

A PSEUDO LAGUERRE METHOD

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Abstract. Newton's method to find the zero of a function in one variable uses the ratio of the function and derivative values, but it does not use the information provided by these quantities separately. It is a natural question to ask what a method would look like that does take into account these values instead of just their ratio. We answer that question in the case of a polynomial with all real zeros, the result being a method that is somewhat reminiscent of Laguerre's method.

1. Introduction

Finding the zeros of a function in one real variable is a classical problem in numerical analysis. There exist many methods to solve it, but probably none are as well-known as Newton's method. For a function $f(z)$, this method generates iterates according to $z_{n+1} = z_n - f(z_n)/f'(z_n)$ that, if one is lucky, converge to a zero of $f(z)$. Geometrically, each iterate is simply the intersection with the z -axis of the tangent to $f(z)$ at the previous iterate.

However, Newton's method does not seem to deal very efficiently with the information it requires: both $f(z)$ and $f'(z)$ need to be computed, but only the ratio of these two values determines the next iterate. In other words, the method generates the same step from some point \bar{z} when, e.g., $f(\bar{z}) = 2$ and $f'(\bar{z}) = 4$ as when $f(\bar{z}) = 1$ and $f'(\bar{z}) = 2$. Taking into account the value of $f(\bar{z})$ would allow one to distinguish between these two situations, and the question arises whether it would be possible to amend Newton's method in a natural way so that it does. We propose one way to achieve this in the case of a polynomial with all real zeros when the starting point lies outside the interval formed by those zeros. Although somewhat uglier, the resulting method is faster than Newton's method and can be interpreted as a downgraded Laguerre method (see below).

The purpose here is to discover what kind of method could result from taking both $f(\bar{z})$ and $f'(\bar{z})$ into account instead of just their ratio, regardless of the merits or lack thereof such a method would exhibit (although we will definitely discuss this

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as well). We are motivated by pure curiosity and our results are more theoretical than practical, although some potential applications are pointed out.

In [6] Newton's method was derived for a polynomial $p(z)$ with all real zeros by asking the following question: given $p'(\bar{z})/p(\bar{z})$ for a point \bar{z} to the right of the largest zero of $p(z)$, what is the largest possible zero of all polynomials of the same degree? The answer to that question yields an upper bound on the largest zero of the polynomial $p(z)$, and that upper bound turns out to be what one obtains by carrying out one Newton step from the point \bar{z} . An analogous situation arises with a point \bar{z} to the left of the smallest zero. A similar question, this time using both $p'(\bar{z})/p(\bar{z})$ and $(p'(\bar{z})/p(\bar{z}))'$, leads to Laguerre's method [3, 6], which is better and faster than Newton's method, but at the price of computing the second derivative. It is this general approach that we will use to obtain our results. We will concentrate on the largest zero, the treatment of the smallest zero being entirely analogous.

2. Definition of the method

Throughout, we assume that the polynomial we seek the zeros of is given by

$$p(z) = z^n + a_{n-1}z^{n-1} + \cdots + a_1z + a_0 = (z - x_1)(z - x_2) \cdots (z - x_n), \quad (1)$$

with $n \geq 3$, and where the zeros $\{x_j\}_{j=1}^n$ are all real and satisfy $x_1 \geq x_2 \geq \cdots \geq x_n$. We define the function $\phi(z)$ as the logarithmic derivative of $p(z)$ for which it can easily be verified that

$$\phi(z) = \frac{p'(z)}{p(z)} = \sum_{j=1}^n \frac{1}{z - x_j}.$$

Clearly, for any $z > x_1$, we have that $p(z) > 0$, $p'(z) > 0$, and $\phi(z) > 0$.

In [6] the following optimization problem was considered for $\bar{z} > x_1$:

$$\sup \left\{ \zeta_1 : \sum_{j=1}^n \frac{1}{\bar{z} - \zeta_j} = \phi(\bar{z}); \zeta_j < \bar{z}, j = 1, 2, \dots, n \right\}, \quad (2)$$

where the variables of the problem are the ζ_j 's. Its solution is obtained for $\zeta_1 = \bar{z} - 1/\phi(\bar{z})$ and $\zeta_j = -\infty$ ($j \neq 1$), resulting in Newton's iteration. Likewise [3, 6], Laguerre's method is obtained from

$$\sup \left\{ \zeta_1 : \sum_{j=1}^n \frac{1}{\bar{z} - \zeta_j} = \phi(\bar{z}); \sum_{j=1}^n \frac{1}{(\bar{z} - \zeta_j)^2} = \phi'(\bar{z}); \zeta_j < \bar{z}, j = 1, 2, \dots, n \right\}. \quad (3)$$

