq.(1):

$$\begin{aligned}
 c &= 1 \\
 a_0 &= \frac{1}{9}e^{-4} - \frac{1}{8}e^{-3} + \frac{1}{72}e^5 \approx 2.0571055639 \\
 r_{\pm} &= \frac{7e^9 + 9e - 16 \pm \sqrt{4096 - 10368e + 6561e^2 - 128e^9 - 162e^{10} + e^{18}}}{e^9 - 9e + 8} \\
 r_1 &= \frac{1}{2}r_- \approx 3.0244254046 \\
 r_2 &= \frac{1}{2}r_+ \approx 3.9908734844
 \end{aligned} \tag{4}$$

Without any loss of generality, we can set  $c = 1$  since this corresponds to a re-scaling of the variable  $x$  and parameters  $a_0$ ,  $r_1$  and  $r_2$  of eq. (1). For these parameters, the roots of eq. (1) are:

$$\begin{aligned}
 x_1 &= -5 \\
 x_2 &= 3 \\
 x_3 &= 4
 \end{aligned} \tag{5}$$

These can be shown in the plot of Figure 3.1. The roots can be seen from the intersection of the plot for  $e^{-x}$  and  $a_0(x - r_1)(x - r_2)$  with the parameters governed by eq. (4). The series expansions [1] made use of a parameter:  $z_0 = \frac{1}{2}\sqrt{c^2/a_0} e^{-cr_m/2}$  where  $r_m = (r_1 + r_2)/2$ . From section 2 the greatest number of real roots eq. (1) can have is 3. The starting approximations [1]:

$$W_0 = \frac{2}{c}W(\pm z_0)$$

where  $W$  on the right-hand-side of the equation above is the standard Lambert  $W$  function. This yields  $z_0 = 0.0603483382$ ,  $r_m = 3.50764944445$  for the parameters in eq. (4) and approximate solutions:

$$\begin{aligned}
 r_m + (W_0)_+ &= 3.62165830 \\
 r_m + (W_0)_- &= 3.37892929
 \end{aligned}$$

This gives us at best an approximation for the roots 3 and 4 but not  $-5$  so readily. The series expansions in our previous work could represent at most two of these roots but not all three roots directly. Thus we need a complimentary scheme to ensure getting *all* the roots. We divide the problem in two regions: one with  $x \geq 0$  and the other  $x < 0$ . For the latter region, note that if we make the 0:

$$x \rightarrow -x \quad c \rightarrow -c \quad r_1 \rightarrow -r_1 \quad r_2 \rightarrow -r_2, \tag{6}$$

eq. (1) becomes:

$$e^{cx} = a_0(x + r_1)(x + r_2)$$

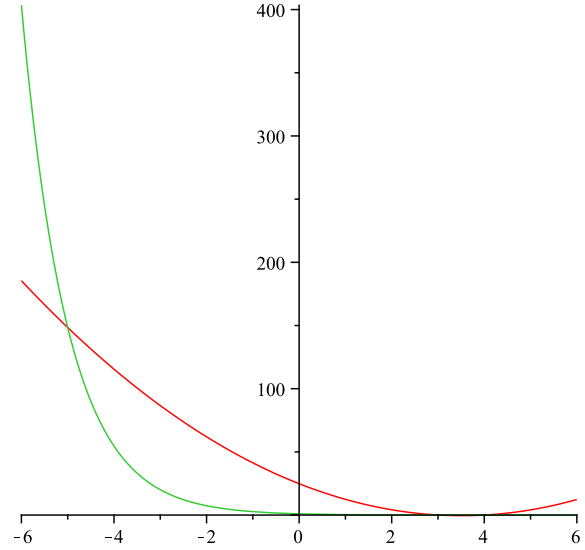


Figure 1: Roots at  $x = -5, 3$  and  $4$  for eq. (1) with parameters in eq. (4).

