4. Root finding and interpolation

With the remainder theory developed in the previous handout, we now have a higher vantage point from which to reexamine the problem of root finding posed in Section 1. Suppose we want to solve $f(x) = 0$ with f sufficiently smooth. Denote by $\{x_n\}$ the sequence of approximations to the simple root x_* and by $\{y_n\}$ the corresponding values of the function; the values of the first derivative, when available, will be denoted $\{y'_n\}$; for higher derivatives we will use the superscript notation $\{y_n^{(l)}\}$. Interpolation theory offers two conceptually different approaches to designing rules for computing x_n from the previously computed data.

4.1. **Direct methods.** Let p be an interpolant of f. For instance, p can be a polynomial of degree m that is forced to agree with f at points x_{n-1}, x_{n-2}, $\ldots$, x_{n-m-1}. If $f \approx p$ then the zero of f should be close to one of the zeros of p. Consequently, we can choose x_n so that $p(x_n) = 0$. Root finding schemes of this type are called *direct* methods.

As an important special case, consider $m = 1$. The Lagrangian interpolant agreeing with f at x_{n-1} and x_{n-2} is:

$$p = y_{n-1}\,\frac{x - x_{n-2}}{x_{n-1} - x_{n-2}} + y_{n-2}\,\frac{x - x_{n-1}}{x_{n-2} - x_{n-1}}.$$

Setting x_n to be the zero of that polynomial leads to

$$x_n = \frac{y_{n-1}\,x_{n-2} - y_{n-2}\,x_{n-1}}{y_{n-1} - y_{n-2}},$$

which is the Secant Method. Now, if we replace Lagrangian interpolation with Taylor (linear) interpolation, we get

$$p = y_{n-1} - y'_{n-1}\,(x - x_{n-1}),$$

which leads to Newton's method:

$$x_n = x_{n-1} - \frac{y_{n-1}}{y'_{n-1}}.$$

Unfortunately, using higher order polynomial interpolants, either Lagrange or Taylor, is problematic for several reasons. Firstly, computing the roots of nonlinear polynomials is computationally expensive even for degree two[5]. Secondly, it may not always be clear which of the several roots of the interpolant should be used to approximate the root of f. Last but not least, polynomial interpolation is unstable—increasing the degree of the interpolating polynomial will not generally result in better approximation of the function. On the contrary, a higher degree

[5]Because of `sqrt`

interpolant may very well end up being a worse approximation of f than a low order one.

One way to overcome the deficiencies of polynomial interpolation is to use rational interpolating functions. Recall that a rational function is a quotient of two polynomials:

$$r(x) = \frac{p(x)}{q(x)} = \frac{a_0 + a_1\,x + \ldots + a_n\,x^n}{b_0 + b_1\,x + \ldots + b_m\,x^m}.$$

Since reducing the numerator and the denominator by the same factor does not change the fraction, our convention will be that $b_m = 1$.

Notice that if $\deg(q) = m = 0$, then r is a polynomial of degree n. Thus rational interpolation includes polynomial interpolation as a special case. In fact, the construction of rational interpolants is based on exactly the same principles as in polynomial interpolation. For instance, to construct a *Padé interpolant* one matches the values of the function and its derivatives at a point—just as in Taylor interpolation. A Padé-Lagrange interpolant matches the values of the function at distinct points. The most general Padé-Hermite interpolant matches the values of the function and its derivatives at prescribed points with the number of matched derivatives dependent on the point.

Let r be a $(1,m)$-rational interpolant of f constructed using the values $\{x_k, y_k, y_k', \ldots, y_k^{(l)}\}_{k=n-1}^{n-N}$. This means that

$$r = \frac{p}{q}, \quad \deg(p) = 1, \quad \deg(q) = m$$

and

$$\begin{aligned} r(x_k) &= y_k, \quad k = n-1, \ldots, n-N, \\ r'(x_k) &= y_k', \quad k = n-1, \ldots, n-N, \\ &\ldots \\ r^{(l)}(x_k) &= y_k^l, \quad k = n-1, \ldots, n-N, \end{aligned}$$

for an appropriate N. To obtain a direct root finding method, one chooses x_n to be the unique root of p. For instance, the $(1,1)$-Padé interpolant of f at $x = x_{n-1}$ has the form

$$r = \frac{a\,x + b}{x + c}$$

with coefficients a, b, and c chosen so that r matches the value of f and its first two derivatives at $x = x_{n-1}$. It is easy to show that:

