SELF-ACCELERATING ROOT SEARCH AND OPTIMISATION METHODS BASED ON RATIONAL INTERPOLATION

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Abstract. Iteration methods based on barycentric rational interpolation are derived that exhibit accelerating orders of convergence. For univariate root search, the derivative-free methods approach quadratic convergence and the first-derivative methods approach cubic convergence. For univariate optimisation, the convergence order of the derivative-free methods approaches 1.62 and the order of the first-derivative methods approaches 2.42. Generally, performance advantages are found with respect to low-memory iteration methods. In optimisation problems where the objective function and gradient is calculated at each step, the full-memory iteration methods converge asymptotically 1.8 times faster than the secant method. Frameworks for multivariate root search and optimisation are also proposed, though without discovery of practical parameter choices.

Key words. convergence acceleration, barycentric rational interpolation, preconditioning

AMS subject classifications. 26C15, 41A20, 65B99, 65D25, 65F08, 65H05, 65H10

1. Introduction. The search for solutions of non-linear equations and related problem of optimisation form routine tasks in numerical analysis. In this paper, families of iterative algorithms are presented that re-use information from an arbitrary number of prior steps in order to accelerate convergence. Furthermore, the iteration parameters are analytically expressed and therefore need no intermediate calibration.

On the history of related work, the general principles of interpolation-based iteration methods for root search problems were studied in the 1960s by Ostrowski [1] and Traub [2]. That same decade, Tornheim [3], Jarratt and Nudds [4] proposed the application of rational interpolation for root searches. However, the general formulations required matrix equations to be solved. In 1980, Larkin [5] then identified a recursive approach for evaluating root search iterations derived from minimal rational interpolants with a linear numerator. Following an alternative approach, in 2008 Sidi [6] presented a root search scheme applying Newton’s method to polynomial interpolants, with the interpolant derivative being calculated by recursion. These recursive schemes can suffer from numerical instabilities though, depending on the distribution and ordering of interpolation points [7].

This paper presents iteration methods based on barycentric representations of rational interpolants [8, 9], which possess useful properties of expressivity, computational efficiency and numerical stability [7, 10]. Applications for both root search and optimisation problems are considered. Frameworks for multivariate cases are also proposed. However, only the univariate methods are of immediate practical use. It is still common though to perform one-dimensional line searches as a subroutine within multivariate root search or optimisation, and so these methods can be applied to many general problems.

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2. Roots of univariate rational interpolants. The simplest approach for solving \( f[x] = 0 \) is to approximate the inverse function \( x[f] \) and then evaluate at the point \( f = 0 \). Given a set of points \( \{x_i, f_i\} \) where \( f_i = f[x_i] \), the barycentric representation of a rational interpolant is stated below,

\[
x[f] \approx \frac{\left( \sum_{i=0}^{n} \omega_i x_i \right)}{\left( \sum_{i=0}^{n} \omega_i f_i \right)}
\]

where \( \omega_i \) are free (non-zero) parameters. The iteration scheme below then follows.

\[
x_{n+1} = \frac{\left( \sum_{i=0}^{n} \omega_i x_i \right)}{\left( \sum_{i=0}^{n} \omega_i f_i \right)}
\]

Now, instead of addressing whether the inverse function is well-defined or not, it’s useful to note that the same iteration formula can also be derived by approximating \( f[x] \). Consider the rational expression in (3), where \( r[x] \) is approximated by (4).

\[
f[x] = \frac{x - c}{r[x]}
\]

\[
r[x] \approx \frac{\left( \sum_{i=0}^{n} \omega_i r_i \right)}{\left( \sum_{i=0}^{n} \omega_i (x - x_i) \right)}
\]

From (3), it is known that \( r_i = (x_i - c)/f_i \). The root of the approximated \( f[x] \) is then given by (2) when applying the following constraint and solving for \( c \).

\[
\sum_{i=0}^{n} \omega_i r_i = 0
\]

Other constraints could be considered, or the right hand side of (5) set to some free parameter, leading to alternative iteration formulae. However, this paper does not seek to exhaustively discuss all such possible iteration schemes. It is chosen to focus on the methods that form a weighted linear average of points, as in (2).

Before exploring how to choose the interpolation parameters, the case where first derivatives \( f'_i \) are also available is presented. The corresponding barycentric rational approximation of the inverse function can be found by taking the limit of (1) for coinciding pairs of interpolation nodes,

\[
x[f] \approx \frac{\left( \sum_{i=0}^{n} \lambda_i x_i + (\gamma_i x_i + \lambda_i/f'_i) (f - f_i) \right)}{\left( \sum_{i=0}^{n} \lambda_i + \gamma_i (f - f_i) \right)}
\]

where \( \{\lambda_i, \gamma_i\} \) are free parameters. The iteration scheme below then follows for \( f = 0 \).

\[
x_{n+1} = \frac{\left( \sum_{i=0}^{n} \lambda_i (x_i - f_i/f'_i) - \gamma_i f_i x_i \right)}{\left( \sum_{i=0}^{n} \lambda_i - \gamma_i f_i \right)}
\]
The same iteration formula can again be derived from $f[x]$ in (3), but now with:

$$r[x] \approx \left( \sum_{i=0}^{n} \hat{\lambda}_i r_i + (\gamma_i r_i + \hat{\lambda}_i r'_i) (x - x_i) \right) / \left( \sum_{i=0}^{n} \hat{\lambda}_i + \gamma_i (x - x_i) \right)$$

and the following constraint,

$$\sum_{i=0}^{n} (\gamma_i r_i + \hat{\lambda}_i r'_i) = 0$$

where the relation $r'_i = (f_i - (x_i - c)f'_i)/f_i^2$ is known by differentiating (3). On solving for $c$ and defining $\lambda_i = \hat{\lambda}_i f'_i$, the iteration formula in (7) is reproduced.

The constraints in (5) and (9) could otherwise be identified by first expressing the $r[x]$ approximations as a ratio of polynomial functions: multiplying the numerators and denominators by $\prod_{i=0}^{n} (x - x_i)^m$ with $m = 1, 2$ respectively. The constraints are then equivalent to setting the coefficient of the highest degree term $x^{m(n+1)-1}$ in the numerator to zero. Again, other constraints may be considered, but for this choice the iteration scheme corresponds to a weighted linear average of the sampled points and respective Newton iterates.

