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Analysis of Traub's method for cubic

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Abstract

The dynamical analysis of the Kurchatov scheme is extended to Traub's method. The difference here is that Traub's method requires two additional starting points. Therefore, the map is 3-dimensional instead of 2-D. We obtain a complete description of the dynamical planes and show that the method is stable for cubic polynomials.

Keywords: Nonlinear equations, simple roots, Derivative-free methods
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1. Introduction

The solution of a single nonlinear equation

$$f(x) = 0 \tag{1}$$

can be found in applied science and engineering. For example, the Colebrook equation [1] to find the friction factor. Most numerical solution methods are based on Newton's scheme, i.e., starting with an initial guess x_0 for the root ξ, we create a sequence $\{x_n\}$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. \tag{2}$$

The convergence is quadratic, that is

$$|x_{n+1} - \xi| \leq C_2 |x_n - \xi|^2. \tag{3}$$

To increase the order, one has to include higher derivatives, such as in Halley's scheme [2] using first and second derivatives to achieve cubic convergence In order

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to avoid higher derivatives, one can use multipoint methods, see e.g. Petković et al. [3].

Derivative-free one-step methods are either linear (such as Picard), super-linear (such as secant) or even quadratic, such as Steffensen's method [4]. Clearly we can construct multipoint methods that are derivative-free. Most of those are based on Steffensen's method to achieve the highest possible order for the least number of function-evaluations.

In a recent article, Neta [5] has shown that there is a better choice for a first step, even though it is NOT second order. Traub's method [6], given by

$$x_{n+1} = x_n - \frac{f(x_n)}{\frac{(f(x_{n-2}) - f(x_n))}{(x_{n-2} - x_n)} - \frac{f(x_{n-2}) - f(x_{n-1})}{x_{n-2} - x_{n-1}} + \frac{f(x_{n-1}) - f(x_n)}{x_{n-1} - x_n}} \tag{4}$$

is of order 1.839 and it runs faster and have better dynamics than several other derivative-free methods. Clearly, one cannot get optimal methods (see Kung and Traub [7]) this way. Kung and Traub [7] conjectured that multipoint methods without memory using d function evaluations could have order no larger than 2^{d-1}. The efficiency index I defined as $p^{1/d}$. Thus an optimal method of order 8 has an efficiency index of $I = 8^{1/4} = 1.6817$ and an optimal method of order 4 has an efficiency index $I = 4^{1/3} = 1.5874$ which is better than Newton's method for which $I = \sqrt{2} = 1.4142$. The efficiency index of optimal method cannot reach a value of 2. In fact realistically one uses methods of order at most 8. For high order derivative-free methods based on Steffensen's method as first step, see Zhanlav and Otgondorj [8] and references there. Such methods are especially useful when the derivative is very expensive to evaluate and, of course, when the function is non-differentiable.

If we denote $x_{n-2} = w$ and $x_{n-1} = z$, then the Traub algorithm can be studied from a dynamical point of view as a three-dimensional map

$$T : \begin{pmatrix} w \\ z \\ x \end{pmatrix} -> \begin{pmatrix} z \\ x \\ x - \frac{f(x)}{\frac{(f(w) - f(x))}{w - x} - \frac{f(w) - f(z)}{w - z} + \frac{f(z) - f(x)}{z - x}} \end{pmatrix}. \tag{5}$$

Our study extends the results of Garijo and Jarque [9] for the secant method and of Campos et al. [10] for Kurchatov's scheme. Both methods require only one memory point.

For the cubic polynomial $p_3(x) = x(x-1)(x-a)$ the map becomes

$$T_a : \begin{pmatrix} w \\ z \\ x \end{pmatrix} -> \begin{pmatrix} z \\ x \\ \dfrac{N(w,z,x)}{D(w,z,x)} \end{pmatrix} \tag{6}$$

where

$$N(w,z,x) = (x^2 - (a-w-z+1)x - wz)x \tag{7}$$

and

$$D(w,z,x) = 2x^2 - (2a-w-z+2)x - wz + a. \tag{8}$$

The set of non-definition of T_a is given by

$$\delta_{T_a} = \left\{(w,z,x) \in \mathbb{R}^3 / 2x^2 - (2a-w-z+2)x - wz + a = 0\right\}. \tag{9}$$

Let

$$E_T = \mathbb{R}^3 \setminus \bigcup_{n\geq 0} T_a^{-n}(\delta_{T_a})$$

Points in E_T define a natural subset of $\mathbb{R}^3$ where all iterates of T_a are well defined and so $T_a : E_T \to E_T$ defines a smooth dynamical system.