$$\begin{aligned} a &= y_{n-1} - 2\,\frac{(y'_{n-1})^2}{y^{(2)}_{n-1}} \\ b &= -x_{n-1}\,y_{n-1} + 2\,x_{n-1}\,\frac{(y'_{n-1})^2}{y^{(2)}_{n-1}} - 2\,y_{n-1}\,\frac{y'_{n-1}}{y^{(2)}_{n-1}} \\ c &= -x_{n-1} - 2\,\frac{y'_{n-1}}{y^{(2)}_{n-1}} \end{aligned}$$

Now set x_n to be the unique root of p:

$$x_n = -\frac{b}{a} = \frac{x_{n-1}\,y_{n-1} - 2\,x_{n-1}\,\frac{(y'_{n-1})^2}{y^{(2)}_{n-1}} + 2\,y_{n-1}\,\frac{y'_{n-1}}{y^{(2)}_{n-1}}}{y_{n-1} - 2\,\frac{(y'_{n-1})^2}{y^{(2)}_{n-1}}}.$$

Simplifying, we can write:

$$x_n = x_{n-1} - \frac{(y_{n-1}/y'_{n-1})}{1 - \frac{1}{2}\,\frac{y_{n-1}\,y^{(2)}_{n-1}}{(y'_{n-1})^2}}. \tag{18}$$

Equation (18) is known as *Halley's method*. Notice that (18) can be thought of as Newton's method applied to f/f'.

4.2. **Inverse methods.** In order to compute the root of f analytically, one needs to find the inverse function $g(y) = f^{-1}(y)$; then $x_* = g(0)$. This suggests basing root finding on the interpolation of g rather than f. For instance, we can use the computed values $\{y_k, x_k\}_{k=n-1}^{n-m-1}$ to approximate $x = g(y)$ with a Lagrange polynomial p of degree m; then $x_n = p(0)$. This class of methods is broadly known as inverse interpolation methods or, simply, *inverse methods*.

As an example, consider the case of inverse linear interpolation:

$$g(y) \approx p(y) = x_{n-1}\,\frac{y - y_{n-2}}{y_{n-1} - y_{n-2}} + x_{n-2}\,\frac{y - y_{n-1}}{y_{n-2} - y_{n-1}}.$$

Setting $x_n = p(0)$ results in the familiar Secant Method. Thus the Secant Method can be thought of as an inverse method—a fact that will be very helpful in later analysis of its convergence.

As another example, consider inverse quadratic interpolation.

$$\begin{aligned} g(y) \approx p(y) = {} & x_{n-1}\,\frac{(y-y_{n-2})(y-y_{n-3})}{(y_{n-1}-y_{n-2})(y_{n-1}-y_{n-3})} \\ & + x_{n-2}\,\frac{(y-y_{n-1})(y-y_{n-3})}{(y_{n-2}-y_{n-1})(y_{n-2}-y_{n-3})} \\ & + x_{n-3}\,\frac{(y-y_{n-1})(y-y_{n-2})}{(y_{n-3}-y_{n-1})(y_{n-3}-y_{n-2})}. \end{aligned}$$

Again, we set $x_n = p(0)$ which leads to:

$$\begin{aligned} x_n = {} & x_{n-1}\,\frac{y_{n-2}\,y_{n-3}}{(y_{n-1}-y_{n-2})(y_{n-1}-y_{n-3})} \\ & + x_{n-2}\,\frac{y_{n-1}\,y_{n-3}}{(y_{n-2}-y_{n-1})(y_{n-2}-y_{n-3})} \\ & + x_{n-3}\,\frac{y_{n-1}\,y_{n-2}}{(y_{n-3}-y_{n-1})(y_{n-3}-y_{n-2})}. \end{aligned}$$

This method—inverse quadratic interpolation—is at the core of MATLAB's `fzero` command; one of the exercises at the end of this section asks you to investigate its convergence properties.

The obvious advantage of inverse methods over direct methods is that the rule $x_n = p(0)$ is both unambiguous and computationally cheap. Unfortunately, the inherent instability of interpolation still remains a limiting factor which has to be reckoned with. One consequence of that instability is that one rarely uses high degree interpolating polynomials. In addition, one has to augment the rule $x_n = p(0)$ with conditional statements to ensure that x_n is, indeed, an improved approximation. For instance, the MATLAB's `fzero` routine generates starting approximations to the root using a combination of bisection and Secant Method. It attempts to switch to inverse quadratic interpolation only after it detects convergence.