Its solution is given by

$$\zeta_1 = \bar{z} - \frac{n}{\phi(\bar{z}) + \sqrt{(n-1)(n\phi'(\bar{z}) - \phi^2(\bar{z}))}}.$$

In other words, both the Newton and Laguerre iteration formulas can be obtained for a polynomial with all real zeros from a starting point outside the interval containing the zeros by considering an appropriate optimization problem. The same

is also true for Ostrowski's "square root" method [6]. This strategy seems tailor-made for what we have in mind since adding requirements simply translates into adding constraints to the same optimization problem. Our requirement to utilize the value $p(\bar{z})$ means adding just one constraint to the problem defining Newton's method. The resulting method can then be seen as belonging to the same family as several classical methods.

Even though this optimization framework is restricted to polynomials with all real zeros and a real starting point outside the interval containing them, the methods it generates can have wider validity and additional properties. For example, both Newton's and Laguerre's methods are valid for general polynomials and starting points, including imaginary ones, but Newton's method does not necessarily converge whereas Laguerre's method converges from any starting point when all zeros are real.

Let us now go back to our original purpose, namely to incorporate the information provided by both $p(\bar{z})$ and $p'(\bar{z})$. Using the aforementioned optimization framework, we compute an upper bound on x_1 by solving

$$\sup \left\{ \zeta_1 : \prod_{j=1}^n (\bar{z} - \zeta_j) = p(\bar{z}); \sum_{j=1}^n \frac{1}{\bar{z} - \zeta_j} = \phi(\bar{z}); \zeta_j < \bar{z}, j = 1, 2, \dots, n \right\}. \quad (4)$$

Looking at the equality constraint in (2), which defined Newton's method, we see that the closer \bar{z} is to x_1 , the more informative that constraint becomes because then $\phi(\bar{z}) \approx 1/(\bar{z} - x_1)$, which implies that $\zeta_1 \approx x_1$, i.e., we can expect a close upper bound on x_1 . A similar situation exists for both constraints in Laguerre's method and a similar situation also exists for (4) since it can equivalently be written as

$$\sup \left\{ \zeta_1 : \sum_{j=1}^n \ln(\bar{z} - \zeta_j) = \ln(p(\bar{z})); \sum_{j=1}^n \frac{1}{\bar{z} - \zeta_j} = \phi(\bar{z}); \zeta_j < \bar{z}, j = 1, 2, \dots, n \right\}. \quad (5)$$

Thus we have two constraints that behave very much like the two constraints in Laguerre's method, although they are not as effective since the less negative the power appearing in the equality constraints, the worse the upper bound. The equality constraints in (5) are like the ones for Laguerre's method but with the exponents increased from -1 to a natural logarithm, and from -2 to -1 , respectively. Similar, but not as good, which is the price for not computing the second derivative, and therefore a "pseudo Laguerre method". We note that it is guaranteed to be better than Newton's method because the defining optimization problem is more constrained, leading to a lower upper bound.

3. Derivation of the method

Next, we need to solve the optimization problem in (4). This is done in the following theorem.

THEOREM 1. *Define $p(z) = (z - x_1)(z - x_2) \cdots (z - x_n)$, where all the x_j are*

real, $n \geq 3$, and $\phi(z) = p'(z)/p(z)$. Then, for any $\bar{z} > x_1$,

$$\sup \left\{ \zeta_1 : \prod_{j=1}^n (\bar{z} - \zeta_j) = p(\bar{z}); \sum_{j=1}^n \frac{1}{\bar{z} - \zeta_j} = \phi(\bar{z}); \zeta_j < \bar{z}, j = 1, 2, \dots, n \right\}$$

is obtained for $\zeta^* = \bar{z} - 1/s_*^{n-1}$, where $s_* > 0$ is the largest zero of the function

$$g(s) = s^n - \phi(\bar{z})s + \frac{n-1}{p(\bar{z})^{\frac{1}{n-1}}}.$$

This defines one iteration of our method, \bar{z} being the current iterate and ζ^* being the next one.