The surface $D = 0$ is a quadric surface. In general, a quadric surface is given by

$$A_1x^2 + A_2w^2 + A_3z^2 + A_4xz + A_5xw + A_6wz + A_7x + A_8w + A_9z + A_{10} = 0 \tag{10}$$

By means of rotation and translation, we can get one of these forms

$$\begin{array}{l} Ax^2 + Bw^2 + Cz^2 + J = 0 \\ Ax^2 + Bw^2 + Iz = 0 \end{array} \tag{11}$$

In our case, $A_1 = 2, A_2 = A_3 = A_8 = A_9 = 0, A_4 = A_5 = 1, A_6 = -1, A_7 = -2(a+1)$ and $A_{10} = a$. If we take the following transformation

$$\begin{array}{l} x = \xi + 3\eta + 2\lambda \\ w = a_2\xi + b_2\eta + c_2\lambda \\ z = 2\eta + \lambda \end{array} \tag{12}$$

we get 3 equations for the unknown whose solution is $a_2 = 4$, $b_2 = -18$, $c_2 = -13$ and the surface becomes

$$6\xi^2 + 6\eta^2 - 3\lambda^2 - 2(a+1)\xi - 6(a+1)\eta - 4(a+1)\lambda + a = 0 \tag{13}$$

Now we do a translation

$$\begin{array}{l} \Xi = \xi - \frac{a+1}{6} \\ H = \eta - \frac{a+1}{2} \\ \Lambda = \lambda + \frac{2}{3}(a+1) \end{array} \tag{14}$$

The equation becomes

$$\Xi^2 + H^2 - \frac{1}{2}\Lambda^2 = \frac{1}{6}(-a + \frac{1}{3}(a+1)^2) \tag{15}$$

This surface is a hyperboloid of one sheet. The axis of symmetry is the Λ axis. The trace of the surface can be obtained by taking Λ constant. If $\Lambda = \Lambda_0$ then the equation of the trace is

$$\Xi^2 + H^2 = \frac{1}{6}(-a + \frac{1}{3}(a+1)^2 + 3\Lambda_0^2) \tag{16}$$

This is a circle centered at $\Xi = 0$, $H = 0$. The radius is

$$r(a) = \sqrt{\frac{1}{6}(-a + \frac{(a+1)^2}{3} + 3\Lambda_0^2)}.$$

Clearly the minimum value of the radius is when $\Lambda_0 = 0$ and $a = \frac{1}{2}$. At that point the radius is $\frac{1}{\sqrt{24}}$, see Figure 2.

Plotting the surface δ_{T_a} (9) (see Figures 1-3), we see a hyperboloid of one sheet for three different values of a. Notice how the radius changes as a function of the value of a.

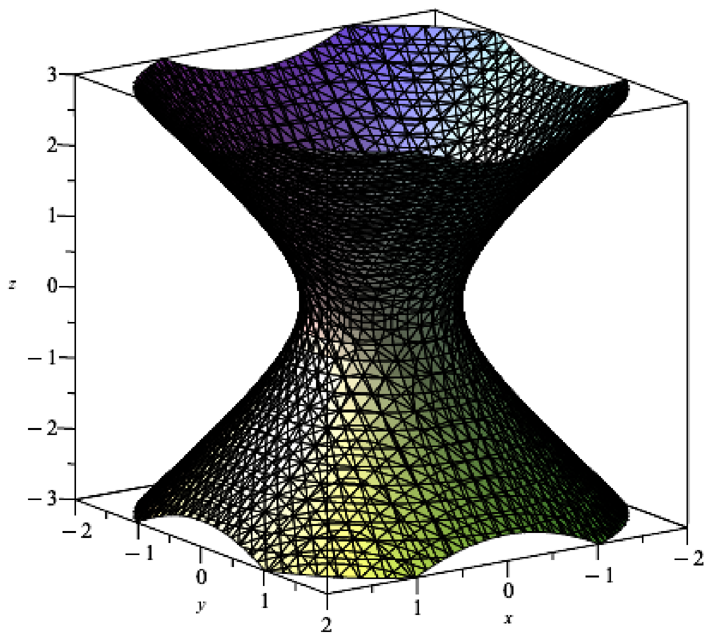


Figure 1: Surfaces on which $D = 0$ for $a = -1.5$. The minimum value of the radius is $r = \sqrt{19/72}$.