For future reference, it is also helpful to stress that polynomial functions form a sub-class of barycentric rational representations. The relevant interpolation parameters can be determined from the following partial fraction expansions:

$$\prod_{i=0}^{n} \frac{1}{z - z_i} = \sum_{i=0}^{n} \frac{u_i}{z - z_i} \quad \text{where} \quad u_i = \prod_{j \neq i} \frac{1}{z_i - z_j}$$

$$\prod_{i=0}^{n} \frac{1}{(z - z_i)^2} = \sum_{i=0}^{n} \frac{u_i^2 + v_i (z - z_i)}{(z - z_i)^2} \quad \text{where} \quad v_i = -2u_i^2 \sum_{j \neq i} \frac{1}{z_i - z_j}$$

The approximations for $r[x]$ or $x[f]$ thus simplify to polynomial expressions when the respective denominators equate to products of inverse polynomials.

To determine convergence properties of the iterative methods, series expansions can be considered about the true root $x_*$ where $x_i = x_* + \epsilon_i$. For the applications presented in this paper, the derivative-free formula in (2) is focused on, as corresponding parameters for (7) will be formed from the limit of coinciding pairs of sampling points.

For derivative-free iteration (2), the leading error is:

$$\epsilon_{n+1} = \left( \sum_{i=0}^{n} \omega_i \right) / \left( \sum_{i=0}^{n} \omega_i^2 \right) + \text{higher-order terms}$$

Given arbitrary choices of $\omega_i$, the leading error is thus $O[\epsilon]$ and so the iterations are only linearly convergent (if they do converge). However, the above error term vanishes when $\sum_i \omega_i = 0$. If then successively requiring the leading error term to vanish, the following constraints are established:

$$\sum_{i=0}^{n} \omega_i \epsilon_i^k = 0 \quad 0 \leq k \leq n - 1$$
Such constraints correspond to finding the kernel of the Vandermonde matrix, whose solution is given by:

$$\omega_i \propto \prod_{j \neq i} \frac{1}{\epsilon_i - \epsilon_j}$$  \hspace{1cm} (13)

Although the $\epsilon_i$ terms are not known directly, it can be chosen to substitute $(\epsilon_i - \epsilon_j)$ consistently by $(x_i - x_j)$ or $(f_i - f_j)$ without re-introducing the eliminated error terms. From (10), it then follows that if the constraints in (12) are satisfied, the leading error for the derivative-free iteration scheme has the following form with $m = 1$:

$$\epsilon_{n+1} = E_{m,n+1} \times \left( \prod_{i=0}^{n} \epsilon_i^m \right) + \text{sub-dominant terms}$$  \hspace{1cm} (14)

where $E_{m,n+1}$ is a factor composed of $k$th derivatives $f_s^{(k)}$ evaluated at the true root. For convenience in later expressing $E_{m,n+1}$, the following notation is introduced:

$$f_s^{(i,j,...,k)} = f_s^{(i)} f_s^{(j)} \cdots f_s^{(k)}$$  \hspace{1cm} (15)

The error relation trivially generalises to cases where $m$ interpolation nodes coincide. In order to then identify the asymptotic order of convergence, the conventional definition that $\epsilon_{n+1} \sim \epsilon_n^\ell$ can be recursively applied to (14) to find $\ell_{n+1} = m \sum_{i=0}^{n} \ell_i$. Equivalently, the geometric sum can be re-expressed to equate $\ell = (m+1) - m \ell_{-(n+1)}$.

Table 1 presents numerical solutions of $\ell$ for the cases where $m = 1$ and 2. The order of convergence accelerates as $n$ increases, tending to $m + 1$. However, a long memory is not needed to raise the convergence order close to its asymptotic limit. In practice, one may then be satisfied with methods that use a limited history of points.

| Data    | Error     | $n = 0$ | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ |
|---------|-----------|---------|---------|---------|---------|---------|
| $\{x_i, f_i\}$ | $\prod_{i=0}^{n} \epsilon_i$ | 1.00000 | 1.61803 | 1.83929 | 1.92756 | 1.96595 |
| $\{x_i, f_i, f'_i\}$ | $\prod_{i=0}^{n} \epsilon_i^2$ | 2.00000 | 2.73205 | 2.91964 | 2.97445 | 2.99165 |

**Table 1**

Convergence indices $(\ell : \epsilon_{n+1} \sim \epsilon_n^\ell)$ for iteration methods with a leading error term given by (14).

It is stressed that the relative efficiency of derivative-free methods and higher-derivative methods depends on the computational costs of obtaining higher derivatives. If each derivative takes a similar or longer time as $f[x]$ to be calculated, the derivative-free methods are generally most efficient. Even for low-memory iterations, note that the order of convergence is 2 for one Newton step given $(f_i, f'_i)$, but 2.62 $(1.62^2)$ for two secant steps given $(f_i, f_{i+1})$ and the respective memory. As $n \to \infty$, the order of convergence is 3 for one first-derivative method step, but 4 $(2^2)$ for two derivative-free method steps.

Conversely, if $f[x]$ is defined by an integral, or $f[x]$ is known to satisfy a differential equation (which could itself be differentiated), or the derivatives assume simple forms, it may be relatively quick to calculate derivatives. In such cases, interpolation-based schemes that minimise the number of references to $f[x]$ could be favourable. The root search schemes detailed in this paper assume that $f[x]$ is determined at every iteration point, but the interpolation-based approach can be adapted to generally consider mixed interpolation conditions.
Tables 2 and 4 present root search schemes with specific parameter choices, and the associated leading error factors $E_{m,n+1}$ for some cases of $n$. The 2-point ($n = 1$) derivative-free methods in Table 2 are equivalent to the secant method. The 1-point ($n = 0$) first-derivative methods in Table 4 are equivalent to Newton’s method. The scheme in the left column of Table 2 is also recognised to result in the same iteration steps formulated by Larkin [5], though without recursive evaluations of divided differences being required. Some of the leading error factors could be cancelled by forming weighted averages of the different iteration schemes. However, the coefficients of the highest degree factors are common for given $n$, and so such averaging does not generally raise the order of convergence further. It is important to note that the $x_i$ or $f_i$ values referenced in the weights must be distinct. Otherwise some weights become infinite.

Tables 3 and 5 demonstrate the convergence behaviours of different iteration sequences. Although the iterations are presented to high precision, there are few practical cases where such precision is needed. If tolerant to 64-bit machine errors ($\sim 10^{-16}$), the interpolation-based methods save a few steps compared to the secant method or Newton’s method. Such savings can still form a useful performance advantage though. The application of non-local information can also further help to enter the convergence phase faster, where robust derivative estimates smooth over localised oscillations.