4.3. **Convergence of one-point schemes.** An iterative scheme of the type $x_n = \phi(x_{n-1})$ is called a *one-point scheme*. In Section 2 we proved that such a scheme converges to a fixed point p as long as there exists a neighborhood of p that ϕ maps into itself. Recall that we also showed (see Theorem 1) that fixed point convergence is linear if $\phi'(p) \neq 0$. If $\phi'(p) = 0$ one can expect higher order of convergence. For instance, Newton's method is quadratically convergent. We will now show that the order of convergence of any one-point scheme is given by the order of the first non-vanishing derivative.

Theorem 5. *Let $x_n = \phi(x_n)$ be a one-step method converging to p and let k be the smallest positive integer for which $\phi^{(k)}(p) \neq 0$. Then the* *order of convergence is k and the asymptotic error constant is given by:*

$$\lambda = \frac{|\phi^{(k)}(p)|}{k!}.$$

Proof. Consider the $(k-1)$-st order Taylor expansion of ϕ centered at the fixed point:

$$\phi(x) = \phi(p) + \phi'(p)\,(x-p) + \ldots + \frac{\phi^{(k-1)}(p)}{(k-1)!}\,(x-p)^{k-1}$$
$$+ \frac{\phi^{(k)}(\xi)}{k!}\,(x-p)^k.$$

Recall that ξ is some number between p and x. By assumption, all derivatives of ϕ of order less than k vanish at the fixed point; also $\phi(p) = p$ by definition of the fixed point. Therefore:

$$\phi(x) = p + \frac{\phi^{(k)}(\xi)}{k!}\,(x-p)^k.$$

Evaluating at x_{n-1}, we get

$$x_n = \phi(x_{n-1}) = p + \frac{\phi^{(k)}(\xi_{n-1})}{k!}\,(x_{n-1}-p)^k,$$

with ξ_{n-1} now some point between x_{n-1} and p. It follows that

$$\frac{|x_n - p|}{|x_{n-1}-p|^k} = \frac{|\phi^{(k)}(\xi_{n-1})|}{k!}.$$

By assumption, $\lim_{n\to\infty} x_{n-1} = p$. Since ξ_{n-1} is bracketed by x_{n-1} and p: $\lim_{n\to\infty} \xi_{n-1} = p$. This in turn implies that

$$\lim_{n\to\infty} \frac{|x_n - p|}{|x_{n-1}-p|^k} = \frac{|\phi^{(k)}(p)|}{k!},$$

as required. □

As an immediate application, consider Newton's method for which $\phi = x - f(x)/f'(x)$. Straightforward computation shows that $f(p) = 0$ implies that $\phi'(p) = 0$. However, in general,

$$\phi''(p) = \frac{f^{(2)}(p)}{f'(p)} \neq 0.$$

Therefore Newton's method is quadratic with the asymptotic error constant:

$$\lambda = \frac{1}{2}\,\frac{|f^{(2)}(p)|}{|f'(p)|}. \tag{19}$$

Here we remind the reader that $f'(p) \neq 0$ for simple roots, which is our default assumption. It turns out that for multiple roots, Newton's method may still converge. However, the order of convergence in that case is usually significantly less than two.

4.4. **Convergence of multi-point schemes.** The analysis of stationary[6] iterative one-point schemes presented in Theorem 5 is relatively simple owing to the fact that for such schemes the error $|x_n - x_*|$ depends only on the error at the previous step $|x_{n-1} - x_*|$. We now turn our attention to stationary multi-point schemes, such as the Secant Method. Here the analysis is more involved because the error term $|x_n - x_*|$ depends not just on $|x_{n-1} - x_*|$ but also on the error in the preceding steps: $|x_{n-2} - x_*|$, $|x_{n-3} - x_*|$, and so on.