and represents a reflected image of Figure 3.1). In this example,  $c > 0$  and thus  $\exp(-cx)$  of (1) will be bounded from below by zero and bounded above by unity for the region  $x \geq 0$ . In other words, defining:

$$Y = e^{-cx} \quad (7)$$

it is understood that  $Y \in [0, 1]$  when  $x > 0$ . For  $x < 0$ , then  $Y \in [1, \infty)$ . We now formally treat  $Y$  as a constant and simply apply the well-known solutions for any quadratic  $aX^2 + bX + c = 0$  whose roots are:

$$X_{\pm} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

For the quadratic polynomial on the right-hand-side of eq. (1), we get:

$$X_{\pm} = \frac{1}{2} \left( r_1 + r_2 \pm \sqrt{(r_1 - r_2)^2 + 4 \frac{Y}{a_0}} \right) \quad (8)$$

where it is understood that  $Y = e^{-cx}$  which brings us back to the *pseudo-quadratic* of Byers-Brown [1, 6–8]. However, unlike Byers-Brown we do not use this pseudo-quadratic for series expansion. The resulting series are slow in convergence because of the branch structure implied in eq. (8) when viewed in the complex plane. Rather, we use eq. (8) directly for computation to establish bounds of the roots. For  $Y = 0$  and  $Y = 1$ , this provides us with 4 points. Note that when  $a_0 > 0$ ,  $X_{\pm}$  will also be real if  $r_1$  and  $r_2$  are real roots to the quadratic polynomial on the right-side of eq. (1). Since both roots share the same square-root term, they are both equally real or equally complex. If  $a_0 < 0$  and  $X_{\pm}$  is complex, this puts into question whether or not eq. (1) has real roots at all and may require some exception processing such as lowering the value of  $Y = 1$  down to  $Y < |a_0(r_1 - r_2)^2/4|$ .

One could argue that the  $\pm$  cases of (8) bound the roots for the individual cases of  $Y = 0$  and  $Y = 1$  giving a total of only 2 possible roots but although true in some cases, this would be hasty in general. For the time being, we compute 4 points and sort them in increasing order for  $x > 0$ . Two of these points correspond to the  $Y = 1$  case and are given by:

$$\begin{aligned} R_{\pm} &= \frac{7e^9 + 9e - 16 \pm \sqrt{4096 - 10368e + 6561e^2 + 2304e^4 - 2592e^5 - 128e^9 - 162e^{10} + 288e^{13} + e^{18}}}{e^9 - 9e + 8} \\ R_1 &= \frac{1}{2} R_- \approx 2.6593420730 \\ R_2 &= \frac{1}{2} R_+ \approx 4.3559568158 \end{aligned}$$

Once sorted, these 4 points are:

$$[R_1, r_1, r_2, R_2] = [2.6593420730, 3.0244254046, 3.9908734844, 4.3559568158] \quad (9)$$

Now it's matter of evaluating:

$$f(x) = \exp(-cx) - a_0(x - r_1)(x - r_2) \quad (10)$$

at these very points in (9):

$$[f(R_1), f(r_1), f(r_2), f(R_2)] = [-0.93000574243, 0.048585730140, 0.018483561518, -0.98716984217] \quad (11)$$

which provide our bounds. By the intermediate value theorem [11], we can see the change in sign between respectively  $R_1$  and  $r_1$  and between  $R_2$  and  $r_2$ , establishing bounds to 2 roots. We now repeat this exercise for the region  $x < 0$ . We now consider the region  $Y \in [1, Y_{max}]$ . The endpoint 5 may seem artificial but it's a matter of ensuring any value  $Y_{max}$  small enough but to that  $f(Y_{max}) > 0$ . This can be guaranteed

since the exponential term  $\exp(-cx)$  rises more quickly in the region  $x < 0$  than any quadratic. We choose  $Y_{max} = 5$  and this choice will turn out to be sufficient.

$$\begin{aligned} S_{\pm} &= \frac{7e^9 + 9e - 16 \pm \sqrt{4096 - 10368e + 6561e^2 + 11520e^4 - 12960e^5 - 128e^9 - 162e^{10} + 1440e^{13} + e^{18}}}{e^9 - 9e + 8} \\ S_1 &= \frac{1}{2}S_- \approx 1.8754407900 \\ S_2 &= \frac{1}{2}S_+ \approx 5.1398580989 \end{aligned}$$

Once sorted, these 4 points are:

$$[-S_2, -R_2, -R_1, -S_1] = [-5.1398580989, -4.3559568159, -2.6593420730, -1.8754407900] \quad (12)$$

at these very points in (12):

$$[f(-S_2), f(-R_2), f(-R_1), f(-S_1)] = [17.342798224, -48.782093196, -63.468163560, -52.606067113] \quad (13)$$

In this case, we see only one change of sign and thus a bound for only one more root. Thus, we can discern 3 roots in all.

