Relations between Rayleigh Quotient Iteration and Classical Root Finding Algorithms

Jens-Peter M. Zemke
zemke@tu-harburg.de

Institut für Numerische Simulation
Technische Universität Hamburg-Harburg

Universiteit Utrecht, The Netherlands
2010/03/03

Outline

Newton's method

The best known method for the computation of a root of a rational function

$$f : \mathbb{C} \to \mathbb{C}, \quad f(z) := \frac{p(z)}{q(z)}, \quad p, q \in \mathbb{P}_m$$

is Newton's method

$$z_{k+1} = z_k - \frac{f(z_k)}{f'(z_k)}.$$

Newton's method corresponds to iteratively computing a root of the Taylor approximation of first order to the given function.

Newton's method mostly converges locally with Q-quadratic order of convergence. The global convergence is more complicated; the arising phenomena are more or less understood since the works of Fatou and Julia.

Newton's method costs two function evaluations per step, one evaluation of the function, one evaluation of its derivative.

The secant method

If the derivative of the function $f : \mathbb{C} \to \mathbb{C}$ is not at hand, we could use the first divided difference which gives the secant method:

$$z_{k+1} = z_k - \frac{f(z_k)}{[z_k, z_{k-1}]f}.$$

The secant method mostly locally has the R-order of convergence given by the golden ratio

$$\phi := \frac{1+\sqrt{5}}{2} \approx 1.618.$$

Two steps of the secant method are as costly as one step of Newton's method. This makes the secant method the winner:

$$\phi^2 = \phi + 1 \approx 2.618 > 2.$$

In general, the secant method locally wins (Raydan, 1993).

Schröder's and König's methods

Newton's method has been generalized to incorporate higher order derivatives and to exhibit a higher order of convergence. Well-known generalized Newton's methods are Halley's and Laguerre's methods.

In 1870 E. Schröder from Pforzheim came up with two infinite families of generalizations with prescribed order of convergence (Schröder, 1870).

In 1884 Julius König proved a theorem on the limiting behavior of certain ratios of Taylor coefficients (König, 1884), which enabled another, but simpler derivation of a family of methods.

This family is nowadays known as "König's method":

$$z_{k+1} = z_k + s\frac{(1/f)^{(s-1)}(z_k)}{(1/f)^{(s)}(z_k)}, \quad s = 1, 2, \dots$$

König's method typically has a Q-convergence order of $s+1$.

König's method for $s=1$ is Newton's method,

$$z_{k+1} = z_k + \frac{(1/f)(z_k)}{(1/f)'(z_k)} = z_k - \frac{1/f(z_k)}{f'(z_k)/(f(z_k))^2} = z_k - \frac{f(z_k)}{f'(z_k)}.$$

The Opitz-Larkin method

There is a natural extension of König's method using divided differences in place of the derivatives.

This natural extension (without the connection to König's method) was published 1958 by Günter Opitz on a two-page article in ZAMM postponing the proofs and details of the derivation (Opitz, 1958):

Die Möglichkeit weitergehender Verallgemeinerungen wird noch untersucht Eine ausführliche Beschreibung des Verfahrens, die Darlegung der Konvergenzverhältnisse und eine Diskussion der angedeuteten Verallgemeinerungen wird an anderer Stelle veröffentlicht.

Opitz never published a detailed version. Independently, 23 years later F. M. Larkin re-developed Opitz' method and published parts of Opitz' results with proofs in (Larkin, 1981) and the predecessor (Larkin, 1980).

We will refer to this method as the Opitz-Larkin method. The Opitz-Larkin method is based on iterations of the form

$$x_{k+1} = z_k + \frac{[z_1, z_2, \ldots, z_{k-1}](1/f)}{[z_1, z_2, \ldots, z_{k-1}, z_k](1/f)}.$$

The Opitz-Larkin method

Mostly, the z_i are all distinct and the next iterate is used as new evaluation point $z_{k+1} = x_{k+1}$,

$$z_{k+1} = z_k + \frac{[z_1, z_2, \dots, z_{k-1}](1/f)}{[z_1, z_2, \dots, z_{k-1}, z_k](1/f)}.$$

This variant of the Opitz-Larkin method converges with R-order 2.

Frequently, the Opitz-Larkin method is used with truncation:

$$z_{k+1} = z_k + \frac{[z_{k-p}, \dots, z_{k-1}](1/f)}{[z_{k-p}, \dots, z_{k-1}, z_k](1/f)},$$

see (Opitz, 1958, Seite 277, Gleichung (9)) and (Larkin, 1981, Section 4, pages 98–99).

The Opitz-Larkin method

It is possible to use confluent divided differences, i.e., multiple points of evaluation, i.e., higher order derivatives of $1/f$.