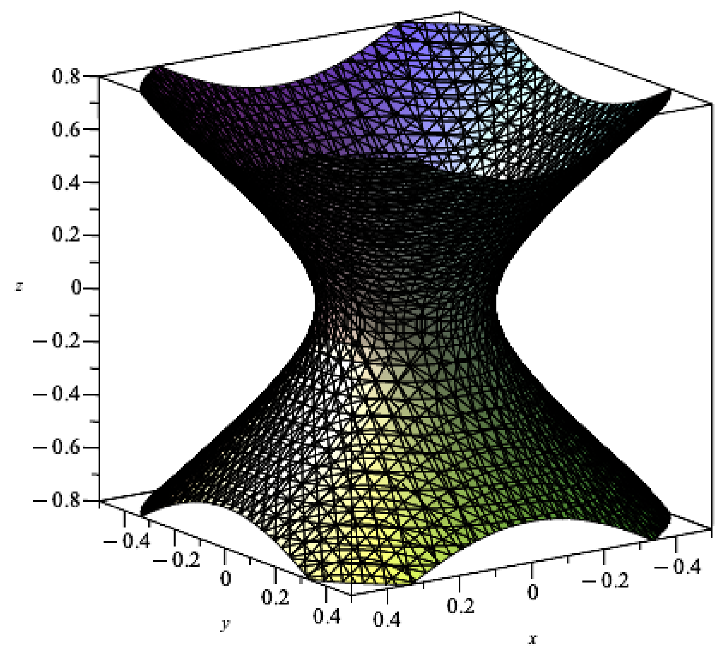


Figure 2: Surfaces on which $D = 0$ for $a = 0.5$. The minimum value of the radius is $r = 1/\sqrt{24}$.

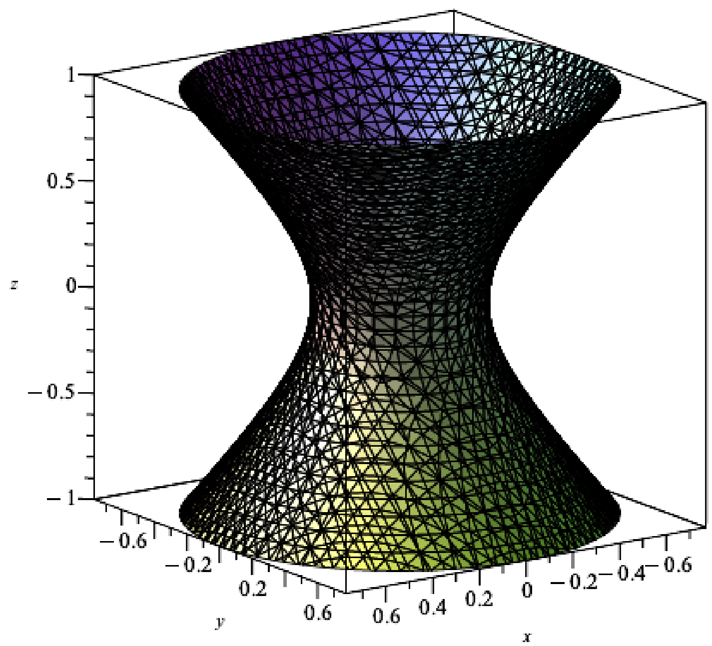


Figure 3: Surfaces on which $D = 0$ for $a = 2.0$. The minimum value of the radius is $r = 1/\sqrt{6}$.

The origin in the $\Xi H \Lambda$ coordinate system corresponds to $x = w = z = \frac{a+1}{3}$.

If $x = 0$ then both (7) and (8) vanish. The limit as x tends to zero is zero, since the numerator is a polynomial in x of degree higher than the denominator. This is called a focal point. A focal point Q is called simple if the tangent planes to the surfaces N and D are **not** parallel. This can be expressed by the condition

$$\|\nabla N \text{x} \nabla D\| \neq 0 \qquad \text{at } Q. \tag{17}$$

We now evaluate the gradient of the surfaces $N(w, z, x)$ and $D(w, z, x)$ at $x = 0$

$$\begin{aligned}
\frac{\partial N}{\partial w} &= x^2 - zx \\
\frac{\partial N}{\partial z} &= x^2 - wx \\
\frac{\partial N}{\partial x} &= 3x^2 - 2(a + 1 - w - z)x - wz \\
\frac{\partial D}{\partial w} &= x - z \\
\frac{\partial D}{\partial z} &= x - w \\
\frac{\partial D}{\partial x} &= 4x - (2a + 2 - w - z)
\end{aligned} \tag{18}$$

Evaluating the derivatives at $x = 0$ and then substituting in (17), we have

$$\|\nabla N \text{x} \nabla D\| = |wz|\sqrt{w^2 + z^2} = |a|\sqrt{w^2 + z^2} \neq 0.$$

The surface $D(w, z, x) = 0$ can be described as follows: If $x = 0$ (on the wz coordinate plane) we have the hyperbola $wz = a$. If $x = z$ (a slanted plane through the w coordinate axis), then $x = z = \alpha_{1,2}$ and w is free. That is, lines through the given points. Similarly, if $x = w$ then $x = w = \alpha_{1,2}$ and we have lines. If $x = w = z$, we get the two points

$$\alpha_{1,2} = \frac{(a + 1) \pm \sqrt{a^2 - a + 1}}{3}$$

If $w = z$ again we get a hyperbola

$$-2x^2 + 2(a + 1)x - 2xw + w^2 - a = 0. \tag{19}$$

If $x = \alpha_{1,2}$ then $D = 0$ but $N \neq 0$. Similarly if $x = z$ or $x = w$, $N \neq 0$. If $w = z$, then when $D = 0$ we can see if there is a point on the hyperbola (19) that will satisfy $N = 0$.