### 3.2 Zeroing on the roots: Kantorovich Theorem

At this stage, a computer algebra systems like Maple which provides a functionality called `fsolve` would readily yield the root once the bounds for the roots are known. However, in case such systems are not available or simply for the sake of completeness of the algorithm, we now consider a scheme for zeroing on the root once the bounds are given. It is well known that when a initial guess for the root of a function is known, if it is sufficiently close, the Newton-Raphson scheme can offer better than quadratic convergence. However, a criteria telling us if this root is sufficiently before applying the Newton-Raphson scheme would be very helpful. This is realized with the Kantorovich theorem. The Newton-Raphson algorithm considers a Taylor series expansion of any general function  $f(x)$  as:

$$f(x + \epsilon) = f(x) + \epsilon f'(x) + \frac{\epsilon^2}{2} f''(x)$$

where  $\epsilon$  is assumed small. Allowing  $f(x + \epsilon) = 0$ , the iteration for successive guesses of the roots  $x_n$  of  $f(x)$  are given:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}, \quad (14)$$

where  $e_i$  is the error of the  $i^{th}$  iteration [12, 13]:

$$\epsilon = e_i = -\frac{f(x_i)}{f'(x_i)}. \quad (15)$$

When this scheme converges:

$$\lim_{i \rightarrow \infty} x_i \rightarrow x^* \quad f(x^*) = 0.$$

If there exists a point  $x_0$  which lines on the closed interval I containing the root  $x^*$  of  $f(x)$  taken as a  $C^2$  function and finite positive constants  $(m_0, M_0, K_0)$  such that [14–16]:

$$\begin{aligned} (i) \quad & \left| \frac{1}{f'(x_0)} \right| \leq m_0 \\ (ii) \quad & \left| \frac{f(x_0)}{f'(x_0)} \right| \leq M_0 \\ (iii) \quad & |f''(x_0)| \leq K_0 \end{aligned} \quad (16)$$

and if  $h_0 = 2 m_0 M_0 K_0 \leq 1$ , Newton's iteration will converge to a root  $x^*$  of  $f(x)$  and

$$|x_i - x^*| < KT(i) \quad \text{where} \quad KT(i) = 2^{1-i} M_0 h_0^{2^{i-1}}. \quad (17)$$

For illustration purposes, we have stated these conditions in parallel to their counterparts for a single function  $f(x)$ . Note that (i) and (ii) are conditions of boundedness. Condition (iii) can also be equivalently expressed as:

$$|f'(x) - f'(y)| \leq K_0 |x - y| \quad \text{for all } x, y \in I \quad (18)$$

As pointed out by Tapia [15], this theorem gives *sufficient* conditions to insure the existence of a root and the convergence of Newton's process. Moreover, if  $h_0 < 1$ , the convergence of  $KT(i)$  is quadratic (the number of good digits of the root is doubled at each iteration).

In this case, we have a critical point for  $m_0$  and  $M_0$  when  $f'(x) = 0$  and solving for  $x$ . Since:

$$f'(x) = -c \exp(-cx) - 2a_0x + a_0(r_1 + r_2) \quad (19)$$

this yields:

$$f'(x) = 0 \rightarrow x_{crit}[k] = \frac{1}{c} W \left( k, -\frac{1}{2} \frac{ce^{-\frac{c}{2}(r_1+r_2)}}{a_0} \right) + \frac{1}{2}(r_1 + r_2) \quad (20)$$