When we use only confluent divided differences in the truncated Opitz-Larkin method with truncation parameter $p = s$, we recover König's method:

$$
\begin{aligned}
z_{k+1} &= z_k + \frac{[\overbrace{z_k, \ldots, z_k}^{s}](1/f)}{[\underbrace{z_k, \ldots, z_k, z_k}_{s+1}](1/f)} \\
&= z_k + \frac{(1/f)^{(s-1)}(z_k)/(s-1)!}{(1/f)^{(s)}(z_k)/s!} = z_k + s\frac{(1/f)^{(s-1)}(z_k)}{(1/f)^{(s)}(z_k)}.
\end{aligned}
$$

The Opitz-Larkin method

Truncated Opitz-Larkin with $p = 1$ is the secant method,

$$\begin{aligned} z_{k+1} &= z_k + \frac{[z_{k-1}](1/f)}{[z_{k-1}, z_k](1/f)} \\ &= z_k + \frac{1}{f(z_{k-1})} \cdot \frac{z_{k-1} - z_k}{1/f(z_{k-1}) - 1/f(z_k)} \\ &= z_k + \frac{f(z_k)f(z_{k-1})}{f(z_{k-1})} \cdot \frac{z_{k-1} - z_k}{f(z_k) - f(z_{k-1})} \\ &= z_k - \frac{f(z_k)}{[z_{k-1}, z_k]f}. \end{aligned}$$

Confluent truncated Opitz-Larkin with $p = 1$ is Newton's method.

The Opitz-Larkin method

In general, the Opitz-Larkin method is closely connected to rational interpolation of the inverse function (Larkin, 1981, Theorem 1, page 96):

Theorem (Larkin 1981)

If, for any integer $k > 1$, there exists a rational function of the form

$$r_k(z) = \frac{q_d(z)}{z-\alpha}, \quad \forall\, z,$$

where q_d is a polynomial of degree $d \leqslant k-2$, such that $q_d(\alpha) \neq 0$ and

$$r_k(z_j) = f(z_j)^{-1}, \quad j = 1, 2, \dots, k,$$

then

$$z_k + \frac{[z_1, z_2, \dots, z_{k-1}](1/f)}{[z_1, z_2, \dots, z_{k-1}, z_k](1/f)} = \alpha.$$

The Opitz-Larkin method

Thus, the Opitz-Larkin method computes the unique root of the inverse of a rational interpolation at the inverse function values.

In the earlier publication (Larkin, 1980) Larkin used another approach to obtain the rational interpolant and gave pointers to articles that investigated the rate of convergence of such (direct and inverse) rational interpolations.

Most important are the articles (Tornheim, 1964) and (Jarratt and Nudds, 1965). We state the main results contained in these articles.

The Opitz-Larkin method

In the paper (Tornheim, 1964), Tornheim considered the case of direct

$$f^{(\ell_j)}(x_{i-j}) = \left(\frac{p}{q}\right)^{(\ell_j)}(x_{i-j})$$

and inverse rational interpolation

$$\left(\frac{1}{f}\right)^{(\ell_j)}(x_{i-j}) = \left(\frac{p}{q}\right)^{(\ell_j)}(x_{i-j}),$$

where

$$\ell_j = 0, 1, \ldots m_j - 1, \quad m = \sum_{j=0}^{k} m_j = \deg(p) + \deg(q) + 1,$$

and k given distinct points $\quad x_{i-j} \quad j = 1, \ldots, k,$

and gave its rate of convergence (Tornheim, 1964, Theorem 2).

The Opitz-Larkin method

Theorem (Tornheim 1964; conditions for the theorem)

Suppose an k-point iterative method is defined by the procedure to solve the equation $f(x) = 0$ by direct or inverse rational interpolation with m_j coincident interpolating points at x_{i-j} ($j = 1, \ldots, k$) for the i-th iteration. Assume that $f(x)$ has $m = m_1 + \cdots + m_k$ continuous derivatives in a neighborhood of $x^\star$, where $f(x^\star) = 0$ and $f'(x^\star) \neq 0$, and that

$$\mathbf{M} = \begin{vmatrix} a_d & a_{d-1} & \cdots & a_{2d+2-m} \\ a_{d+1} & a_d & \cdots & \\ \vdots & \vdots & & \vdots \\ a_{m-2} & & \cdots & a_d \end{vmatrix} \neq 0.$$

Here d is the degree of the numerator and e is the degree of the denominator of the rational function used; $d + e + 1 = m$; a_i is 0 if $i < 0$, otherwise it is the ith derivative of $f(x)$ (for direct interpolation) or of its inverse function (for inverse interpolation) at $x = x^\star$.

The Opitz-Larkin method

Theorem (Tornheim 1964; result of the theorem)

Then there is a neighborhood $N^\star$ of $x^\star$ such that if $x_1, \dots, x_k$ are in $N^\star$, the sequence $\{x_i\}$ converges to $x^\star$. Moreover, the order of convergence u, if it exists, is the positive root of the equation

$$x^k = m_1 x^{k-1} + m_2 x^{k-2} + \cdots + m_k.$$

In the context of the Opitz-Larkin method, we have to consider the limit of the positive root for $k \to \infty$.