Returning to the topic of parameter constraints in derivative-free schemes, it was previously argued for the terms of $O(\epsilon^k)$ to cancel each other for $k < n$. However, it was then identified that the derivative-free schemes exhibit sub-quadratic convergence. Any $O(\epsilon^k)$ error terms for $k \geq 2$ are thus sub-dominant. The constraints in (16) can then be generally applied without compromising the order of convergence, where $g_j = O(\epsilon_n)$ and $h_j = O(\epsilon_n)$.

\[
\begin{pmatrix}
1 & \cdots & 1 & 1 \\
\epsilon_0 & \cdots & \epsilon_{n-1} & g_1 \\
\vdots & \vdots & \vdots & \vdots \\
\epsilon_{n-1} & \cdots & \epsilon_{n-1} & g_{n-1}
\end{pmatrix}
\begin{pmatrix}
\omega_0 \\
\vdots \\
\omega_{n-1} \\
\omega_n
\end{pmatrix}
= 
\begin{pmatrix}
0 \\
\vdots \\
\vdots \\
h_n
\end{pmatrix}
\]  

(16)

If $g_j = (\alpha \epsilon_n)^j$ for some free variable $\alpha$ and $h_j = 0$, it follows from (13) that the parameter set below has asymptotic behaviours satisfying the above constraints.

\[
\omega_{i(\neq n)} = \frac{1}{f_i - \alpha f_n} \prod_{j \neq \{i, n\}} \frac{1}{f_i - f_j} \\
\omega_n = \prod_{j \neq n} \frac{1}{\alpha f_n - f_j}
\]  

(17)

The limit of coinciding pairs of interpolation nodes could also be considered in order to find parameters suitable for the iteration scheme with first derivatives. However, this paper does not seek to comprehensively explore such cases. It is simply emphasised that other parameter sets can be applied that have similar convergence properties.
Method:  
\[ x_{n+1} = \left( \sum_{i=0}^{n} \frac{\omega_i x_i}{f_i} \right) \bigg/ \left( \sum_{i=0}^{n} \frac{\omega_i}{f_i} \right) \]

Weights:  
\[ \omega_i = \prod_{j \neq i} \frac{1}{x_i - x_j} \quad \omega_i = \prod_{j \neq i} \frac{1}{f_i - f_j} \]

Interpolant:  
\[ f[x]: (1,n-1) \text{ rational} \quad f[x]: (n+1,n-1) \text{ rational} \]
\[ x[f]: (n,n) \text{ rational} \quad x[f]: (n) \text{ polynomial} \]

| n+1 | Leading error factor \((E_{1,n+1})\) | Leading error factor \((E_{1,n+1})\) |
|-----|--------------------------------|--------------------------------|
| 2   | \( \frac{f_s^{(2)}}{2 f_s^{(1)}} \) | \( \frac{f_s^{(2)}}{2 f_s^{(1)}} \) |
| 3   | \( \frac{3 f_s^{(2,2)} - 2 f_s^{(1,3)}}{12 f_s^{(1,1)}} \) | \( \frac{6 f_s^{(2,2)} - 2 f_s^{(1,3)}}{12 f_s^{(1,1)}} \) |
| 4   | \( \frac{3 f_s^{(2,2,2)} - 4 f_s^{(1,2,3)} + f_s^{(1,1,4)}}{24 f_s^{(1,1,1)}} \) | \( \frac{15 f_s^{(2,2,2)} - 10 f_s^{(1,2,3)} + f_s^{(1,1,4)}}{24 f_s^{(1,1,1)}} \) |

Table 2  
Root search schemes based on derivative-free rational interpolation.

| Picard \(n = 1\) | Secant \(n = 2\) | Secant \(n = 3\) | Newton \(n = 3\) |
|------------------|------------------|------------------|------------------|
| \(i\)            |                  |                  |                  |
| 0                | 2.26             | 2.26             | 2.26             | 2.26             |
| 1                | 1.73             | 1.73             | 1.73             | 1.73             |
| 2                | \(1.90 \times 10^{-1}\) | \(6.19 \times 10^{-1}\) | \(6.19 \times 10^{-1}\) | \(6.19 \times 10^{-1}\) |
| 3                | \(1.14 \times 10^{-1}\) | \(8.35 \times 10^{-1}\) | \(3.47 \times 10^{-1}\) | \(3.47 \times 10^{-1}\) |
| 4                | \(8.15 \times 10^{-2}\) | \(1.01 \times 10^{-1}\) | \(6.61 \times 10^{-2}\) | \(1.77 \times 10^{-2}\) |
| 5                | \(5.24 \times 10^{-2}\) | \(1.23 \times 10^{-2}\) | \(1.73 \times 10^{-3}\) | \(2.00 \times 10^{-4}\) |
| 6                | \(3.63 \times 10^{-2}\) | \(2.91 \times 10^{-4}\) | \(4.27 \times 10^{-6}\) | \(1.78 \times 10^{-8}\) |
| 7                | \(2.40 \times 10^{-2}\) | \(7.94 \times 10^{-7}\) | \(5.60 \times 10^{-11}\) | \(4.40 \times 10^{-16}\) |
| 8                | \(1.63 \times 10^{-2}\) | \(5.09 \times 10^{-11}\) | \(4.80 \times 10^{-20}\) | \(6.06 \times 10^{-31}\) |
| 9                | \(1.09 \times 10^{-2}\) | \(8.90 \times 10^{-18}\) | \(1.33 \times 10^{-36}\) | \(2.08 \times 10^{-59}\) |

Table 3  
Error magnitudes for the root of \(f[x] = \cos x - x\) \((x_0 = 3)\), where Picard’s method corresponds to fixed-point iteration: \(x_{i+1} = \cos x_i\). Newton’s method is applied in the right column using \(f'_s\) information, and the central sequences are generated by the method and weights defined in the left column of Table 2 using only the latest \(n+1\) points.
Method: 
\[ x_{n+1} = \left( \sum_{i=0}^{n} \frac{\lambda_i (x_i - f_i / f_i') - \gamma_i f_i x_i}{f_i'^2} \right) / \left( \sum_{i=0}^{n} \frac{\lambda_i - \gamma_i f_i}{f_i'^2} \right) \]

Weights: 
\[ \lambda_i = f_i' \prod_{j \neq i} \frac{1}{(x_i - x_j)^2} \quad \lambda_i = \prod_{j \neq i} \frac{1}{(f_i - f_j)^2} \]

\[ \gamma_i = -\frac{2\lambda_i}{f_i'} \sum_{j \neq i} \frac{1}{x_i - x_j} \quad \gamma_i = -\frac{2\lambda_i}{f_i - f_j} \]