where  $W$  is the standard Lambert  $W$  function and  $k$  is an integer representing all the branches in which the  $W$  function is real. For this particular example,  $k = -1, 0$  with  $k = 0$  representing the principal branch and  $k = -1$  has a branch point at  $-e^{-1}$ . The formula in eq. (20) is general for arbitrary  $c, a_0, r_1$  and  $r_2$ . Thus, we can expect the principle branch of the  $W$  function to be amongst the roots and for  $|k|$  to be small in magnitude. In view of section 2, eq. (20) establishes regions of roots and the number of roots even more so than the bounds we found in section 3.1. For this particular 3-root example, (20) is:

$$\begin{aligned} x_{crit}[-1] &= -3.3380708176 \dots \\ x_{crit}[0] &= 3.5003119589 \dots \end{aligned} \quad (21)$$

The location of these two critical points divides the  $x$ -axis into 3 regions. The left most point can tell us what  $Y_{max} > e^{|-3.33870|} \approx 27$ . However our choice of  $Y_{max} = 5$  is good enough in this example. Moreover, it reinforces the notion that no roots exist between  $x = r_1$  and  $x = r_2$ . However, for the intervals in the bounds we established, the Kantorovich conditions hold very well.

$$[h_0(R_1), h_0(r_1), h_0(r_2), h_0(R_2)] = [0.6430829954, 0.1050235098, 0.03760437762, 0.6599106776]$$

$$[h_0(-S_2), h_0(-R_2), h_0(-R_1), h_0(-S_1)] = [0.3164937840, 3.465689765, 10.50792320, 1.038566654] \quad (22)$$

Clearly the Kantorovich conditions tell us when a root applies and turn out to be even more important than the bounds we established in section 3.1. Table 3.2 shows that for all 3 roots, the Kantorovich bound holds up and we get very rapid convergence from the bounds established in the first section to the actual root.

## 4 Solutions to Cubic Transcendental Equation in Eq. (2)

Consider a particular case of eq. (2) where  $N = 3$  and  $M = 0$  or equivalently where the quadratic polynomial on right-hand-side of eq. (1) is replaced by a cubic polynomial:

$$e^{-cx} = a_o (x - r_1)(x - r_2)(x - r_3) \quad (23)$$

Table 1: Convergence of Newton-Raphson/Kantorovich bound for eq. (1)

	$x^* = -5$ $x_0 = -5.13985809890$		$x^* = 3$ $x_0 = 3.0244254047250$		$x^* = 4$ $x_0 = 3.9908734842$	
i	$ x_i - x^* $	$KT(i)$	$ x_i - x^* $	$KT(i)$	$ x_i - x^* $	$KT(i)$
1	1.1501196897e-2	4.0624161631e-2	6.2524266166e-4	2.630906913e-3	8.50086025e-5	3.4639364290e-4
2	8.3588049471e-5	6.4286473200e-3	3.8918002348e-7	1.381535391e-4	7.239366092e-9	6.5129586747e-5
3	4.4447310177e-9	3.2197338607e-4	1.509723032e-13	7.619124596e-7	5.25109317e-17	4.6049523112e-9

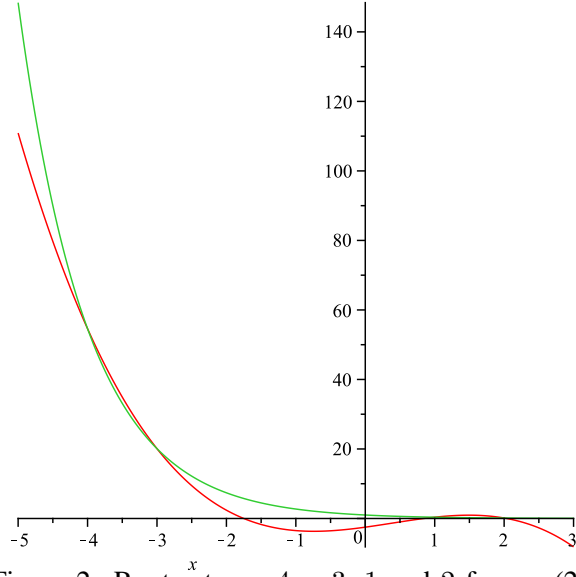


Figure 2: Roots at  $x=-4$ ,  $-3$ ,  $1$  and  $2$  for eq. (23) with parameters in eq. (24).