He also gave a “comparison result” that predicts faster convergence when the (inverse) function is evaluated to higher order at the last iterates.

The Opitz-Larkin method

Lemma (Tornheim 1964)

Suppose that the coefficients of

$$a(x) := x^n - a_1 x^{n-1} - \cdots - a_n$$

satisfy

$$a_1 + a_2 + \cdots + a_n > 1, \quad a_1 \geqslant a_2 \geqslant \cdots \geqslant a_n \geqslant 0.$$

By Descartes' rule of signs the polynomial a has a unique positive root $u > 1$. If the coefficients b_i of

$$b(x) := x^n - b_1 x^{n-1} - \cdots - b_n$$

are a permutation of the coefficients a_i, then the positive root v of b is less than u.

The Opitz-Larkin method

In the paper (Jarratt and Nudds, 1965), Jarratt and Nudds give a detailed treatment of the case of rational interpolation with

$$r(z) = \frac{z-\alpha}{q_{k-2}(z)}, \quad q_{k-2} \in \mathbb{P}_{k-2}.$$

Larkin proves in (Larkin, 1981) that the Opitz-Larkin method is just a stable and cheap way to compute this rational interpolation.

As you might already have guessed: We are going to prove that RQI is the Opitz-Larkin method. One instance of RQI actually is the Opitz-Larkin method applied to the characteristic polynomial of the given matrix.

Original RQI

In the second edition of the first volume of his book "The Theory of Sound" (Strutt, 1894), John William Strutt, 3rd Baron Rayleigh included on page 110 the following passage:

> The stationary property of the roots of Lagrange's determinant (3) § 84, suggests a general method of approximating to their values. Beginning with assumed rough approximations to the ratios $A_1 : A_2 : A_3 \ldots\ldots$ we may calculate a first approximation to p^2 from
>
> $$p^2 = \frac{\frac{1}{2} c_{11} A_1^2 + \frac{1}{2} c_{22} A_2^2 + \ldots + c_{12} A_1 A_2 + \ldots}{\frac{1}{2} a_{11} A_1^2 + \frac{1}{2} a_{22} A_2^2 + \ldots + a_{12} A_1 A_2 + \ldots} \quad \ldots\ldots (3).$$
>
> With this value of p^2 we may recalculate the ratios $A_1 : A_2 \ldots$ from any $(m-1)$ of equations (5) § 84, then again by application of (3) determine an improved value of p^2, and so on.]

Original RQI

In modern notation, stated for the Hermitean algebraic eigenvalue problem

$$\mathbf{A}\mathbf{v} = \mathbf{v}\lambda, \quad \mathbf{A} = \mathbf{A}^{\mathsf{H}},$$

Lord Rayleigh starts with an approximate eigenvector $\mathbf{v}_k$, computes its Rayleigh quotient

$$\rho(\mathbf{v}_k) := \frac{\mathbf{v}_k^{\mathsf{H}}\mathbf{A}\mathbf{v}_k}{\mathbf{v}_k^{\mathsf{H}}\mathbf{v}_k}$$

and uses the linear system

$$(\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)\mathbf{v}_{k+1} = \mathbf{e}_j$$

for some standard unit vector $\mathbf{e}_j$ to compute a new approximate eigenvector $\mathbf{v}_{k+1}$. He was, of course, only interested in its direction.

Original RQI

This is repeated several times, i.e.,

$$\mathbf{v}_{k+1} = (\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{e}_j, \quad k = 0, 1, \ldots$$

As Lord Rayleigh only was interested in the ratios between eigenvector components, he definitely had used some sort of scaling between several steps.

Classical RQI can thus be stated in modern notation as

$$\mathbf{v}_{k+1} = \frac{(\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{e}_j}{\|(\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{e}_j\|}, \quad k = 0, 1, \ldots$$

for some suitably chosen $j \in \{1, 2, \ldots, n\}$, which might vary, depending on the computed approximate eigenvector.

Classical Rayleigh quotient iteration mostly converges locally with quadratic order of convergence.

Inverse Iteration

Closely connected to RQI is inverse iteration. Inverse iteration was developed by Helmut Wielandt in 1944, (Wielandt, 1944).

In the most basic variant of inverse iteration the shift τ is never updated, but the right-hand side is replaced by the latest approximate eigenvector:

$$\mathbf{v}_{k+1} = \frac{(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k}{\|(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k\|}, \quad k = 0, 1, \ldots$$

There exist variants which use other scalings, mostly using as left vector some standard unit vector $\boldsymbol{\ell} = \mathbf{e}_j$:

$$\mathbf{v}_{k+1} = \frac{(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k}{\mathbf{e}_j^{\mathsf{T}}(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k}, \quad k = 0, 1, \ldots$$

In the latter context, $\mathbf{e}_j^{\mathsf{T}}(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k \approx (\lambda - \tau)^{-1}$ gives an eigenvalue approximation.