Since $x \neq 0$ and $w = z$, we have the set of equations

$$\begin{array}{l} x^2 - (a+1)x - w^2 + 2wx = 0 \\ -2x^2 + 2(a+1)x + w^2 - 2wx = a \end{array} \tag{20}$$

Adding the two equation we have

$$-x^2 + (a+1)x = a$$

whose two solutions are $x = a$ and $x = 1$. For $x = a$ we get $w = z = a \pm \sqrt{a(a-1)}$. For $x = 1$ we get $w = z = 1 \pm \sqrt{1-a}$.

The fixed points of the map

$$T_a(w_0, z_0, x_0) = (w_0, z_0, x_0)$$

are

$$\begin{aligned} w &= z \\ z &= x \\ x &= \frac{(x^2 - (a - w - z + 1)x - wz)x}{2x^2 - (2a - w - z + 2)x - wz + a} \end{aligned}$$

or

$$x(2x^2 - (2a - 2x + 2)x - x^2 + a) = x(x^2 - (a + 1 - 2x)x - x^2)$$

One solution is $x = 0$ and the other two are the solution of

$$x^2 - (a+1)x + a = 0$$

which are $x = 1$ and $x = a$. The fixed points coincide with the roots of $p_3(x)$.

In order to study their stability, we build the Jacobian matrix

$$JT_a(w, z, x) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ \frac{\partial G}{\partial w} & \frac{\partial G}{\partial z} & \frac{\partial G}{\partial x} \end{pmatrix} \tag{21}$$

where $G(w, z, x) = \dfrac{x(x^2 - (a + 1 - w - z)x - wz)}{(2x^2 - (2a + 2 - w - z)x - wz + a)}$ and the partial derivatives are

$$\frac{\partial G}{\partial w} = -\frac{1}{4} \frac{x(x-1)(x-z)(a-x)}{(-x^2 + (a - w/2 - z/2 + 1)x + wz/2 - a/2)^2}$$

$$\frac{\partial G}{\partial z} = \frac{1}{4}\frac{x(x-1)(w-x)(a-x)}{(-x^2+(a-w/2-z/2+1)x+wz/2-a/2)^2}$$

$$\frac{\partial G}{\partial x} = \frac{1}{4}\frac{(2x^4+(-4a+2w+2z-4)x^3+q_2(x,w,z)x^2-q_1(w,z,x))}{(-x^2+(a-w/2-z/2+1)x+wz/2-a/2)^2}$$

with

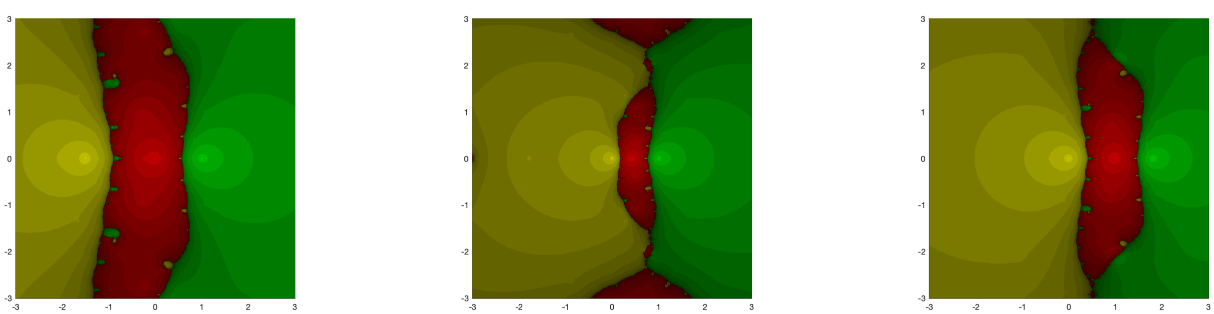
$$q_2(w,z,x) = w^2+(-3a+z-3)w+z^2+(-3a-3)z+2a^2+7a+2$$

$$q_1(w,z,x) = 2(a+1-w-z)(-wz+a)x+(wz)^2-awz.$$

The partial derivatives at the roots are $\dfrac{\partial G}{\partial w} = \dfrac{\partial G}{\partial z} = 0$ and

$$\frac{\partial G}{\partial x} = \begin{cases} \dfrac{wz}{wz-a} & \text{at} \quad x=0 \\ \dfrac{(w-1)(z-1)}{(w-1)(z-1)+a-1} & \text{at} \quad x=1 \\ \dfrac{(w-a)(z-a)}{(w-a)(z-a)+(1-a)a} & \text{at} \quad x=a \end{cases}$$

Therefore the fixed points are attractive.