The solutions for a cubic polynomial are well known and readily implemented in a system like Maple using the `RootOf` implementation.

$$\begin{aligned}
 c &= 1 \\
 a_0 &= \frac{1}{30}e^{-2} - \frac{1}{20}e^{-1} + \frac{1}{20}e^3 - \frac{1}{30}e^4 \\
 &\approx -0.8295442842 \\
 r_1 &\approx -1.7498372963 \\
 r_2 &\approx 2.0376547064 \\
 r_3 &\approx 0.8445802935
 \end{aligned} \tag{24}$$

The numbers  $r_i$  with  $i = 1, 2, 3$  are too lengthy to write here and so only the floating point approximations are given. The roots of eq. (23) are:

$$\begin{aligned}
 x_1 &= -4 \\
 x_2 &= -3 \\
 x_3 &= 1 \\
 x_4 &= 2
 \end{aligned} \tag{25}$$

These can be shown in the plot of Figure 4. The roots can be seen from the intersection of the plot for  $e^{-x}$  and  $a_0(x - r_1)(x - r_2)(x - r_3)$  with the parameters governed by eq. (24). For eq. (23), reflection symmetry yields:

$$\begin{aligned}
 x &\rightarrow -x & c &\rightarrow -c & a_0 &\rightarrow -a_0 \\
 r_1 &\rightarrow -r_1 & r_2 &\rightarrow -r_2 & r_3 &\rightarrow -r_3,
 \end{aligned} \tag{26}$$

eq. (23) becomes:

$$e^{cx} = -a_0 (x + r_1)(x + r_2)(x + r_3) \tag{27}$$

and represents a reflected image of Figure 4). Note the minus sign in contradistinction to the quadratic case of section 3 because of the change in sign of  $a_0$ . We repeat the analysis given in section 3 but show only the highlights. Care must be taken for the cubic case because the roots of cubic polynomials are expressed in terms of cubic roots and these roots are often in the complex plane. Thus we must be careful to extract real bounds from the possible bounds. For the regime  $x > 0$  where  $Y = e^{-c x} \in [0, 1)$ , we obtain:

$$\begin{aligned}
 &[u_1, r_1, r_3, u_2, u_3, r_2] \\
 &= [-1.8585722629, -1.7498372963, 0.8445802935, 1.49092364, 1.5000463207, 2.0376547064]
 \end{aligned} \tag{28}$$

Table 2: Convergence of Newton-Raphson/Kantorovich bound for eq. (23)

		$x^* = -4$ $x_0 = -4.1177608579$		$x^* = -3$ $x_0 = -3.3500642513$	
i		$ x_i - x^* $	$KT(i)$	$ x_i - x^* $	$KT(i)$
1		1.7962719444e-2	5.46044101e-2	0.1546358144	1.7111102871
2		5.0758675434e-4	1.4938362841e-2	3.9625707509e-2	2.9005874531
3		4.2129220718e-7	2.2360605911e-3	4.880109845e-6	16.669857343

		$x^* = 1$ $x_0 = 0.8445802935$		$x^* = 2$ $x_0 = 2.0376547064$	
i		$ x_i - x^* $	$KT(i)$	$ x_i - x^* $	$KT(i)$
1		1.2052125422e-2	3.0777915006e-2	1.6326953295e-3	6.020339117e-3
2		9.7459148339e-5	4.9776391861e-2	3.2995757618e-2	5.030880003e-4
3		6.5464896532e-9	1.7282074285e-4	1.352200184e-11	7.026191162e-6

For the Kantorovich analysis,

$$[h_0(u_1), h_0(r_1), h_0(r_3), h_0(u_2), h_0(u_3), h_0(r_2)] \quad (29)$$

$$= [6.0536283540, 9.6767648688, 0.2635125024, 133.22056221, 216.11264014, 0.1671294559]$$