Inverse Iteration

Either variant of inverse iteration with fixed shift τ converges linearly. The shift can be updated by using the approximate eigenvalues obtained by the latter, i.e., by using the shift update strategy

$$\tau_{k+1} := \tau_k - \frac{1}{\mathbf{e}_j^{\mathsf{T}}(\mathbf{A} - \tau\mathbf{I}_n)^{-1}\mathbf{v}_k}.$$

In both variants also the Rayleigh quotient can be used, the Rayleigh quotient uniquely solves the least squares problem

$$\rho(\mathbf{v}_k) = \operatorname{argmin}_{\rho\in\mathbb{C}} \|\mathbf{A}\mathbf{v}_k - \mathbf{v}_k\rho\|$$

and thus gives the “best” eigenvalue approximation matching the given approximate eigenvector $\mathbf{v}_k$.

Both these methods typically exhibit a quadratic convergence behavior.

Symmetric RQI

When automatic computers became available, the combination of inverse iteration with Rayleigh's original RQI resulted in the locally Q-cubically convergent (symmetric) RQI

$$\mathbf{v}_{k+1} = \frac{(\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{v}_k}{\|(\mathbf{A} - \rho(\mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{v}_k\|}, \quad k = 0, 1, \ldots$$

Crandall was the first who investigated the three variants (the original Rayleigh quotient iteration; inverse iteration with fixed shift; symmetric RQI) and proved their convergence rates to be quadratic, linear, and cubic, respectively, see (Crandall, 1951).

Ostrowski proved that unsymmetric RQI still has a quadratic convergence rate, (Ostrowski, 1959e). In (Ostrowski, 1959c), he also gave a variant that recovers the cubic convergence rate at the expense of the necessity to solve two linear systems every step instead of only one.

Two-Sided RQI

When $\mathbf{A} \in \mathbb{C}^{n \times n}$ is no longer Hermitean, the cubic convergence is lost and Ostrowski suggested in (Ostrowski, 1959c) the use of a two-sided RQI.

Two-sided RQI is based on the two-sided Rayleigh quotient

$$\rho(\mathbf{w}_k, \mathbf{v}_k) := \frac{\mathbf{w}_k^{\mathsf{H}} \mathbf{A} \mathbf{v}_k}{\mathbf{w}_k^{\mathsf{H}} \mathbf{v}_k}.$$

The iteration involves two sequences of vectors,

$$\begin{aligned} \mathbf{v}_{k+1} &= (\mathbf{A} - \rho(\mathbf{w}_k, \mathbf{v}_k)\mathbf{I}_n)^{-1}\mathbf{v}_k, \\ \mathbf{w}_{k+1} &= (\mathbf{A} - \rho(\mathbf{w}_k, \mathbf{v}_k)\mathbf{I}_n)^{-\mathsf{H}}\mathbf{w}_k, \end{aligned} \qquad k = 0, 1, \ldots$$

This trick recovers the cubic convergence of RQI at the price of the solution of an additional system.

Two-Sided RQI

Ostrowski worked out a more detailed analysis than Crandall. He published a series of six papers on RQI, (Ostrowski, 1959b; Ostrowski, 1959c; Ostrowski, 1959d; Ostrowski, 1959e; Ostrowski, 1959a). He measured the rate of convergence with respect to the number of solutions of linear systems, which he called one “Horner”. He was a little unfair to the two-sided variant, as these two Horners are related to each other (one decomposition, two forward and backward substitutions with the same two triangular matrices).

The proofs by Crandall and Ostrowski are beautiful and worth reading.

But we feel that a more direct proof of convergence for the different variants of RQI and related algorithms would be very helpful, especially when we want to investigate the overall behavior: the basins of attraction; global convergence; effects of perturbation and inexact methods, . . .

Simplification

Hessenberg matrices are in some sense the closest computable normal form of square matrices under unitary similarity transformations.

The implicit Q-Theorem gives uniqueness of the upper part of the reduction to Hessenberg form in case of given first column $\mathbf{q}$, if we fix the signs of the elements in the lower diagonal, e.g., to be non-negative real.

We use the implicit Q-Theorem to unitarily transform the pair $(\mathbf{A}, \mathbf{q})$ with $\|\mathbf{q}\|_2 = 1$ to the pair $(\mathbf{H}_n, \mathbf{e}_1)$, where $\mathbf{H}_n$ is upper Hessenberg and $\mathbf{e}_1$ denotes the first standard unit vector.

The following Matlab-code gives the transformed pair:

```
[Q,R] = qr(q);
[P,H] = hess(Q'*A*Q);
signs = sign(diag(H,-1));
S = diag(cumprod([1;signs]));
P = P*S;
H = S'*H*S;
```

Simplification

When $\mathbf{A}$ is non-derogatory, the Hessenberg matrix $\mathbf{H}_n$ is unreduced and uniquely determined. In other cases, only the leading part of $\mathbf{H}_n$ up to the first zero in the lower diagonal is uniquely determined.