Proof. With the change of variables $\eta_j = 1/(\bar{z} - \zeta_j)$, the optimization problem is equivalent to solving

$$\sup \left\{ \eta_1 : \prod_{j=1}^n \eta_j = \frac{1}{p(\bar{z})}; \sum_{j=1}^n \eta_j = \phi(\bar{z}); \eta_j > 0, j = 1, 2, \dots, n \right\}, \quad (6)$$

where $p(\bar{z}), \phi(\bar{z}) > 0$. Replacing the constraints $\eta_j > 0$ in (6) by $\eta_j \geq 0$ does not change the optimal value because $\eta_j = 0$ is not feasible for any j , but it does make the feasible set closed and bounded and therefore compact. Since the functions in the constraints and the objective function are all differentiable on this compact feasible set, the supremum will be attained on that set and can be found among the points satisfying the first order (Karush-Kuhn-Tucker) optimality conditions (see, e.g., [2, Ch. 2]). These conditions state that there exist Lagrange multipliers λ and μ such that

$$1 + \lambda \prod_{j=2}^n \eta_j + \mu = 0 \quad \text{and} \quad \lambda \prod_{\substack{j=1 \\ j \neq k}}^n \eta_j + \mu = 0 \quad \text{for } k = 2, \dots, n.$$

The multipliers corresponding to the nonnegativity constraints do not play a role because they are zero since $\eta_j = 0$ is not feasible. If, for $k = 2, \dots, n$, we multiply the k th equation by η_k , then the first constraint in (6) gives $\lambda/p(\bar{z}) + \mu\eta_k = 0$, which in turn means that $\eta_k = -\lambda/(\mu p(\bar{z}))$, a value independent of k , because $\mu \neq 0$ (otherwise $\lambda = 0$ also and that would violate the first optimality condition). Setting $u = -\lambda/(\mu p(\bar{z}))$, the optimal solution is therefore obtained for $\eta_2 = \eta_3 = \dots = \eta_n = u$, and we have

$$\eta_1 u^{n-1} = \frac{1}{p(\bar{z})} \quad \text{and} \quad \eta_1 + (n-1)u = \phi(\bar{z}).$$

Eliminating u yields

$$\eta_1^{\frac{n}{n-1}} - \phi(\bar{z})\eta_1^{\frac{1}{n-1}} + \theta(\bar{z})\eta_1^{\frac{n}{1-n}} = 0, \quad \text{where } \theta(\bar{z}) = \frac{((n-1)p(\bar{z}))^{\frac{1}{n}}}{n-1}. \quad (7)$$

The equation for η_1 can be written as $g(\eta_1^{1/(n-1)}) = 0$, where $g(s) = s^n - \phi(\bar{z})s + \theta(\bar{z})\frac{n}{1-n}$. We note that this is the same function $g(s)$ as in the statement of the theorem. It is easy to verify that $g'(0) < 0$ and that $g''(s) > 0$ for $s > 0$, which implies that the function $g(s)$ has a unique minimum at $\bar{s} = (\phi(\bar{z})/n)^{1/(n-1)} > 0$ (see Figure 1). For $g(s) = 0$ to have real solutions, one must have that $g(\bar{s}) \leq 0$. To show that this is indeed the case, we denote by G and A the geometric and arithmetic means of the positive numbers η_j , respectively, and observe that $p(\bar{z}) = 1/G^n$ and $\phi(\bar{z}) = nA$. Because $G \leq A$, this means that $p(\bar{z})^{\frac{1}{n}}\phi(\bar{z}) = nA/G \geq n$. We have

$$\begin{aligned} g(\bar{s}) &= \left(\frac{\phi(\bar{z})}{n}\right)^{\frac{n}{n-1}} - \phi(\bar{z})\left(\frac{\phi(\bar{z})}{n}\right)^{\frac{1}{n-1}} + \frac{((n-1)p(\bar{z}))^{-\frac{1}{n-1}}}{(n-1)^{-\frac{n}{n-1}}} \leq 0 \\ \iff (1-n)\left(\frac{\phi(\bar{z})}{n}\right)^{\frac{n}{n-1}} + (n-1)p(\bar{z})^{-\frac{1}{n-1}} &\leq 0 \\ \iff p(\bar{z})^{-\frac{1}{n-1}} &\leq \left(\frac{\phi(\bar{z})}{n}\right)^{\frac{n}{n-1}} \\ \iff p(\bar{z})^{\frac{1}{n}} &\geq \frac{n}{\phi(\bar{z})}, \end{aligned}$$

which is precisely the arithmetic-geometric means inequality. We have obtained that $g(\bar{s}) \leq 0$ and the equation $g(s) = 0$ therefore has two solutions $s_1 \leq \bar{s} \leq s_2$, which means that the solution of (6) is given by $\eta_1 = s_2^{n-1}$. Setting $s_* = s_2$ and using the change of variables introduced at the beginning concludes the proof. ■

Theorem 1 defines the raw form of the method we obtained for a polynomial $p(z)$ when the values of both $p(z)$ and $p'(z)$ are taken into account, rather than just their ratio.