Thus only points  $r_2$  and  $r_3$  are acceptably close to a root. The critical points for which the derivative  $f'(x)$  are zero:

$$x_{crit} = [-3.5794772231, -1.2520736568, 1.5336103231] \quad (30)$$

and are obtained by recursive use of the approach in section 3 since the derivative of eq. (23) with respect to  $x$  yields a quadratic for the right-hand-side. This establishes 4 different regions and also tells us we must take extra care for the region  $x \leq 0$  and that the region  $Y = e^{cx} \in [1, Y_{max}]$  needs some extra granularity by which to extra two more roots. Evaluating the eq. (23) at  $Y = 1, \frac{1}{2}Y_{max}, Y_{max}$  where  $Y_{max} = 60$  and collecting only the real results:

$$[t_1, t_2, t_3, t_4, t_5, t_6] \quad (31)$$

$$= [-4.1177608579, -3.3500642513, -1.8639130872, 1.4981553954, 2.2412309775, 2.6250792807]$$

and for these points, the Kantorovich  $h_0$  values are respectively:

$$[h_0(t_1), h_0(t_2), h_0(t_3), h_0(t_4), h_0(t_5), h_0(t_6)] \quad (32)$$

$$= [0.5471485847, 3.3902986514, -5.5923736326, 193.56899958, 0.6673918032, 0.9881773857]$$

The results are shown in Table 4). Note that we present the case where  $t_2 = -3.3400642513$  as a starting case even if  $h_0(t_2) > 1$ . However, the Newton-Raphson converges nonetheless to a root. It is important to know that the Kantorovich theorem provides sufficient rather than necessary conditions. In principle, we could go as far as quartic polynomial for the right-hand-side of eq. (2) namely  $N = 4$  and  $M = 0$  but no further since a fourth degree polynomial is the highest degree polynomial for which the roots can be expressed in terms of the coefficients according to the Abel-Rufini theorem. The determinations of bounds could be improved especially for higher-order polynomials using known methods for polynomials.

## 5 Outline of General Algorithm

From sections 3 and 4, we can infer the general algorithm for obtaining the real roots of eq. (2) for  $M = 0$  and  $N = 1 \dots 4$ :



1. Obtain coefficient  $a_0$  and roots  $r_i$  for  $i = 1 \dots N$  of polynomial on right-hand-side of eq. (2).
2. Differentiate eq. (2) with respect to  $x$ . This creates an equation just like eq. (2) but with the right-hand-side replaced by a polynomial of degree  $N - 1$ . Solve for the real roots yielding the critical points  $f'(x) = 0$  for the Kantorovich algorithm.
3. Divide region of  $x$  into  $x \geq 0$  and  $x < 0$ .
4. Obtain *real* bounds for  $Y = e^{-c x} \in [0, 1)$ , namely the values  $Y = 0$  and  $Y = 1$  for region  $x \geq 0$ . Sort the results.
5. Apply reflection symmetry  $x \rightarrow -x$  and see what happens to  $a_0$  and  $r_i$  for  $i = 1 \dots N$ .
6. Obtain real bounds for  $Y = e^{c x} \in [1, Y_{max}]$  where  $Y_{max}$  is greater in magnitude than the absolute value of the small critical value of Step 2. Sort the results.
7. For the bounds determined in the last step, add if need be, intermediate points for steps 4 and 6.
8. Evaluate the eq. (2) and  $h_0$  for these points obtained in steps 4 and 6.
9. Apply Newton-Raphson scheme for cases when  $h_0 \leq 1$  and for points when Newton-Raphson scheme converges.
10. Collect and sort all real roots obtained.

## 6 Conclusions

We have outlined a method for obtaining all the roots of special cases of eq. (2) for  $M = 0$ ,  $N = 2$  (specifically eq. (1)) and  $N = 3, 4$ . We make use of the explicit formulae for obtaining roots of respectively quadratic, cubic and quartic polynomials and also the Kantorovich theorem within the Newton-Raphson scheme. The method is *recursive* that in solving eq. (2), it requires finding the critical points of the Kantorovich theorem, namely  $f'(x) = 0$  and thus the solution for eq. (2) for a polynomial of one degree less i.e.  $N - 1$ . For  $N = 2$  or eq. (1), these critical points are expressed in terms of the standard Lambert  $W$  function, namely eq. (20). The method here could serve as functionality for e.g. Maple's `fsolve` implementation for real roots.