Any left vector used for the Rayleigh quotient is modified accordingly.

We define as abbreviation

$$^{z}\mathbf{H}_n := (z\mathbf{I}_n - \mathbf{H}_n).$$

The first resolvent identity (Chatelin, 1993, Lemma 2.2.1, p. 63), valid for $z_1 \neq z_2$ from the resolvent set, gives

$$\begin{aligned} (^{z_1}\mathbf{H}_n)^{-1}(^{z_2}\mathbf{H}_n)^{-1} &= (z_1\mathbf{I}_n - \mathbf{H}_n)^{-1}(z_2\mathbf{I}_n - \mathbf{H}_n)^{-1} && \text{(1a)} \\ &= \frac{(^{z_1}\mathbf{H}_n)^{-1} - (^{z_2}\mathbf{H}_n)^{-1}}{z_2 - z_1} = -[z_1, z_2](^{z}\mathbf{H}_n)^{-1}. && \text{(1b)} \end{aligned}$$

The first resolvent identity is based on the trivial observation that

$$(z_2\mathbf{I}_n - \mathbf{H}_n) - (z_1\mathbf{I}_n - \mathbf{H}_n) = (z_2 - z_1)\mathbf{I}_n.$$

Simplification

This identity can be generalized to k distinct points of evaluation:

$$\prod_{i=1}^{k} ({}^{z_i}\mathbf{H}_n)^{-1} = (-1)^{k-1}[z_1, \ldots, z_k]({}^{z}\mathbf{H}_n)^{-1}. \tag{2}$$

The inverse of the characteristic matrix ${}^{z}\mathbf{H}_n$ is the rational function

$$({}^{z}\mathbf{H}_n)^{-1} = \frac{\mathrm{adj}({}^{z}\mathbf{H}_n)}{\chi(z)} =: \frac{\mathbf{P}_n(z)}{\chi(z)}, \quad \chi(z) := \det({}^{z}\mathbf{H}_n), \tag{3}$$

where the elements $p_{ij}(z)$ of $\mathbf{P}_n(z)$ are polynomials. The matrix-valued function $({}^{z}\mathbf{H}_n)^{-1}$ is meromorphic and analytic in the resolvent set.

Thus, confluent divided differences are well-defined and we do not need to restrict the points $\{z_i\}_{i=1}^{k}$ from the resolvent set.

Simplification

The adjugate of unreduced Hessenberg matrices has been investigated in (Z, 2006) and the results have been applied to Krylov subspace methods in (Z, 2007).

A similar approach predating these papers can be found in the technical report (Ericsson, 1990). Unfortunately, the report by Ericsson has never been published in a journal. We use here the notation of (Z, 2006).

We only need here a well-known result on a recurrence for the determinants of unreduced Hessenberg matrices, see, e.g., (Franklin, 1968, Section 7.11, p. 252, Eqn. (8)), or, the probably earliest reference (Schweins, 1825, Erste Abtheilung, IV. Abschnitt, § 154, Seite 361, Gleichung 560)).

There exist short proofs based on Laplace expansion and Cramer's rule.

Simplification

For simplicity we assume that $\mathbf{H}_n$ is unreduced.

We denote products of sub-diagonal elements of the unreduced Hessenberg matrices $\mathbf{H}_n \in \mathbb{C}^{n\times n}$ by

$$h_{i:j} := \prod_{\ell=i}^{j} h_{\ell+1,\ell}.$$

Polynomial vectors ν and $\check{\nu}$ are defined by

$$\nu(z) := \left(\frac{\chi_{j+1:n}(z)}{h_{j:n-1}}\right)_{j=1}^{n} \quad \text{and} \quad \check{\nu}(z) := \left(\frac{\chi_{1:j-1}(z)}{h_{1:j-1}}\right)_{j=1}^{n}. \tag{4}$$

The elements are denoted by $\nu_j(z)$ and $\check{\nu}_j(z)$, $j = 1, \ldots, n$. We remark that $\nu_n \equiv 1 \equiv \check{\nu}_1$.

The polynomials $\chi_{i:j}$ are the characteristic polynomials of submatrices of $\mathbf{H}_n$,

$$\chi_{i:j}(z) := \det\left({}^{z}\mathbf{H}_{i:j}\right) = \det\left(z\mathbf{I}_{j-i+1} - \mathbf{H}_{i:j}\right).$$

Simplification

By (Z, 2006, Lemma 3.1, Eqn. (3.5)) for z in the resolvent set

$$({}^{z}\mathbf{H}_n)\nu(z) = \frac{\chi(z)}{h_{1:n-1}}\mathbf{e}_1 \quad \Leftrightarrow \quad \frac{\nu(z)h_{1:n-1}}{\chi(z)} = ({}^{z}\mathbf{H}_n)^{-1}\mathbf{e}_1, \tag{5a}$$

$$\check{\nu}(z)^{\mathsf{T}}({}^{z}\mathbf{H}_n) = \mathbf{e}_n^{\mathsf{T}}\frac{\chi(z)}{h_{1:n-1}} \quad \Leftrightarrow \quad \frac{h_{1:n-1}\check{\nu}(z)}{\chi(z)} = \mathbf{e}_n^{\mathsf{T}}({}^{z}\mathbf{H}_n)^{-1}. \tag{5b}$$