We remark that if $x_1 = x_2 = \dots = x_n$, then in the proof of the previous theorem we have $\bar{s} = (\bar{z} - x_1)^{-1/(n-1)}$ and $g(\bar{s}) = 0$, so that $s_1 = s_2 = \bar{s}$. This means that $\eta_1 = 1/(\bar{z} - x_1)$ and therefore $\zeta_1 = x_1$, i.e., the method converges in one iteration. The same property is not true for Newton’s method, although it does hold for Laguerre’s method. Therefore, unless specifically included, we will exclude this trivial case in what follows.

Let us now recast our method in a more convenient form. Since the point \bar{s} at which the function $g(s)$ in the proof of Theorem 1 achieves its minimum becomes unbounded in the limit as the iterates approach the largest zero of $p(z)$, so does s_2 , which is larger than \bar{s} . It would therefore be more practical to set $\eta_1 = (\theta(\bar{z})y)^{-1}$, with $\theta(\bar{z})$ as defined in (7), which turns computing the largest of the two zeros of $g(\eta_1^{1/(n-1)}) = 0$ on $(0, +\infty)$ into computing the smallest zero y_* of the two zeros of $f(y) = 0$ on $(0, +\infty)$, where

$$f(y) = y^{\frac{n}{n-1}} - \theta(\bar{z})\phi(\bar{z})y + 1. \tag{8}$$

The next iterate is then given by $\bar{z} - \theta(\bar{z})y_*$. The function $f(y)$ satisfies $f'(0) < 0$ and $f''(y) > 0$ for $y > 0$, so that $f'(y) < 0$ on $[0, y_*]$ (see Figure 1). Because of

these properties, Newton's method can be used to solve $f(y) = 0$ with guaranteed convergence from any starting point in $[0, y_*]$. Such a starting point could be $\bar{y} = 1/(\theta(\bar{z})\phi(\bar{z}))$ because $\bar{y} > 0$, $f(\bar{y}) \geq 0$, and $f'(\bar{y}) < 0$, which implies that $0 < \bar{y} \leq y_*$. It corresponds to the Newton step at \bar{z} for the original problem $p(z) = 0$, which is never larger than y_* because our method is guaranteed to be no worse than Newton's. In practice, a few Newton iterations usually suffice to solve $f(y) = 0$.

The following theorem formally states our method, which we have called the PL method ("pseudo Laguerre"), and summarizes its properties. We note that, as was our goal, the PL method uses the values of both $p(z)$ and $p'(z)$ separately unlike Newton's method, which uses just their ratio.

THEOREM 2. *Consider a polynomial $p(z) = \prod_{j=1}^n (z - x_j)$ with all real zeros $x_1 \geq x_2 \geq \dots \geq x_n$, and $n \geq 3$. Then the PL method, defined by the iteration formula*

$$z_{k+1} = z_k - \left(1 + y_k^{\frac{n}{n-1}}\right) \frac{p(z_k)}{p'(z_k)}, \quad (9)$$

where y_k is the smallest positive solution of

$$y^{\frac{n}{n-1}} - \frac{((n-1)p(z_k))^{\frac{1}{n}}}{n-1} \cdot \frac{p'(z_k)}{p(z_k)} y + 1 = 0, \quad (10)$$

converges monotonically to x_1 from any starting point $z_0 > x_1$. This method is at least as fast as Newton's method and when $p(z)$ has at least two distinct zeros, then it has the same order of convergence as Newton's method. When $x_1 = x_2 = \dots = x_n$, then the PL method converges in one iteration from any $z_0 > x_1$.