(a) $a < 0$ (b) $0 < a < 1$ (c) $a > 1$

Figure 4: Dynamical planes of Traub's method for different values of a

2. Dynamical study of the methods

Let us firstly analyze the curves or surfaces that are mapped on fixed points of operator $T_a(w,z,x)$:

$$\begin{aligned} T_a(w,z,x) = (0,0,0) &\Leftrightarrow z = x = 0 \text{ and } G(w,z,x) = 0, \\ &\Leftrightarrow G(w,0,0) = 0, \\ &\Leftrightarrow G(w,0,0) = \frac{0}{a} = 0, \end{aligned}$$

therefore, $T_a(w,z,x)$ maps to the fixed point at the origin if and only if $z = x = 0$. On the other hand,

$$\begin{aligned} T_a(w,z,x) = (1,1,1) &\Leftrightarrow z = x = 1 \text{ and } G(w,1,1) = 1, \\ &\Leftrightarrow \frac{1-a}{1-a} = 1. \end{aligned}$$

So, $T_a(w,z,x) = (1,1,1) \Leftrightarrow z = x = 1$. Finally,

$$\begin{aligned} T_a(w,z,x) = (a,a,a) &\Leftrightarrow z = x = a \text{ and } G(w,a,a) = a, \\ &\Leftrightarrow \frac{a(a^2 - (a+1-w-a)a - wa)}{2a^2 - (2a+2-w-a)a - wa + a} = a, \end{aligned}$$

then, $T_a(w,z,x) = (a,a,a) \Leftrightarrow z = x = a$ and plane $z = x$ maps $T_a(w,z,x)$ to its fixed points.

2.1. Focal points and prefocal curves

Taking into account that focal points are those satisfying that at least one component is 0/0 with finite limit, focal points of T_a satisfy

$$x(x^2 - (a - w - z + 1)x - wz) = 0, \qquad (22)$$

$$2x^2 - (2a - w - z + 2)x - wz + a = 0. \qquad (23)$$

- Therefore, if in (22) we consider $x = 0$ and replace it in (23), we get the hyperbola $wz = a$, see Figure 5.

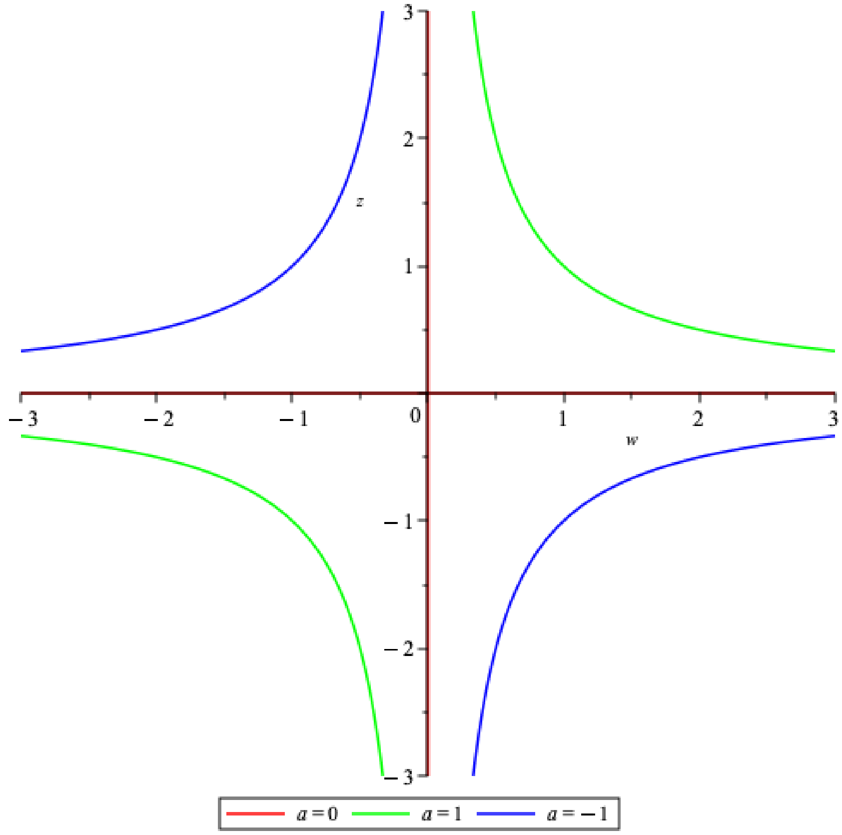


Figure 5: Focal curve for $x = 0$ for various values of a

- $N = 0$ also if $x^2 - (a - w - z + 1)x - wz = 0$, then $x^2 - ax - x = wz - wx - zx$ and replacing in (23), we get the surface in $\mathbb{R}^3$,