The repeated application of resolvents to $\mathbf{e}_1$ results in

$$\Bigl(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\Bigr)\mathbf{e}_1 = (-1)^{k-1}[z_1,\dots,z_k]({}^{z}\mathbf{H}_n)^{-1}\mathbf{e}_1 \tag{6}$$

$$= (-1)^{k-1}[z_1,\dots,z_k]\frac{\nu(z)h_{1:n-1}}{\chi(z)}. \tag{7}$$

We note that $z\mathbf{I}_n - {}^{z}\mathbf{H}_n = z\mathbf{I}_n - (z\mathbf{I}_n - \mathbf{H}_n) = \mathbf{H}_n$.

Simplification

For the sake of eased understanding, we look at inverse iteration with a two-sided Rayleigh quotient where the left vector is the last standard unit vector $\mathbf{e}_n^{\mathsf{T}}$. For this method we have the iterates

$$\mathbf{v}_{k+1} = \Big(\prod_{i=1}^{k} ({}^{z_i}\mathbf{H}_n)^{-1}\Big)\mathbf{e}_1, \quad x_{k+1} = \frac{\mathbf{e}_n^{\mathsf{T}}\mathbf{H}_n\mathbf{v}_{k+1}}{\mathbf{e}_n^{\mathsf{T}}\mathbf{v}_{k+1}},$$

and thus the approximate eigenvalues are given by the Opitz-Larkin method:

$$x_{k+1} = \frac{\mathbf{e}_n^{\mathsf{T}}\mathbf{H}_n\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1}{\mathbf{e}_n^{\mathsf{T}}\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1} = \frac{\mathbf{e}_n^{\mathsf{T}}(z_k\mathbf{I}_n - ({}^{z_k}\mathbf{H}_n))\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1}{\mathbf{e}_n^{\mathsf{T}}\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1} \tag{8a}$$

$$= z_k - \frac{\mathbf{e}_n^{\mathsf{T}\,z_k}\mathbf{H}_n\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1}{\mathbf{e}_n^{\mathsf{T}}\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1} = z_k - \frac{\mathbf{e}_n^{\mathsf{T}}\big(\prod_{i=1}^{k-1}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1}{\mathbf{e}_n^{\mathsf{T}}\big(\prod_{i=1}^{k}({}^{z_i}\mathbf{H}_n)^{-1}\big)\mathbf{e}_1} \tag{8b}$$

$$= z_k + \frac{[z_1, \ldots, z_{k-1}](1/\chi)}{[z_1, \ldots, z_{k-1}, z_k](1/\chi)}. \tag{8c}$$

Simplification

When we update the shifts by choosing $z_{k+1} = x_{k+1}$ we obtain the standard variant of the Opitz-Larkin method. This method has asymptotically second order convergence against the roots of the characteristic polynomial χ.

Inverse iteration with fixed shift $\tau = z_1 = z_2 = \ldots = z_k$ results in the recurrence

$$x_{k+1} = \tau + \frac{[\tau, \ldots, \tau](1/\chi)}{[\tau, \ldots, \tau, \tau](1/\chi)} = \tau + k \frac{(1/\chi)^{(k-1)}(\tau)}{(1/\chi)^{(k)}(\tau)}. \tag{9}$$

Inverse iteration with fixed shift performs one step of König's method. Restarting inverse iteration every s steps with updated shift given by the current eigenvalue approximation converges with order s.

This knowledge together with an estimate for the cost of preprocessing (computing the LU decomposition; initializing a Krylov method using a seed system) and the cost of the (approximate) solutions of the systems enables to decide when to compute an update of the shift.

Simplification

The original Rayleigh quotient iteration (Strutt, 1894) with the symmetric Rayleigh quotient and, because of the symmetry, a tridiagonal Hermitean Hessenberg matrix $\mathbf{H}_n$, gives the update

$$z_{k+1} = \frac{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-\mathsf{H}} \mathbf{H}_n ({}^{z_k}\mathbf{H}_n)^{-1} \mathbf{e}_1}{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-\mathsf{H}} ({}^{z_k}\mathbf{H}_n)^{-1} \mathbf{e}_1} = \frac{\mathbf{e}_1^{\mathsf{T}} \mathbf{H}_n ({}^{z_k}\mathbf{H}_n)^{-2} \mathbf{e}_1}{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-2} \mathbf{e}_1} \tag{10a}$$

$$= \frac{\mathbf{e}_1^{\mathsf{T}} (z_k \mathbf{I}_n - {}^{z_k}\mathbf{H}_n)({}^{z_k}\mathbf{H}_n)^{-2} \mathbf{e}_1}{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-2} \mathbf{e}_1} \tag{10b}$$

$$= z_k - \frac{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-1} \mathbf{e}_1}{\mathbf{e}_1^{\mathsf{T}} ({}^{z_k}\mathbf{H}_n)^{-2} \mathbf{e}_1} = z_k + \frac{[z_k](\chi_{2:n}/\chi)}{[z_k, z_k](\chi_{2:n}/\chi)} \tag{10c}$$

$$= z_k - \frac{r(z_k)}{r'(z_k)}, \qquad r(z) := \frac{\chi(z)}{\chi_{2:n}(z)}. \tag{10d}$$