Interpolant: 
\( f[x] \): (1,2n) rational  
\( f[x] \): (2n+2,2n) rational  
\( x[f] \): (2n+1,2n+1) rational  
\( x[f] \): (2n+1) polynomial

| \( n+1 \) | Leading error factor \( (E_{2,n+1}) \) | Leading error factor \( (E_{2,n+1}) \) |
|---|---|---|
| 1 | \( \frac{f_*^{(2)}}{2 f_*^{(1)}} \) | \( \frac{f_*^{(2)}}{2 f_*^{(1)}} \) |
| 2 | \( \frac{3 f_*^{(2,2,2)} - 4 f_*^{(1,2,3)} + f_*^{(1,1,4)}}{24 f_*^{(1,1,1)}} \) | \( \frac{15 f_*^{(2,2,2)} - 10 f_*^{(1,2,3)} + f_*^{(1,1,4)}}{24 f_*^{(1,1,1)}} \) |

Table 4  
Root search schemes based on rational interpolation with first derivatives.

| Newton | Halley |
|---|---|
| \( i \) | \( n = 0 \) | \( n = 1 \) | \( n = 2 \) | \( n = 3 \) |
| 0 | 2.26 | 2.26 | 2.26 | 2.26 | 2.26 |
| 1 | 1.24 | 1.24 | 1.24 | 8.72 \( \times 10^{-1} \) |
| 2 | 1.39 | 1.18 \( \times 10^{-1} \) | 1.18 \( \times 10^{-1} \) | 5.27 \( \times 10^{-2} \) |
| 3 | 4.94 \( \times 10^{-2} \) | 6.85 \( \times 10^{-4} \) | 2.44 \( \times 10^{-5} \) | 1.65 \( \times 10^{-5} \) |
| 4 | 5.68 \( \times 10^{-4} \) | 1.35 \( \times 10^{-10} \) | 9.33 \( \times 10^{-15} \) | 4.76 \( \times 10^{-15} \) |
| 5 | 7.12 \( \times 10^{-8} \) | 1.88 \( \times 10^{-28} \) | 2.87 \( \times 10^{-43} \) | 6.73 \( \times 10^{-44} \) |
| 6 | 1.12 \( \times 10^{-15} \) | 1.41 \( \times 10^{-77} \) | 1.56 \( \times 10^{-126} \) | 7.76 \( \times 10^{-131} \) |

Table 5  
Error magnitudes for the root of \( f[x] = \cos x - x \ (x_0 = 3) \). Halley’s method is applied in the right column using \( f'' \) information, and the other sequences are generated by the method and weights defined in the left column of Table 4 using only the latest \( n+1 \) points.
3. Approximate roots of univariate rational interpolants. In the previous section, the exact roots of interpolating functions were selected for subsequent iteration. However, such functions fundamentally are approximations. An alternative approach is to apply local iteration schemes about a specific point of the interpolant. The local scheme then approximates the interpolant root, but if the associated errors are of similar order to the interpolation errors, the iteration should be similarly effective.

Table 6 summarises the choices for derivative-free interpolation made in this section. The derivatives are deduced by performing a series expansion about the respective points. The leading error terms for Newton iteration \( (x_{n+1} = x_n - f_n/f'_n) \) with interpolant derivatives are then also presented for arbitrary \( \omega_i \).

| Direct function interpolation | Inverse function interpolation |
|-------------------------------|-------------------------------|
| \( f[x] \approx \left( \sum_{i=0}^{n} \omega_i f_i \right)/\left( \sum_{i=0}^{n} \omega_i (x - x_i) \right) \) | \( x[f] \approx \left( \sum_{i=0}^{n} \omega_i x_i \right)/\left( \sum_{i=0}^{n} \omega_i (f - f_i) \right) \) |
| \( f'_i \approx -\frac{1}{\omega_i} \sum_{j \neq i} \omega_j \frac{f_i - f_j}{x_i - x_j} \) | \( \frac{1}{f'_i} \approx -\frac{1}{\omega_i} \sum_{j \neq i} \omega_j \frac{x_i - x_j}{f_i - f_j} \) |

\[ \epsilon_{n+1} \sim \epsilon_n \left( \sum_{i=0}^{n} \omega_i \right)/\left( \sum_{j \neq n} \omega_j \right) \quad \epsilon_{n+1} \sim \left( \sum_{i=0}^{n} \omega_i \right) \frac{\epsilon_n}{\omega_n} \]

Table 6

Interpolants with corresponding first derivatives, and leading error terms for Newton iteration.

As in the previous section, the leading error is generally \( O[\epsilon] \), but that term vanishes when \( \sum \omega_i = 0 \). In such cases, the interpolant derivative becomes a weighted average of finite differences. If then successively requiring the leading error to vanish up to \( O[\epsilon^2] \) terms, the following constraints also apply:

\[ \sum_{j \neq n} \omega_j \epsilon_j^k = O[\epsilon_n] \quad 1 \leq k \leq n - 1 \quad (18) \]

The constraints take the same form as (16), and so the weights identified in the previous section can again be used. Similarly, it follows that when these constraints are satisfied, the leading error term takes the form of (14) for which the asymptotic order of convergence was previously discussed.

Tables 7 and 8 present iteration schemes based on the above interpolating functions. The leading error factors for the schemes in Table 7 are common to those when taking the exact interpolant root of \( x[f] \) (Table 2). However, the sub-dominant error terms differ, so the iteration sequences are generally distinct. The scheme in the left column of Table 8 is also noted to be equivalent to the method described by Sidi [6], though with the polynomial interpolant derivative being constructed here without recursion. This method should be generally favoured amongst the derivative-free root search methods detailed in this paper, as its leading error factor contains only the highest degree term common to all methods, and so the error tends to be suppressed.
Method: \( x_{n+1} = x_n - \frac{f_n}{f_n'} \) 

\[
\frac{1}{f_n'} \approx \left( \sum_{k \neq n} \omega_k \frac{x_n - x_k}{f_n - f_k} \right) / \left( \sum_{k \neq n} \omega_k \right)
\]

Weights: \( \omega_i = \prod_{j \neq i} \frac{1}{x_i - x_j} \) \( \omega_i = \prod_{j \neq i} \frac{1}{f_i - f_j} \)

Interpolant: \( x[f] \): (n,n) rational \( x[f] \): (n) polynomial

\[
\begin{array}{c|c|c}
\text{n+1} & \text{Leading error factor (} E_{1,n+1} \text{)} & \text{Leading error factor (} E_{1,n+1} \text{)} \\
\hline
2 & \frac{f_2}{2 f_1} & \frac{f_2}{2 f_1} \\
3 & \frac{3 f_3^{(2,2)} - 2 f_3^{(1,3)}}{12 f_1} & \frac{6 f_3^{(2,2)} - 2 f_3^{(1,3)}}{12 f_1} \\
4 & \frac{3 f_4^{(2,2,2)} - 4 f_4^{(1,2,3)} + f_4^{(1,1,4)}}{24 f_1^{(1,1,1)}} & \frac{15 f_4^{(2,2,2)} - 6 f_4^{(1,2,3)} + f_4^{(1,1,4)}}{24 f_1^{(1,1,1)}} \\
\end{array}
\]

Table 7
Root search schemes based on Newton’s method for \( x[f] \) interpolant.