  $$w(z - x) - zx + a = 0.$$

  However, $x^2 - ax - x = wz - wx - zx$, so

  $$x^2 - (a + 1)x + a = 0 \Leftrightarrow x = a \ \text{ or } x = 1.$$

  If $x = 1$, the focal curve is $wz - w - z + a = 0$ (Figure 6) and, if $x = a$, $wz - aw - az + a = 0$, (Figure 7).

Thus, in all cases the focal curve is a hyperbola. Notice that in Figure 7 we have plotted the cases that $a = 0$ and $a = 1$. Those plots are just the asymptotes of the hyperbolas in Figures 5 and 6, respectively.

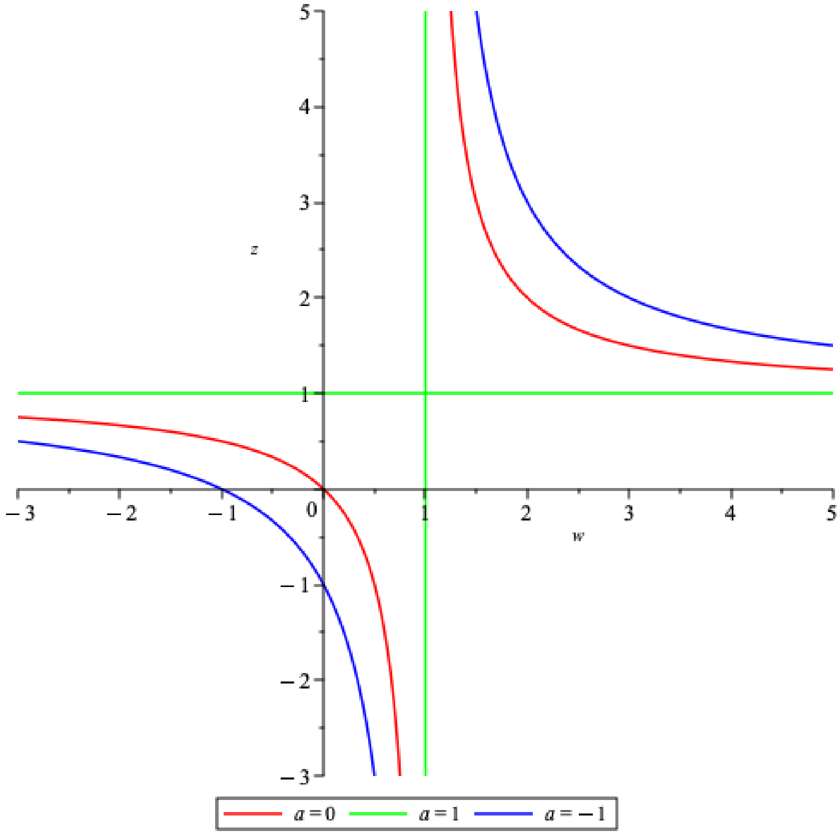


Figure 6: Focal curve for $x = 1$ for various values of a

$$\text{focal curves} \qquad \begin{cases} wz = a & x = 0 \\ wz - w - z + a = 0 & x = 1 \\ wz - a(w+z) + a = 0 & x = a \end{cases} \tag{24}$$

To show that these points on the focal curves are all simple, we use (17)

$$\|\nabla N \text{ x } \nabla D\| = \begin{cases} |a|\sqrt{w^2 + z^2} \neq 0 & \text{at} \quad x = 0 \\ \\ |(w-1)(1-z)|\sqrt{(w-1)^2 + (z-1)^2} \\ = |a-1|\sqrt{(w-1)^2 + (z-1)^2} \neq 0 & \text{at} \quad x = 1 \\ \\ |(w-a)(a-z)|\sqrt{(w-a)^2 + (z-a)^2} \\ = |a(1-a)|\sqrt{(w-a)^2 + (z-a)^2} \neq 0 & \text{at} \quad x = a \end{cases}$$