This is Newton's method on the meromorphic function r. As the poles of this meromorphic function are the eigenvalues of a submatrix, they interlace by Cauchy's interlace theorem the roots, which are the eigenvalues.

Simplification

Symmetric RQI for Hermitean matrices gives the update

$$z_{k+1} = z_k + \frac{[z_1, z_1, \ldots, z_{k-1}, z_{k-1}, z_k](\chi_{2:n}/\chi)}{[z_1, z_1, \ldots, z_{k-1}, z_{k-1}, z_k, z_k](\chi_{2:n}/\chi)}. \tag{11}$$

This update has by the result of Tornheim asymptotically a cubic convergence rate, as we have to compute the limit of the real roots of the equations

$$x^k - 2x^{k-1} - 2x^{k-2} - \cdots - 2 = 0,$$

i.e., the maximal eigenvalue of a Hessenberg matrix with ones in the lower diagonal and twos in the last column. The approximate eigenvector of all ones to the approximate eigenvalue 3 gives the backward error $1/\sqrt{k}$ and the only real positive eigenvalue of the matrix is well separated, the other eigenvalues lie close to a circle of radius one around zero.

Simplification

The picture changes if we apply the special inverse iteration to a general unreduced Hessenberg matrix, not necessarily Hermitean or symmetric.

If we take another standard unit vector $\mathbf{e}_\ell$ as left vector, we obtain the Opitz-Larkin method applied to the meromorphic function

$$m_\ell(z) = \frac{\chi(z)}{h_{1:\ell-1}\chi_{1+\ell:n}(z)}. \tag{12}$$

If we take an arbitrary left vector $\mathbf{y}$, we obtain the Opitz-Larkin method applied to the meromorphic function

$$r(z;\mathbf{y}) = \frac{\chi(z)}{\sum_{i=1}^n y_i h_{1:i-1}\chi_{1+i:n}(z)} = \frac{\chi(z)}{p(z;\mathbf{y})}, \quad p(z;\mathbf{y}) \in \mathbb{P}_{<n}. \tag{13}$$

The polynomials $\chi_{1+i:n}$ have degree $\deg(\chi_{1+i:n}) = n - i$ and leading coefficient one, thus they form a basis of the space of polynomials of degree less n.

Simplification

Every polynomial of degree less than n can be expressed by exactly one choice of starting vector ($\mathbb{C}^n$ and $\mathbb{P}_{<n}$ are isomorphic).

By luck or accident, we can construct a polynomial that is zero (of any order up to order $n-1$) at one eigenvalue. This is of interest in case of (algebraically) multiple eigenvalues. In theory, there is always a left starting vector which ensures that the root is simple, as the multiple zero is reduced to a simple one.

The best choice is the starting vector $\mathbf{y}$ that represents the derivative of χ, i.e., the vector $\bar{\mathbf{y}}$ such that

$$p(z; \bar{\mathbf{y}}) = \chi'(z). \tag{14}$$

In this special case the rational function is the Newton's update

$$r(z; \bar{\mathbf{y}}) = \frac{\chi(z)}{\chi'(z)} \tag{15}$$

which has only simple zeros and poles between the eigenvalues.

Simplification

The Academic Example: The matrix $\mathbf{H}_4 = \mathrm{triu}(\mathrm{ones}(4), -1)$ has the eigenvalues 0 (double), 1, and 3, and the vector

$$\mathbf{y} = \begin{pmatrix} 4 \\ 0 \\ 2 \\ 2 \end{pmatrix} \tag{16}$$

picks the derivative of the characteristic polynomial.

The two-sided RQI with left-hand vector $\mathbf{e}_1$ and right-hand vector $\mathbf{y}$ performs confluent Opitz-Larkin with double nodes on the Newton's update χ/χ'.

A variant of original RQI with starting vector $\mathbf{e}_1$ and test vector $\mathbf{y}$ and updated shifts performs Newton's method on the Newton's update χ/χ'.

Simplification

The two-sided RQI method corresponds to a confluent Opitz-Larkin method with double nodes. In this method the left vector determines a polynomial, which is formed as a linear combination of characteristic polynomials of trailing submatrices.

Measured in Horners, single-sided RQI applied to non-Hermitean matrices performs better. In the QR algorithm we implicitly perform a single-sided RQI in every step.