Earlier we noted that the Secant Method can be regarded as an inverse linear interpolation method

$$x_n = p(0),$$

with $p(y)$ being the linear Lagrangian interpolant of $g(y) = f^{-1}(y)$ computed from $\{x_{n-k}, y_{n-k}\}_{k=1}^{2}$. Using the remainder for Lagrangian interpolation of order one, we can write

$$x_n = p(0) = g(0) - r(0) = x_* - \frac{g^{(2)}(\eta)}{2}\, y_{n-1}\, y_{n-2},$$

with $\min\{0, y_1, y_2\} \leq \eta \leq \max\{0, y_1, y_2\}$. From this follows that

$$x_n - x_* = -\frac{g^{(2)}(\eta)}{2}\, y_{n-1}\, y_{n-2}.$$

Using MVT, we can write

$$y_{n-1} = f(x_{n-1}) - f(x_*) = f'(\xi_1)\,(x_{n-1} - x_*),$$

with ξ_1 located somewhere between x_{n-1} and x_*. Similarly,

$$y_{n-2} = f(x_{n-2}) - f(x_*) = f'(\xi_2)\,(x_{n-2} - x_*),$$

with ξ_2 between x_{n-2} and x_*. It follows that

$$x_n - x_* = -\frac{g^{(2)}(\eta)}{2}\, f'(\xi_1)\, f'(\xi_2)\,(x_{n-1} - x_*)\,(x_{n-2} - x_*).$$

Let us introduce the following notation:

$$\begin{aligned} e_n &= x_n - x_*, \\ K_n &= -\frac{g^{(2)}(\eta)}{2}\, f'(\xi_1)\, f'(\xi_2). \end{aligned}$$

[6]Stationary means that the rule ϕ which produces x_n from x_{n-1}, x_{n-2}, ... does not depend on n. Bisection is an example of a non-stationary method.

Our analysis shows that the error at step n is proportional to the product of the errors at the preceding two steps

$$e_n = K_n\, e_{n-1}\, e_{n-2}, \tag{20}$$

with the constant of proportionality depending on n through η, ξ_1, and ξ_2. Furthermore, since we are assuming convergence, the Squeeze Theorem implies:

$$\begin{aligned}\lim_{n\to\infty} \eta &= 0,\\ \lim_{n\to\infty} \xi_1 &= \lim_{n\to\infty} \xi_2 = x_*.\end{aligned}$$

Consequently,

$$\lim_{n\to\infty} K_n = -\frac{g^{(2)}(0)}{2}\,(f'(x_*))^2 = K,$$

which shows that $e_n \approx K\, e_{n-1}\, e_{n-2}$ in the limit for large n. Now assume that the order of convergence is α and the asymptotic error constant is λ. From Equation (20) follows

$$\lim_{n\to\infty} \frac{|e_n|}{|e_{n-1}|^\alpha} = \lim_{n\to\infty} |K_n|\,\frac{|e_{n-1}|\,|e_{n-2}|}{|e_{n-1}|^\alpha}.$$

The limit on the left-hand side is λ, by assumption. On the right, we get:

$$\begin{aligned}\lim_{n\to\infty} |K_n|\,\frac{|e_{n-1}|\,|e_{n-2}|}{|e_{n-1}|^\alpha} &= \lim_{n\to\infty}|K_n|\,\lim_{n\to\infty}\frac{|e_{n-2}|}{|e_{n-1}|^{\alpha-1}}\\ &= |K|\,\lim_{n\to\infty}\frac{|e_{n-2}|}{|e_{n-1}|^{\alpha-1}}\,\frac{|e_{n-2}|^{\alpha\,(\alpha-1)-1}}{|e_{n-2}|^{\alpha\,(\alpha-1)-1}}\\ &= |K|\,\lim_{n\to\infty}\frac{|e_{n-2}|^{\alpha\,(\alpha-1)}}{|e_{n-1}|^{\alpha-1}}\,\lim_{n\to\infty}\frac{1}{|e_{n-2}|^{\alpha\,(\alpha-1)-1}}\\ &= |K|\,\lim_{n\to\infty}\left(\frac{|e_{n-1}|}{|e_{n-2}|^\alpha}\right)^{1-\alpha}\lim_{n\to\infty}|e_{n-2}|^{1-\alpha\,(\alpha-1)}\\ &= |K|\,\left(\lim_{n\to\infty}\frac{|e_{n-1}|}{|e_{n-2}|^\alpha}\right)^{1-\alpha}\lim_{n\to\infty}|e_{n-2}|^{1-\alpha\,(\alpha-1)}\\ &= |K|\,\lambda^{1-\alpha}\,\lim_{n\to\infty}|e_{n-2}|^{1-\alpha\,(\alpha-1)}.\end{aligned}$$