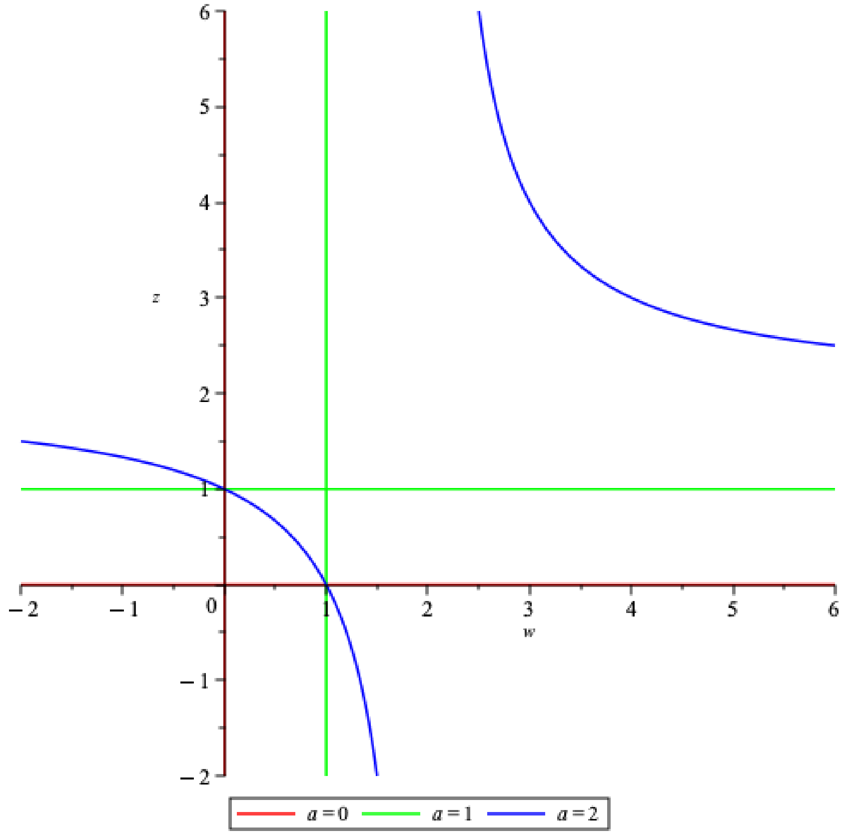


Figure 7: Focal curve for $x = a$ for various values of a

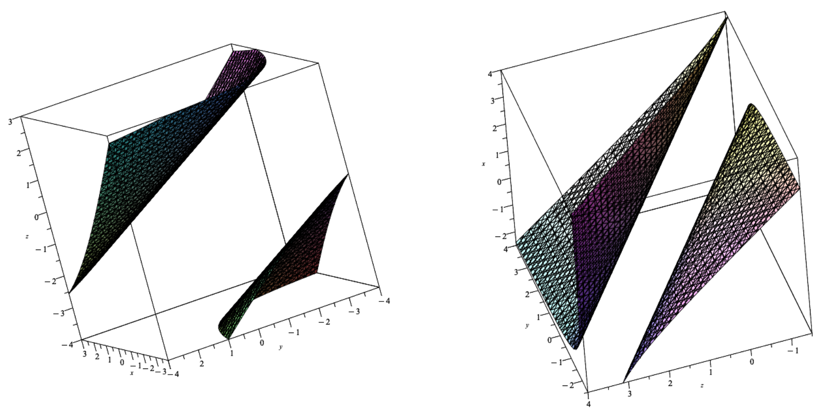
We now look at the prefocal surface. A point Q in δ_{T_a} is a prefocal point if T_3, the third component of T_a (see (6)), evaluated at Q takes the form 0/0 (i.e. $N(Q) = D(Q) = 0$), and there exists a smooth simple arc $\gamma := \gamma(t)$, $t \in (-\epsilon, \epsilon)$, with $\gamma(0) = Q$ such that $\lim_{t\to 0} T_3(\gamma)$ exists and it is finite. Moreover, the line $L_Q = (w, z, x) \in R^3, (w, z) = F(Q)$, where $F(Q)$ is the first two components of T_a. The line is the intersection of the two plane $w = z$ and $z = x$ evaluated at Q when $x = a$. The equations of the line are

$$\begin{aligned} w &= w_0 + t \\ z &= z_0 + t \\ x &= a + t \end{aligned} \tag{25}$$

On δ_{T_a}, $x = a$ (for $a \neq 0$ and $a \neq 1$) and $wz - a(w + z) + a = 0$. Given w_0 on this hyperbola, we get $z_0 = a\frac{w_0-1}{w_0-a}$ and the line for each w_0 is

$$\begin{array}{l} w = w_0 + t \\ z = a\frac{w_0-1}{w_0-a} + t \\ x = a + t \end{array} \tag{26}$$

The set of all these lines (for all possible $w_0 \neq a$ on the focal curve) is the prefocal surface. This surface is a cylinder and the lines are called rulings, see the definition in [13]. In the next figure we show the prefocal surface for a given a value.