Method: \( x_{n+1} = x_n - \frac{f_n}{f_n'} \) 

\[
\frac{1}{f_n'} \approx \left( \sum_{k \neq n} \omega_k \frac{x_n - x_k}{f_n - f_k} \right) / \left( \sum_{k \neq n} \omega_k \right)
\]

Weights: \( \omega_i = \prod_{j \neq i} \frac{1}{x_i - x_j} \) \( \omega_i = \prod_{j \neq i} \frac{1}{f_i - f_j} \)

Interpolant: \( f[x] \): (n) polynomial \( f[x] \): (n,n) rational

\[
\begin{array}{c|c|c}
\text{n+1} & \text{Leading error factor (} E_{1,n+1} \text{)} & \text{Leading error factor (} E_{1,n+1} \text{)} \\
\hline
2 & \frac{f_2}{2 f_1} & \frac{f_2}{2 f_1} \\
3 & \frac{- f_3^{(3)}}{6 f_1^{(1)}} & \frac{3 f_3^{(2,2)} - 2 f_3^{(1,3)}}{12 f_1^{(1,1)}} \\
4 & \frac{f_4^{(4)}}{24 f_1} & \frac{6 f_4^{(2,2,2)} - 6 f_4^{(1,2,3)} + f_4^{(1,1,4)}}{24 f_1^{(1,1,1)}} \\
\end{array}
\]

Table 8
Root search schemes based on Newton’s method for \( f[x] \) interpolant.
However, the iteration sequences are generally distinct. In order to deduce present iteration schemes based on interpolation with first derivatives, using (6) for $x[f]$ and its counterpart form for $f[x]$. The leading error factors in Table 9 are common to those when taking the exact interpolant root of $x[f]$ (Table 2). However, the iteration sequences are generally distinct. In order to deduce the second derivative $f''_i$ from the $x[f]$ interpolant, $x''[f]$ can be first determined by a series expansion about $f_i$ and then the following relation used:

$$\frac{\partial^2 x}{\partial f^2} = \frac{\partial}{\partial f} \left( \frac{\partial x}{\partial f} \right) = \frac{\partial x}{\partial f} \frac{\partial}{\partial x} \left( \frac{1}{f'} \right) = -\frac{f''}{f'}$$

(19)

The Chebyshev-Halley family [12] of root search methods is applied to the interpolant, as these are known to be cubically convergent when the true second derivative is used. For the iteration schemes based on exact interpolant roots, the orders of convergence were identified to be super-quadratic (for $n > 0$) but sub-cubic. It is then sufficient to

| Method: | $x_{n+1} = x_n - \left( \frac{f''_n + (\frac{1}{2} - \beta) f_n f''_n}{f''_n - \beta f_n f''_n} \right) \frac{f_n}{f'_n}$ | $\beta$ free parameter | $\beta = 1$ recommended |
|---|---|---|---|
| $f''_i \approx \frac{2f_i^2}{\lambda_i} \left( \gamma_i + \sum_{k \neq i} \lambda_k (x_i - x_k) + (\gamma_k (x_i - x_k) - \lambda_k f'_k) (f_i - f_k) \right)$ | $\lambda_i = \prod_{j \neq i} \frac{1}{f_i - f_j}$ | $\gamma_i = -2 \lambda_i \sum_{j \neq i} \frac{1}{f_i - f_j}$ |
| Error: | $\epsilon_1 \approx \frac{f^{(2)}_n}{2 f^{(1)}_n} \epsilon_0^2$ | $\epsilon_2 \approx \frac{15 f^{(2,3,2)}_n - 10 f^{(1,3,3)}_n + f^{(1,1,4)}_n}{24 f^{(1,1,1)}_n} \epsilon_0^2 \epsilon_1^2$ |

**Table 9**

*Root search scheme based on Chebyshev-Halley methods for $x[f]$ interpolant.*

| Method: | $x_{n+1} = x_n - \left( \frac{f''_n + (\frac{1}{2} - \beta) f_n f''_n}{f''_n - \beta f_n f''_n} \right) \frac{f_n}{f'_n}$ | $\beta$ free parameter | $\beta = 1$ recommended |
|---|---|---|---|
| $f''_i \approx - \frac{2}{\lambda_i} \left( \gamma_i f'_i + \sum_{k \neq i} \lambda_k (f_i - f_k) + (\gamma_k (f_i - f_k) - \lambda_k f'_k) (x_i - x_k) \right)$ | $\lambda_i = \prod_{j \neq i} \frac{1}{x_i - x_j}$ | $\gamma_i = -2 \lambda_i \sum_{j \neq i} \frac{1}{x_i - x_j}$ |
| Error: | $\epsilon_1 \approx \frac{f^{(2)}_n}{2 f^{(1)}_n} \epsilon_0^2$ | $\epsilon_2 \approx \frac{f^{(4)}_n}{24 f^{(1)}_n} \epsilon_0^2 \epsilon_1^2$ (which is independent) |

**Table 10**

*Root search scheme based on Chebyshev-Halley methods for $f[x]$ interpolant.*
use Chebyshev-Halley methods for schemes referencing approximate interpolant roots, without compromising the order of convergence. Special cases of the Chebyshev-Halley family include Chebyshev’s method ($\beta = 0$), Halley’s method ($\beta = \frac{1}{2}$) and the super-Halley method ($\beta = 1$). The super-Halley method is generally recommended despite the leading errors for the interpolation-based schemes being $\beta$-independent, as certain next-to-leading order error terms then vanish. Note though that higher-order local methods [13, 14] should otherwise be applied if the interpolant uses derivatives beyond first order.

4. Univariate optimisation methods. For optimisation problems, it is first noted that interpolation-based methods derived from inverse objective functions would be unreliable. Since, if the extremum is not approached from a common direction, the multi-valued nature of the inverse function in the neighbourhood of the solution would result in a poorly constructed interpolant. Furthermore, it is non-trivial to identify the exact extremum of rational interpolants for the direct function. However, local iteration schemes about a specific point of the direct function interpolant do allow for suitable approximation of stationary points. This section presents methods based on the latter framework.