In single-sided RQI for non-Hermitean matrices, we change the vector $\mathbf{y}$ that determines the denominator polynomial of the rational function

$$r(z;\mathbf{y}) = \frac{\chi(z)}{p(z;\mathbf{y})}$$

in every step and apply one step of the Opitz-Larkin method without confluent nodes. This gives second order convergence.

Conclusions and Outlook

- We sketched some well known and some less well known classical root finding algorithms, among these a method we refer to as the Opitz-Larkin method.
- We gave a really short account of RQI and related algorithms.
- We used our knowledge of Hessenberg matrices and the first resolvent identity to show that RQI is a clever implementation of the Opitz-Larkin method.

- We omitted the details of an impact analysis to deflation strategies in the QR algorithm.
- Much remains to be done ...

Thank you very much for your attention!

Hartelijk dank!

Chatelin, F. (1993).
Eigenvalues of matrices.
John Wiley & Sons Ltd., Chichester.
With exercises by Mario Ahués and the author, Translated from the French and with additional material by Walter Ledermann.

Crandall, S. H. (1951).
Iterative procedures related to relaxation methods for eigenvalue problems.
Proceedings of the Royal Society. London. Series A. Mathematical, Physical and Engineering Sciences, 207:416–423.

Ericsson, T. (1990).
On the eigenvalues and eigenvectors of Hessenberg matrices.
Numerical Analysis Group, Göteborg, Report 10, Chalmers University of Technology and the University of Göteborg, Department of Computer Sciences, S-412 96 Göteborg, Sweden.
Online available at
`http://www.cs.chalmers.se/pub/num_analysis/reports/`.

Franklin, J. N. (1968).
Matrix theory.
Prentice-Hall Inc., Englewood Cliffs, N.J.

Jarratt, P. and Nudds, D. (1965).
The use of rational functions in the iterative solution of equations on a digital computer.
Comput. J., 8:62–65.

König, J. (1884).
Ueber eine Eigenschaft der Potenzreihen.
Mathematische Annalen, 23:447–449.
Scanned article online available at the Göttinger Digitalisierungszentrum (GDZ): `http://resolver.sub.uni-goettingen.de/purl?GDZPPN002248026`.

Larkin, F. M. (1980).
Root-finding by fitting rational functions.
Mathematics of Computation, 35(151):803–816.

Larkin, F. M. (1981).
Root finding by divided differences.
Numer. Math., 37(1):93–104.

Opitz, G. (1958).
Gleichungsauflösung mittels einer speziellen Interpolation.
Z. Angew. Math. Mech., 38:276–277.

Ostrowski, A. M. (1958/1959b).
On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. I, II.
Arch. Rational Mech. Anal. 1 (1958), 233–241, 2:423–428.

Ostrowski, A. M. (1959a).
On the convergence of the Rayleigh quotient iteration for the computation of characteristic roots and vectors. VI. (Usual Rayleigh quotient for nonlinear elementary divisors).
Arch. Rational Mech. Anal., 4:153–165 (1959).

Ostrowski, A. M. (1959c).
On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. III. (Generalized Rayleigh quotient characteristic roots with linear elementary divisors).
Arch. Rational Mech. Anal., 3:325–340.

Ostrowski, A. M. (1959d).
On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. IV. (Generalized Rayleigh quotient for nonlinear elementary divisors).
Arch. Rational Mech. Anal., 3:341–347 (1959).

Ostrowski, A. M. (1959e).
On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. V. Usual Rayleigh quotient for non-Hermitian matrices and linear elementary divisors.
Arch. Rational Mech. Anal., 3:472–481 (1959).

Raydan, M. (1993).
Exact order of convergence of the secant method.
Journal of Optimization Theory and Applications, 78(3):541–551.

Schröder, E. (1870).
Ueber unendlich viele Algorithmen zur Auflösung der Gleichungen.
Math. Ann., 2(2):317–365.

Schweins, F. (1825).
Theorie der Differenzen und Differentiale.
Verlag der Universitäts-Buchhandlung von C. F. Winter, Heidelberg.
Digitized by Google, online available at
http://books.google.de/books?id=dntNAAAAMAAJ.

Strutt, J. W. (1894).
The Theory of Sound, volume one.
Macmillan, London, 2nd edition.

Tornheim, L. (1964).
Convergence of multipoint iterative methods.
J. Assoc. Comput. Mach., 11:210–220.

Wielandt, H. (1944).
Beiträge zur mathematischen Behandlung komplexer Eigenwertprobleme, Teil V: Bestimmung höherer Eigenwerte durch gebrochene Iteration.
Bericht B44/J/37, Aerodynamische Versuchsanstalt Göttingen.

Zemke, J.-P. M. (2006).
Hessenberg eigenvalue–eigenmatrix relations.
Linear Algebra Appl., 414(2-3):589–606.

Zemke, J.-P. M. (2007).
Abstract perturbed Krylov methods.
Linear Algebra Appl., 424(2-3):405–434.