(a) $a = -2.0$ (b) $a = 1.5$

Figure 8: Prefocal surfaces of Traub's method for different values of a

2.2. Inverse of T_a and its properties

In order to understand the global dynamics of the map T_a, it is important to find the inverse map T_a^{-1} and in which regions of the phase space the inverse is defined. Let (w', z', x') be a given point, then

$$T_a^{-1}\begin{pmatrix} w' \\ z' \\ x' \end{pmatrix} = \begin{pmatrix} w = \frac{z'^3-(a+1-w'-2x')z'^2+(2a+2-w')z'x'-ax'}{(x'-z')(z'-w')} \\ z = w' \\ x = z' \end{pmatrix}. \tag{27}$$

The value of w is obtained by solving $x' = \frac{N(w,w',z')}{D(w,w',z')}$. We now look at the signs of the following 3 functions:

1. $x - z$
2. $z - w$
3. $z^3 - (a - w + 1 - 2x)z^2 + (2a + 2 - w)xz - ax$

If all 3 or just one of them is positive then $w > 0$, otherwise $w < 0$. The two planes $z = x$ and $z = w$ and the surface defined by the cubic $z^3 - (a - w + 1 - 2x)z^2 + (2a + 2 - w)xz - ax = 0$ are the boundaries of the regions. See Figure 9 for the surface defined by the cubic for two different values of the parameter a.

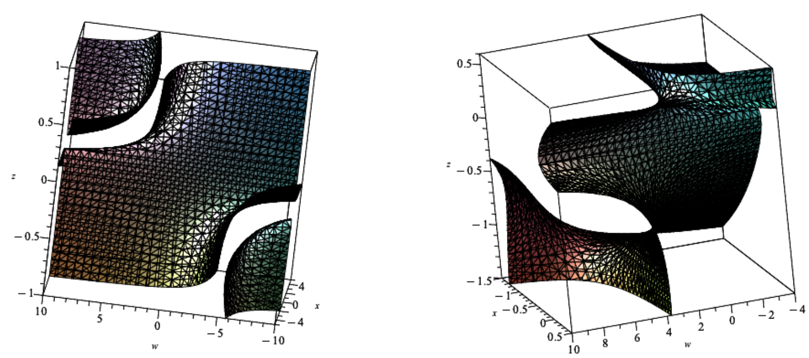
The three surfaces meet at 3 possible points, the first is $z = x = w = 0$ and the other two solutions are given by solving the quadratic equation (using $x = z = w$)

$$3x^2 + (a + 1)x - a = 0. \tag{28}$$

This equation has two complex roots as long as $a \in (-7 - \sqrt{48}, -7 + \sqrt{48})$. For other values of a the real roots are

$$\frac{-a - 1 \pm \sqrt{a^2 + 14a + 1}}{6}. \tag{29}$$

Notice that unlike the secant [9] and Kurchatov's [10] schemes, the solutions are not the 3 fixed points.



(a) $a = -1.5$ (b) $a = 1.5$

Figure 9: One of the boundaries of the region for different values of a. The other two boundaries are the planes $x = z$ and $w = z$.

These surfaces form the boundary of the regions but they are not a locus of critical points where the two inverses are defined and merged, since the denominator vanishes when $x = z = w$. The locus is

$$LC = \left\{ (w.z,x) \in \mathbb{R}^3 / x = \frac{z^3 - (a+1-w)z^2}{-2z^2 - (2a+2-w)z + a} \right\}.$$

Merging preimages are also in another set, denoted LC_{-1}, that it is included in the set of points for which the determinant of the Jacobian vanishes, i.e. $x = z$ or which is the same $\frac{\partial G}{\partial w} = 0$ (see (21).) The set $LC_{-1} = \{(w.z,x) \in \mathbb{R}^3 / det(J(T_a) = 0\}$ has critical points $z = x$ identical to the points of intersection of the boundaries above. In the case $z = 0$ then w can take any value. In the case z satisfies (28) then w satisfies the quadratic equation

$$zw^2 + (2z^2 + 2a - 3(a+1)w)z = 2z^3 + 4(a+1)z^2 - 3az - 2(a+1)^2 z + 2a(a+1).$$

Conclusions

The oldest method with memory is probably the secant method where one replaces the slope of the tangent line in Newton's method by the slope of the secant. This, in turn, requires the use of an additional point beside the previous one. We have generalized the analysis for two methods having one memory point (namely the secant and Kurchatov's schemes) to a method requiring two memory points. In this paper we chose to study Traub's method, which received a lot of attention recently. The analysis in 3-dimensions is not a trivial extension of the 2-dimensional analysis in the literature. But the generalization to methods using more than two memory points is relatively simple.

We have proved that Traub's method is completely stable for any polynomial of degree three, since the only attractors for any value of the parameter are the roots of the polynomial.

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