Consider the following derivative-free approximation of an objective function:

$$
\phi[x] \approx \left( \sum_{i=0}^{n} \frac{\omega_i \phi_i}{x - x_i} \right) \left/ \left( \sum_{i=0}^{n} \frac{\omega_i}{x - x_i} \right) \right.
$$

(20)

The interpolant derivative can be deduced by performing a series expansion about a given point, which can itself be expressed by a series expansion as follows,

$$
\phi'[n] \approx -\frac{1}{\omega_n} \sum_{j \neq n} \omega_j \frac{\phi_n - \phi_j}{x_n - x_j} = -\frac{1}{\omega_n} \sum_{k=0}^{\infty} \left( \frac{\phi_{n+1}}{(k+1)!} \sum_{j \neq n} \omega_j \epsilon_{jn}^k \right)
$$

(21)

where $\epsilon_{jn} = (x_j - x_n)$. In order to find general constraints for the interpolation parameters that raise the order of convergence of iteration methods, the leading errors of such schemes with respect to the true solution should be considered. However, those constraints are found to take complicated forms. This paper thus restricts its scope of discussion to identifying parameters where the derivative estimate is produced to highest order.

For (21) to reproduce the true derivative at zeroth order, it is necessary that the relation $\sum_{j \neq n} \omega_j = -\omega_n$ holds, or equivalently that $\sum_{i} \omega_i = 0$. If series expansions for $\omega_i$ trivially terminate at zeroth order, the subsequent constraints for eliminating leading errors are then equivalent to (16). As discussed previously, (13) offers a solution to such constraints and given the extra conditions on $\omega_i$ series expansions, it follows that $\omega_i \propto \prod_{j \neq i} (x_i - x_j)^{-1}$ may be applied. This choice corresponds to polynomial interpolation. From (10), it then follows that the interpolant derivative equals:

$$
\phi_{n+1}^{(1)} = (-1)^n \frac{\phi_{n+1}}{(n + 1)!} \left( \prod_{j=0}^{n-1} \epsilon_{jn} \right) + \text{sub-dominant terms}
$$

(22)

The leading error when applying Newton’s method with the interpolant derivatives has the following form with $m = 1$:

$$
\epsilon_{n+1} = \epsilon_{m,n+1} \times \left( \epsilon_{m-1,n} \prod_{i=0}^{n-1} \epsilon_{i} \right) + \text{sub-dominant terms}
$$

(23)
where $E_{m,n+1}$ is a factor composed of $k^{th}$ derivatives $\phi^{(k)}$ evaluated at the true stationary point. It is postulated that the error relation generalises as above when $m$ interpolation nodes coincide, which is indeed later confirmed for cases with $m = 2$. In order to then identify the asymptotic order of convergence, the conventional definition that $\epsilon_{n+1} \sim \epsilon_n^\ell$ can be recursively applied to (23) to find $\ell^{n+1} = (m-1) \ell^n + m \sum_{i=0}^{n-1} \ell^i$. Equivalently, the geometric sum can be re-expressed to equate $\ell^2 = 1 + m (\ell - \ell^{-n})$.

| Data | Error | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n \to \infty$ |
|------|-------|---------|---------|---------|---------|----------------|
| $\{x_i, \phi_i\}$ | $\epsilon_n^0 \prod_{i=0}^{n-1} \epsilon_i^1$ | 1.00000 | 1.32472 | 1.46557 | 1.53416 | 1.61803 |
| $\{x_i, \phi_i, \phi'_i\}$ | $\epsilon_n^1 \prod_{i=0}^{n-1} \epsilon_i^2$ | 2.00000 | 2.26953 | 2.35930 | 2.39246 | 2.41421 |
| $\{x_i, \phi_i, \phi'_i, \phi''_i\}$ | $\epsilon_n^2 \prod_{i=0}^{n-1} \epsilon_i^3$ | 3.00000 | 3.22069 | 3.27902 | 3.29571 | 3.30278 |

Table 11

$\ell : \epsilon_{i+1} \sim \epsilon_i^\ell$ for iteration methods with a leading error given by (23).

Table 11 presents numerical solutions of $\ell$. The order of convergence accelerates as $n$ increases, tending to $\frac{1}{2} \left( m + \sqrt{4 + m^2} \right)$. However, as for the root search methods, a long memory is not needed to raise the convergence order close to its asymptotic limit. In practice, one may again be satisfied with methods using a limited history of points.

Note that for problems where algorithmic differentiation [15] is being performed to calculate gradients, the objective function is also necessarily calculated. However, many standard optimisation methods neglect the information associated with objective function values. It is inferred here that the asymptotic order convergence for methods with memory of $\{\phi_i, \phi'_i\}$ is 2.42, compared to 1.62 for the secant method. Given that the same information is calculated for both, the methods with memory converge asymptotically $1.83 \left( \log[2.42]/\log[1.62] \right)$ times faster. There may also be further advantages if the convergence phase is entered faster by using non-local information.

Again, the relative efficiency of derivative-free methods and higher-derivative methods depends on the computational costs of obtaining higher derivatives. If each derivative takes a similar or longer time as $\phi[x]$ to be calculated, the derivative-free methods are generally most efficient. However, if line search optimisation is being performed as a subroutine of multi-dimensional optimisation, it will remain important to calculate gradients for directional information at certain steps. The interpolation-based approach can be adapted to consider mixed interpolation conditions, but this paper focuses on methods where the same type of information is available at each point.

Table 12 presents an optimisation scheme based on applying Newton’s method to derivative-free interpolants given by (20). Table 13 presents an optimisation scheme based on applying Chebyshev-Halley methods [12] to interpolants with first derivatives, as defined below:

$$\phi[x] \approx \frac{\left( \sum_{i=0}^{n} \lambda_i \phi_i + (\gamma_i \phi_i + \lambda_i \phi'_i)(x-x_i) \right)}{\left( \sum_{i=0}^{n} \lambda_i + \gamma_i (x-x_i) \right)^2} \left( \sum_{i=0}^{\infty} \frac{\lambda_i \phi(x-x_i^2)}{(x-x_i)^2} \right) \quad (24)$$
The leading errors in Table 13 are observed to be consistent with (23), and so the Chebyshev-Halley methods are appropriate for \( n > 1 \) in order to not compromise the order of convergence. If Newton’s method was instead applied in Table 13, the iteration scheme would be limited to quadratic convergence.