We are not ruling out the possibility that the method shown here could be generalized to the complex plane. The formulae for the roots of quadratic, cubic and quartic polynomials apply equally to the complex plane. Moreover, the Newton-Raphson scheme and the Kantorovich theorem can be generalized to the complex plane. However, establishing the bounds becomes more different likely requiring bounds according to a norm definition and these bounds need to be vindicated. It is likely that the complex plane needs to be separated into four quadrants for  $\Re x \geq 0$  and  $\Re x \leq 0$  as well as  $\Im x \geq 0$  and  $\Im x \leq 0$ . At any rate, one would need an incentive to make this challenging generalization to the complex; the original incentive having come from physical problems involving real quantities.

The results herein combined out previous results [1] reinforce the notion that our generalization is *natural* and shows how the various cases of the generalization are connected to each other, not unlike the way polynomials are connected to each other.

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## References

- [1] T. C. Scott, G. J. Fee and J. Grotendorst, *Asymptotic series of Generalized Lambert W Function*, accepted by SIGSAM, (2013).
- [2] T. C. Scott, J. F. Babb, A. Dalgarno, and J. D. Morgan III, *The Calculation of Exchange Forces: General Results and Specific Models*, J. Chem. Phys. **99**, (1993), 2841-2854.
- [3] R. B. Mann and T. Ohta, *Exact solution for the metric and the motion of two bodies in  $(1 + 1)$ -dimensional gravity*, Phys. Rev. D. **55**, (1997), 4723-4747.
- [4] P. S. Farrugia, R. B. Mann, and T. C. Scott, *N-body Gravity and the Schrödinger Equation*, Class. Quantum Grav. **24**, (2007), 4647-4659.
- [5] T. C. Scott, R. B. Mann and R. E. Martinez II, *General Relativity and Quantum Mechanics: Towards a Generalization of the Lambert W Function*, AAECC, **17**, (2006) 41-47.
- [6] A. A. Frost, *Delta-Function Model. I. Electronic Energies of Hydrogen-Like Atoms and Diatomic Molecules*, J. Chem. Phys. **25**, (1956), 1150-1154.
- [7] P. R. Certain and W. Byers Brown, *Branch Point Singularities in the Energy of the Delta-Function Model of One-Electron Diatoms*, Intern. J. Quantum Chem. **6**, (1972), 131-142.
- [8] W. N. Whitton and W. Byers Brown, *The Relationship Between the Rayleigh-Schrödinger and Asymptotic Perturbation Theories of Intermolecular Forces*, Int. J. Quantum Chem. **10**, (1976), 71-86.
- [9] T. C. Scott, M. Aubert-Frécon and J. Grotendorst, *New approach for the electronic energies of the hydrogen molecular ion*, Chem. Phys. **324**, (2006), 323-338.
- [10] B. W. Char, K. O. Geddes, G. H. Gonnet, B. L. Leong, M. B. Monagan and S. M. Watt, *First Leaves: A Tutorial Introduction to Maple V*, Springer-Verlag, New York, (1992).
- [11] <http://en.wikipedia.org/wiki/Intermediate-value-theorem>
- [12] M. Abramowitz, I. A. Stegun, Handbook of Mathematical Functions (9th printing), p.18, New York, Dover (1972).
- [13] <http://mathworld.wolfram.com/NewtonsMethod.html>
- [14] P. Sebah and X. Gourdon, "Newton's method and higher order iterations", (Oct.3 2001) <http://numbers.computation.free.fr/Constants/Algorithms/newton.html>
- [15] R. A. Tapia, "the Kantorovich theorem for Newton's method", American Mathematical Monthly **78**, No. 4, 389-392 (Apr. 1971).
- [16] M. Giusti, G. Lecerf, B. Salvy and J. C. Yakoubsohn, "On Location and Approximation of Clusters of Zeroes of Analytic Function", Foundations of Computational Mathematics, **5**, 257-311 (2005).