Thus α and λ should be such that

$$\lambda = |K|\,\lambda^{1-\alpha}\,\lim_{n\to\infty}|e_{n-2}|^{1-\alpha\,(\alpha-1)},$$

which is equivalent to:

$$\lambda^\alpha = |K|\,\lim_{n\to\infty}|e_{n-2}|^{1-\alpha\,(\alpha-1)}. \tag{21}$$

Now, convergence implies that the error goes to zero:

$$\lim_{n\to\infty} |e_{n-2}| = 0.$$

However, $\lambda > 0$ and therefore the limit on the right-hand side of Equation (21) cannot be zero. This means that the power $1 - \alpha\,(\alpha - 1)$ cannot be positive. Nor can it be negative, for in this case the limit becomes infinite. We conclude that the order of convergence α must satisfy the quadratic equation

$$1 - \alpha\,(\alpha - 1) = 0,$$

whose only positive root is $\frac{1+\sqrt{5}}{2}$. The order of convergence of the Secant Method is thus given by the *golden ratio*. Having found the order α, we can easily find the asymptotic error constant. From Equation (21) follows at once that:

$$\lambda = |K|^{\frac{1}{\alpha}} = \left(\frac{|g^{(2)}(0)|}{2}\,(f'(x_*))^2\right)^{\frac{2}{1+\sqrt{5}}}.$$

Now, to obtain the final expression for λ, we need to relate $g^{(2)}(0)$ to the derivatives of f. To this end, differentiate $x = g(y)$ with respect to x using the Chain Rule. Differentiating once, we get

$$1 = \frac{dg}{dx} = \frac{dg}{dy}\,\frac{dy}{dx} = \frac{dg}{dy}\,f'(x),$$

from which follows the familiar relation: $\frac{dg}{dy} = \frac{1}{f'(x)}$. Differentiating $x = g(y)$ twice, produces:

$$0 = \frac{d}{dx}\left(\frac{dg}{dy}\,f'(x)\right) = g^{(2)}(y)\,(f'(x))^2 + g'(y)\,f^{(2)}(x).$$

Therefore

$$g^{(2)}(y) = -\frac{g'(y)\,f^{(2)}(x)}{(f'(x))^2} = -\frac{f^{(2)}(x)}{(f'(x))^3}.$$

In particular,

$$g^{(2)}(0) = -\frac{f^{(2)}(x_*)}{(f'(x_*))^3},$$

which means that the asymptotic error constant of the Secant Method is given by:

$$\lambda = \left(\frac{|f^{(2)}(x_*)|}{2\,|f'(x_*)|}\right)^{\frac{2}{1+\sqrt{5}}}.$$

As a parting remark, we offer the following observation. The analysis of the Secant Method, though involved, is completely straightforward once the scheme is classified sa an inverse interpolation method: one simply unravels the remainder in the Lagrangian interpolation using MVT and implicit differentiation. This analysis would be difficult, if not impossible, without the connection between root finding and interpolation. The moral, therefore, is to always seek such connections. If you don't pay close attention to the organizational principles behind numerical schemes, you won't see the proverbial forest behind the trees.

Exercises

(1) Contrive an example which convincingly demonstrates that Newton's method is quadratic with asymptotic error constant given by (19).

(2) Find a function f with a double root at zero which can be found using Newton's method despite the fact that $f'(0) = 0$. Investigate the order of convergence and present your findings in the form of a report.

(3) Find the order of convergence and the asymptotic error constant of Halley's method. Confirm your computations with a well chosen example.

(4) In the text we derived Halley's method using Padé interpolant of order $(1, 1)$. Formulate a direct root finding method based on Padé interpolant of order $(1, 2)$. Illustrate the method using a few well chosen examples. What can you say about the order of convergence based on the data?

(5) Repeat the previous exercise with Padé-Lagrange interpolant of order $(1, 1)$.

(6) Repeat the previous exercise with Padé-Hermite interpolant of order $(1, 1)$ which matches the function and its first derivative at appropriate number of points.

(7) Find the order of convergence and the asymptotic error constant of the inverse quadratic interpolation. Confirm your findings numerically using your own version of `fzero`.

(8) Formulate an inverse interpolation scheme using Padé interpolant of order $(1, 1)$. Compare it numerically to the Secant Method and `fzero`. How do these three methods seem to rank in order of convergence?