### Table 12

Optimisation scheme based on derivative-free interpolation.

| Method: \( x_{n+1} = x_n - \frac{\phi_n'}{\phi_n''} : \phi_n' \approx \left( \sum_{k \neq n} \omega_k \frac{\phi_n - \phi_k}{x_n - x_k} \right) / \left( \sum_{k \neq n} \omega_k \right) \) |
|---|
| \( \phi_n'' \approx -2 \left( \sum_{k \neq n} \omega_k \frac{(\phi_n - \phi_k) - \phi_n'(x_n - x_k)}{(x_n - x_k)^2} \right) / \left( \sum_{k \neq n} \omega_k \right) \) |
| Weights: \( \omega_i = \prod_{j \neq i} \frac{1}{x_i - x_j} \) |
| Error: \( \epsilon_{n+1} \sim (\frac{(-1)^n}{(n+1)!})^2 \phi_0^{(n+1)} / \phi_0^{(2)} \left( \prod_{i=0}^{n-1} \epsilon_i \right) \) |

| Table 13 |

Optimisation scheme based on interpolation with first derivatives.

| Method: \( x_{n+1} = x_n - \left( \frac{\phi_n'^2 + (\frac{1}{\beta} - 1) \phi_n' \phi_n'''}{\phi_n''^2 - \beta \phi_n' \phi_n''''} \right) \phi_n' \phi_n'' : \beta \) free parameter |
|---|
| \( \beta = 1 \) recommended |
| \( \phi_n'' \approx \frac{2}{\lambda_i} \left( \gamma_i \phi_i' + \sum_{k \neq i} \left( \frac{\gamma_k (\phi_i - \phi_k) - \lambda_k \phi_k'}{(x_i - x_k)^2} + \lambda_k (\phi_i' - \phi_k') (x_i - x_k)^2 \right) \right) \) |
| \( \phi_n''' \approx -\frac{6}{\lambda_i} \left( \frac{\gamma_i \phi_i''}{2} + \sum_{k \neq i} \left( \frac{\gamma_k \phi_i'}{(x_i - x_k)} - \frac{\gamma_k (\phi_i' - \phi_k') (x_i - x_k)^2}{(x_i - x_k)^2} - \frac{2 \lambda_k (\phi_i' - \phi_k') (x_i - x_k)^3}{(x_i - x_k)^3} \right) \right) \) |
| Weights: \( \lambda_i = \prod_{j \neq i} \frac{1}{x_i - x_j} \) |
| \( \gamma_i = -2 \lambda_i \sum_{j \neq i} \frac{1}{x_i - x_j} \) |
| Error: \( \epsilon_2 \sim -\frac{2 \phi_0^{(4)}}{4! \phi_0^{(2)}} \epsilon_0 \epsilon_1^2 + \frac{\phi_0^{(3)}}{2 \phi_0^{(2)}} \epsilon_0^2 \) (\( \beta \)-independent) |
| \( \epsilon_3 \sim -\frac{2 \phi_0^{(6)}}{6! \phi_0^{(2)}} \epsilon_0^2 \epsilon_1 \epsilon_2 \) |
| \( \epsilon_4 \sim -\frac{2 \phi_0^{(8)}}{8! \phi_0^{(2)}} \epsilon_0^2 \epsilon_1 \epsilon_2 \epsilon_3 \) |
5. Multivariate optimisation methods. A framework for multivariate optimisation is now proposed. However, systematic rules for parameter selection that ensure good convergence properties have not been identified. It is expected though that the univariate schemes should form a special case of suitable multivariate schemes.

The following approximation is differentiable if \( \lambda_i \) are non-zero parameters,

\[
\phi[x] \approx \left( \sum_{i=0}^{n} \frac{\lambda_i \phi_i + (\phi_i k_i + \lambda_i g_i)^T(x - x_i)}{\|x - x_i\|_M}\right) \left( \sum_{i=0}^{n} \frac{\lambda_i + k_i^T(x - x_i)}{\|x - x_i\|_M^2} \right)
\]

(25)

where \( g_i \) is the gradient of the objective function at \( x_i \), and \( \{\lambda_i, k_i\} \) are free parameters. The notation of the norm terms is clarified below, where the \( M_i \) metrics should be sign-definite in order for the interpolation to be well-behaved.

\[
\|\Delta\|^2_M = \Delta^T M \Delta
\]

(26)

On performing a series expansion about \( x_i \), the interpolant derivatives are found to be:

\[
\frac{\partial \phi}{\partial x^\alpha} |_{x=x_i} = g_i^\alpha
\]

(27)

\[
H_i^{\mu\nu} = \frac{\partial^2 \phi}{\partial x^\mu \partial x^\nu} |_{x=x_i} = - s_i M_i^{\mu\nu} + \frac{g_i^\mu k_i^\nu + k_i^\mu g_i^\nu}{\lambda_i}
\]

(28)

where \( s_i = 2 \sum_{j \neq i} \left( \frac{\lambda_j (\phi_i - \phi_j) + ((\phi_i - \phi_j) k_j - \lambda_j g_j)^T(x_i - x_j)}{\|x_i - x_j\|^2_M} \right) \)

(29)

The interpolant Hessian \( H_i \) possesses a sufficient number of degrees of freedom so that it could tend to the true Hessian. Depending on the dimension, and number of interpolation points, it may be convenient to decompose \( M_i \) into low rank terms plus a term proportional to the identity matrix. However, it is not obvious what basis to choose for such decompositions.

The inverse Hessian can be calculated by repeated use of the Sherman-Morrison formula, resulting in a form where \( H_i^{-1} = M_i^{-1} W_i M_i^{-1} \) with the following definitions:

\[
W_i^{\mu\nu} = - \frac{\lambda_i}{s_i} \left( M_i^{\mu\nu} + \frac{g_i^\mu g_i^\nu \|k_i\|^2_{M_i^{-1}} + k_i^\mu k_i^\nu \|g_i\|^2_{M_i^{-1}} - (g_i^\mu k_i^\nu + k_i^\mu g_i^\nu) t_i}{t_i^2 - \|k_i\|^2_{M_i^{-1}} \|g_i\|^2_{M_i^{-1}}} \right)
\]

(30)

where \( t_i = g_i^T M_i^{-1} k_i + s_i \)

(31)

On applying Newton’s method to the interpolant in (25), the following iteration scheme is then established:

\[
x_{n+1} = x_n - H_n^{-1} g_n = x_n + \lambda_n M_n^{-1} \left( \frac{t_n g_n - k_n \|g_n\|^2_{M_n^{-1}}}{t_n^2 - \|k_n\|^2_{M_n^{-1}} \|g_n\|^2_{M_n^{-1}}} \right)
\]

(32)

Although the above formula is motivated by interpolation, it may be helpful to simply assume the Hessian form in (28) and then require that certain higher derivatives are constant. Constraints can then be set for a subset of parameters. However, the question of how to ensure good convergence properties still remains.
6. Multivariate root search methods. The approaches considered for univariate root search can also be applied in the multivariate case. However, as for the proposed multivariate optimisation framework, systematic rules for parameter selection that ensure good convergence properties have not been identified.