Proof. The iterate obtained from z_k is given by $z_k - \theta(z_k)y_k$, where y_k is the smallest positive solution of

$$y^{\frac{n}{n-1}} - \theta(z_k)\phi(z_k)y + 1 = 0. \quad (11)$$

Since y_k solves equation (11), it satisfies

$$\theta_k y_k = \frac{1 + y_k^{\frac{n}{n-1}}}{\phi(z_k)},$$

so that the iteration formula can also be written as

$$z_{k+1} = z_k - \left(1 + y_k^{\frac{n}{n-1}}\right) \frac{p(z_k)}{p'(z_k)}.$$

This, together with the definition of $\theta(z)$, reformulates the PL method as in the statement of the theorem. It is clear from the optimization problem defining the method in (4) and from (9) that it is at least as good as Newton's method and that it converges monotonically from any starting point $z_0 > x_1$.

Since y_k corresponds to the largest positive zero s_* of the function $g(s)$ in the proof of Theorem 1 (here with $\bar{z} = z_k$) through the transformation

$s_* = (\theta(z_k)y_k)^{-1/(n-1)}$, and because we also have from that proof that $s_* \geq (\phi(z_k)/n)^{1/(n-1)}$, we obtain

$$y_k \leq \frac{n}{\theta(z_k)\phi(z_k)}. \quad (12)$$

We now show that $\theta(z_k)\phi(z_k)$ becomes unbounded as $z_k \rightarrow x_1^+$ when the multiplicity of x_1 is $\rho < n$. In that case, we have

$$\begin{aligned} \theta(z_k)\phi(z_k) &= (n-1)^{\frac{1-n}{n}} p(z_k)^{\frac{1}{n}} \sum_{j=1}^n \frac{1}{z_k - x_j} \\ &= (n-1)^{\frac{1-n}{n}} \prod_{j=1}^n (z_k - x_j)^{\frac{1}{n}} \sum_{j=1}^n \frac{1}{z_k - x_j} \\ &= (n-1)^{\frac{1-n}{n}} (z_k - x_1)^{\rho/n} \prod_{j=\rho+1}^n (z_k - x_j)^{\frac{1}{n}} \left(\frac{\rho}{z_k - x_1} + \sum_{j=\rho+1}^n \frac{1}{z_k - x_j} \right). \end{aligned} \quad (13)$$

This means that

$$\lim_{z_k \rightarrow x_1^+} \theta(z_k)\phi(z_k) = \lim_{z_k \rightarrow x_1^+} \frac{\rho(n-1)^{\frac{1-n}{n}} \prod_{j=\rho+1}^n (x_1 - x_j)^{\frac{1}{n}}}{(z_k - x_1)^{\frac{n-\rho}{n}}},$$

since the rest of the expression in (13) vanishes in the limit. Because $n > \rho$, this limit is unbounded. With inequality (12) we have therefore obtained that $y_k \rightarrow 0^+$ when $z_k \rightarrow x_1^+$, so that the PL method asymptotically becomes Newton's method and therefore has the same order of convergence.

The last point in the statement of the theorem was already demonstrated in the comments following the proof of Theorem 1. We will nonetheless show how it also follows from the formal statement of the method. Assume that x_1 has multiplicity n . Then

$$p(z_0) = (z_0 - x_1)^n, \quad \phi(z_0) = \frac{n}{z_0 - x_1}, \quad \text{and} \quad \theta(z_0) = (n-1)^{\frac{1-n}{n}} (z_0 - x_1),$$

which turns equation (11) into

$$y^{\frac{n}{n-1}} - n(n-1)^{\frac{1-n}{n}} y + 1 = 0.$$

This equation has a single real zero at $y_0 = (n-1)^{\frac{n-1}{n}}$. Substituting this value in the iteration formula (9) yields

$$z_1 = z_0 - \left(1 + y_0^{\frac{n}{n-1}}\right) \frac{p(z_0)}{p'(z_0)} = z_0 - (1 + (n-1)) \frac{z_0 - x_1}{n} = x_1.$$

This completes the proof. ■

We note that in (9), y_k can be replaced by any number w with $0 \leq w \leq y_k$ to yield an iterate that is greater than z_{k+1} (and therefore also an upper bound on the

largest zero x_1), but never worse than a Newton iterate. Candidates for w could be any inexact solution obtained while solving (11), such as the starting point \bar{y} we mentioned above.