To derive methods based on inverse interpolation, consider the following relation:

\[
x[f] \approx \left( \sum_{i=0}^{n} \Lambda_i + \Gamma_i (f - f_i) \right)^{-1} \left( \sum_{i=0}^{n} \Lambda_i x_i + \left( \Gamma_i x_i + \Lambda_i J_i^{-1} \right) (f - f_i) \right)
\]

(33)

where \( J_i \) are (possibly approximated) Jacobian matrices, \( \Lambda_i \) are free matrices, and \( \Gamma_i \) free tensors such that \( \Gamma_i f_i = \Gamma_i^{\mu\nu} f_i^{\rho} \) and \( \Gamma_i x_i f_i = \Gamma_i^{\mu\nu} x_i^{\rho} f_i^{\sigma} \). Note that for the interpolant to be differentiable, the \( \Lambda_i \) matrices must be non-zero. On notation conventions, it is assumed in this section that pairs of (Greek) dimension indices are summed over when appearing in a given term. The following iteration formula is then found on setting \( f = 0 \):

\[
x_{n+1} = \left( \sum_{i=0}^{n} \frac{\Lambda_i - \Gamma_i f_i}{f_i^T M_i f_i} \right)^{-1} \left( \sum_{i=0}^{n} \frac{\Lambda_i (x_i - J_i^{-1} f_i) - \Gamma_i x_i f_i}{f_i^T M_i f_i} \right)
\]

(34)

A sub-family of the above iteration scheme can also be derived by approximating the direct function in (35), given the relation for the \( R \) matrix function in (36):

\[
f[x] = (R^{-1}[x]) (A x + b)
\]

(35)

\[
(R f)[x] \approx \left( \sum_{i=0}^{n} \frac{\Lambda_i}{\|x - x_i\|^2} \right)^{-1} \left( \sum_{i=0}^{n} \frac{\Lambda_i (R_i f_i + (R_i f_i' + R_i J_i) (x - x_i))}{\|x - x_i\|^2} \right)
\]

(36)

where \( R_i' \) is the derivative of the \( R \) matrix function at \( x_i \), and \( (R_i' f_i)^{\mu\nu} = R_i^{\mu\sigma\nu} f_i^{\sigma} \).

If the conditions below hold, (35) and (36) are guaranteed to be consistent.

\[
A = R_i' f_i + R_i J_i \quad \forall i
\]

\[
b = R_i f_i' - (R_i f_i' + R_i J_i) x_i \quad \forall i
\]

(37)

Solutions for (37) are given by:

\[
R_i^{\mu\nu} = \sum_{k=0}^{n} \left( \frac{\Lambda_k^\mu \alpha}{a_k} - \frac{\Lambda_k^\mu \gamma (z_k^z - z_i^z)}{a_k} \right) \frac{f_i^{\nu} M_i^{\sigma\alpha}}{a_k a_i}
\]

(38)

\[
R_i^{\mu\sigma\nu} = \sum_{k=0}^{n} \left( \frac{\Lambda_k^\mu \gamma (z_k^z - z_i^z)}{a_k} \right) M_i^{\sigma\nu}
\]

(39)

where \( a_i = f_i^T M_i J_i^{-1} f_i \)

\[
z_i = x_i - J_i^{-1} f_i
\]

(40)

The \( A, b \) factors are then equal to:

\[
A = \left( \sum_{k=0}^{n} \frac{\Lambda_k}{f_k^T M_k J_k^{-1} f_k} \right) \quad b = - \left( \sum_{k=0}^{n} \frac{\Lambda_k (x_k - J_k^{-1} f_k)}{f_k^T M_k J_k^{-1} f_k} \right)
\]

(41)
The iteration formula in (34) is thus reproduced by solving for $f = 0$ given (35) \((x_{n+1} = -A^{-1}b)\) and defining $M_i = \tilde{M}_i J^{-1}$, though without the $\Gamma_i$ terms.

Alternatively, root search methods can be constructed by applying local iteration schemes with interpolant derivatives, either of $x[f]$ as in (33), or its counterpart form for $f[x]$. On convergence behaviours of the proposed approaches, naive extensions of the univariate parameter choices do not achieve convergence acceleration, and also tend to delay the convergence phase. Of course the univariate method parameters were required to obey specific constraints. A full set of corresponding constraints for multivariate schemes has not yet been determined.

7. Conclusions. The convergence order of univariate root search and optimisation schemes can be accelerated by re-using accumulated function information, given certain constraints identified in this paper. However, a long memory is not required in order to approach the asymptotic limits. For univariate root search, the presented derivative-free methods approach quadratic convergence and the first-derivative methods approach cubic convergence. For univariate optimisation, the derivative-free methods approach a convergence order of 1.62 and the first-derivative methods approach an order of 2.42. There are general performance advantages with respect to low-memory iteration methods, most notably in the case where optimisation routines calculate the objective function and gradient at each step: the full-memory methods converge asymptotically 1.8 times faster than the secant method. For problems where the time required to calculate derivatives is similar or longer than that for function evaluations, it is stressed that the derivative-free methods are most efficient.

Frameworks to extend the iteration schemes to multivariate problems have also been proposed, but without identification of practically useful parameter choices. Further study is therefore required to answer if/how the approaches can be suitably extended to multivariate problems. There are also various other ways that this work can be extended. Although not listed in this paper, iteration formulae with mixed interpolation conditions can be defined. Furthermore, problems with non-simple roots or stationary points with null second derivatives require adaptations to the interpolation-based schemes presented. Another restriction within this paper was that only ‘greedy’ approaches were considered, where the leading error of the next step was required to be maximally suppressed. It may be expected though that the error tolerance will not be met in the subsequent step (given knowledge of the convergence rates), and so multi-point methods with memory should then be favoured.

For final emphasis, the univariate iteration schemes presented in this paper are advocated for common use. The associated parameters are defined analytically, and so require no intermediate calibration operations. The formulae can also be applied to an arbitrary history of points. Primarily though, performance advantages are achieved when the iteration evaluations form a negligible component of the computation efforts.

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