Our method clearly lacks some of the niceties of Newton's or Laguerre's method: to obtain the iterates, one needs to solve a nonlinear equation and n th roots need to be computed. It is also not immediately clear if and how it could be extended to the complex plane. On the other hand, it is guaranteed to be faster than Newton's method, it does not require second derivatives, and the nonlinear equation that needs to be solved to obtain the next iterate will, in general, be much easier to solve than $p(z) = 0$. One also has the option to only approximately solve (11) and still improve over Newton's method. Once the largest (or smallest) zero is computed, and if so desired, some or all of the other zeros may be computed by deflation or zero suppression.

One area where the PL method could be useful is in the computation of the zeros of the characteristic polynomial of a matrix for which the second derivative is expensive to compute. While this is certainly not the preferred method to compute the eigenvalues of a general matrix, there are special structured matrices such as Toeplitz matrices for which this is a valid approach (see, e.g, [5]). There are, of course, other ways to avoid computing the second derivative, usually involving the computation of function and derivative values at more than one point (see, e.g., [1, 4]).

4. Example

In this section we illustrate the properties of the PL method by comparing it to the Newton and Laguerre methods for an 8th order polynomial with zeros at $-10, -4, -2, -1, 2, 3, 8, 9$. The PL method is denoted by "L" when the solution of (11) is exact (in this case, a relative accuracy of around 10^{-15}), and by "PL1" when that solution is approximated by \bar{y} from the previous section. When one or two additional Newton steps are carried out from \bar{y} to approximate the solution of (11), it is denoted by "PL2" and "PL3", respectively. For an initial point $z_0 = 40$, we obtain the following first few iterates:

Newton:	40, 35.1871, 30.9915, 27.3383, 24.1622, ...
PL1:	40, 32.0982, 25.8829, 21.0213, 17.2536, ...
PL2:	40, 22.6422, 14.2023, 10.6687, 9.4450, ...
PL3:	40, 15.8395, 10.7316, 9.4496, 9.0742, ...
PL:	40, 13.2656, 10.1379, 9.2713, 9.0332, ...
Laguerre:	40, 12.4542, 9.5003, 9.0183, 9.0000, ...

It is also interesting to compare the number of iterations until convergence when the starting point moves away from the largest zero $x_1 = 9$. Situations where starting points are relatively far from the zero are encountered in the aforementioned application to Toeplitz matrices [5]. Here are the number of iterations for each method for $z_0 = 40, 100, \text{ and } 1000$.

	Newton	PL	PL1	PL2	PL3	Laguerre
$z_0 = 40$	20	8	14	9	8	6
$z_0 = 100$	27	8	18	11	9	6
$z_0 = 1000$	44	8	28	15	11	6

As we can see from these results, the PL method's main strength is to improve situations where the starting point lies far from the zero and Newton's method takes many small steps. Like Laguerre's method, it is fairly insensitive to the choice of the initial point and this remains true if the solution of equation (11) is approximated with just one Newton iteration. For higher order polynomials, the number of iterations increases, but its performance relative to the other methods remains very similar. Not surprisingly, Laguerre's method is faster than all the other methods. In Figure 1, we have graphed the functions $g(s)$ and $f(y)$ for the above polynomial when $\bar{z} = 15$.

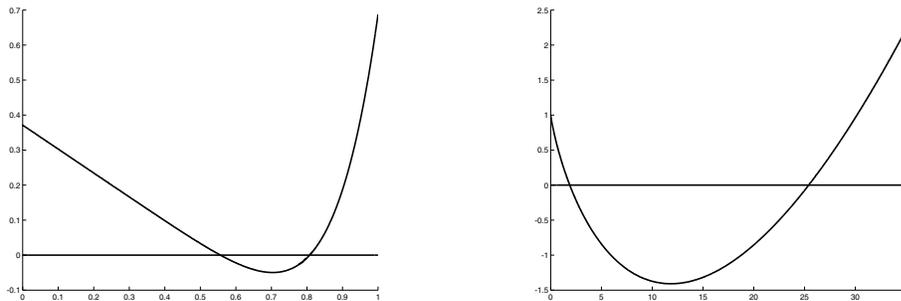


Fig. 1. The functions $g(s)$ (left) and $f(y)$ (right) for $\bar{z} = 15$ in the example.

CONCLUSION. In the case of a polynomial with all real zeros, we have found an answer to the question of what a zerofinder would look like if it truly exploited all the information available from the function and derivative values, instead of just the ratio of the two as in Newton's method. The resulting method is better but more complicated than Newton's method and reminiscent of Laguerre's method.

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