Relations between Rayleigh Quotient Iteration and Classical Root Finding Algorithms

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Outline

Classical Root Finding

Newton’s Method
The Secant Method
König’s Method
The Opitz-Larkin Method

Rayleigh Quotient Iteration

John William Strutt’s RQI
Inverse Iteration
Symmetric RQI
Two-Sided RQI

The Hessenberg-Matrix Point Of View
Outline

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- The Secant Method
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Rayleigh Quotient Iteration

- John William Strutt’s RQI
- Inverse Iteration
- Symmetric RQI
- Two-Sided RQI

The Hessenberg-Matrix Point Of View
The best known method for the computation of a root of a rational function

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

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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:

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In general, the secant method locally wins (Raydan, 1993).
Schröder’s and König’s methods

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\[ z_{k+1} = z_k + \frac{s}{f(z_k)} \left( \frac{1}{f(z_k)} - s \right) \]

König’s method typically has a Q-convergence order of \( s + 1 \).

König’s method for \( s = 1 \) is Newton’s method,

\[ z_{k+1} = z_k - \frac{1}{f(z_k)} \left( z_k - \frac{1}{f(z_k)} f'(z_k) \right) = z_k - \frac{f(z_k)}{f'(z_k)} \]
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This family is nowadays known as “König’s method”:

\[ z_{k+1} = z_k + s \frac{(1/f)^{(s-1)}(z_k)}{(1/f)^{(s)}(z_k)}, \quad s = 1, 2, \ldots \]
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\[ z_{k+1} = z_k + \frac{(1/f)(z_k)}{(1/f)'(z_k)} = z_k - \frac{1/f(z_k)}{f'(z_k)/(f(z_k))^2} = z_k - \frac{f(z_k)}{f'(z_k)}. \]
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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).
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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, \ldots, z_{k-1}](1/f)}{[z_1, z_2, \ldots, z_{k-1}, z_k](1/f)}.
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Frequently, the Opitz-Larkin method is used with truncation:

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

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

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

$$z_{k+1} = z_k + \left[ \frac{[z_k, \ldots, z_k] (1/f)}{[z_k, \ldots, z_k, z_k] (1/f)} \right]^{s+1}$$

$$= z_k + \frac{(1/f)^{(s-1)}(z_k)/(s - 1)!}{(1/f)^{(s)}(z_k)/s!} = z_k + s \frac{(1/f)^{(s-1)}(z_k)}{(1/f)^{(s)}(z_k)}.$$
The Opitz-Larkin method

Truncated Opitz-Larkin with \( p = 1 \) is the secant method,

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

\[
= z_k + \frac{1}{f(z_{k-1})} \cdot \frac{1}{1/f(z_{k-1}) - 1/f(z_k)} \cdot \frac{z_{k-1} - z_k}{z_{k-1} - z_k}
\]

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

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

Confluent truncated Opitz-Larkin with $p = 1$ is Newton’s method.
In general, the Opitz-Larkin method is closely connected to rational interpolation of the inverse function (Larkin, 1981, Theorem 1, page 96):
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**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 \( d \leq k - 2 \), such that \( q_d(\alpha) \neq 0 \) and

\[
r_k(z_j) = f(z_j)^{-1}, \quad j = 1, 2, \ldots, k,
\]

then

\[
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)} = \alpha.
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Thus, the Opitz-Larkin method computes the unique root of the inverse of a rational interpolation at the inverse function values.
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Most important are the articles (Tornheim, 1964) and (Jarratt and Nudds, 1965). We state the main results contained in these articles.
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

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

and gave its rate of convergence (Tornheim, 1964, Theorem 2).
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.
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\[
M = \begin{vmatrix}
    a_d & a_{d-1} & \cdots & a_{2d+2-m} \\
    a_{d+1} & a_d & \cdots & \vdots \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{m-2} & \cdots & a_d \\
\end{vmatrix} \neq 0.
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\]

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 \( i \)-th derivative of \( f(x) \) (for direct interpolation) or of its inverse function (for inverse interpolation) at \( x = x^* \).
The Opitz-Larkin method

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$$x^k = m_1 x^{k-1} + m_2 x^{k-2} + \cdots + m_k.$$
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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.
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Lemma (Tornheim 1964)

Suppose that the coefficients of

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

satisfy

\[ a_1 + a_2 + \cdots + a_n > 1, \quad a_1 \geq a_2 \geq \cdots \geq a_n \geq 0. \]
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\[ a_1 + a_2 + \cdots + a_n > 1, \quad a_1 \geq a_2 \geq \cdots \geq a_n \geq 0. \]

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

\[ r(z) = \frac{z - \alpha}{q_{k-2}(z)}, \quad q_{k-2} \in \mathbb{P}_{k-2}. \]
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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.
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The Hessenberg-Matrix Point Of View
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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

$$p^2 = \frac{1}{2} a_{11} A_1^2 + \frac{1}{2} a_{22} A_2^2 + \ldots + a_{12} A_1 A_2 + \ldots \ldots (3).$$

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.]
In modern notation, stated for the Hermitean algebraic eigenvalue problem

\[ \mathbf{A}\mathbf{v} = \mathbf{v}\lambda, \quad \mathbf{A} = \mathbf{A}^H, \]
In modern notation, stated for the Hermitean algebraic eigenvalue problem

\[ A v = v \lambda, \quad A = A^\text{H}, \]

Lord Rayleigh starts with an approximate eigenvector \( v_k \), computes its Rayleigh quotient

\[ \rho(v_k) := \frac{v_k^\text{H} A v_k}{v_k^\text{H} v_k} \]
In modern notation, stated for the Hermitean algebraic eigenvalue problem

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Lord Rayleigh starts with an approximate eigenvector \( v_k \), computes its Rayleigh quotient

\[ \rho(v_k) := \frac{v_k^H Av_k}{v_k^H v_k} \]

and uses the linear system

\[ (A - \rho(v_k)I_n)v_{k+1} = e_j \]

for some standard unit vector \( e_j \) to compute a new approximate eigenvector \( v_{k+1} \). He was, of course, only interested in its direction.
This is **repeated several times**, i.e.,

\[ v_{k+1} = (A - \rho(v_k)I_n)^{-1}e_j, \quad k = 0, 1, \ldots \]
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Original RQI

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Classical RQI can thus be stated in modern notation as

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for some suitably chosen $j \in \{1, 2, \ldots, n\}$, which might vary, depending on the computed approximate eigenvector.
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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.
Closely connected to RQI is inverse iteration. Inverse iteration was developed by Helmut Wielandt in 1944, (Wielandt, 1944).
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In the most basic variant of inverse iteration the shift $\tau$ is never updated, but the right-hand side is replaced by the latest approximate eigenvector:

$$v_{k+1} = \frac{(A - \tau I_n)^{-1}v_k}{\| (A - \tau I_n)^{-1}v_k \|}, \quad k = 0, 1, \ldots$$
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There exist variants which use other scalings, mostly using as left vector some standard unit vector $\ell = e_j$:

$$v_{k+1} = \frac{(A - \tau I_n)^{-1}v_k}{e_j^T (A - \tau I_n)^{-1}v_k}, \quad k = 0, 1, \ldots$$
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In the latter context, $e_j^T (A - \tau I_n)^{-1}v_k \approx (\lambda - \tau)^{-1}$ gives an eigenvalue approximation.
Either variant of inverse iteration with fixed shift $\tau$ converges linearly.
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\tau_{k+1} := \tau_k - \frac{1}{\mathbf{e}_j^T (A - \tau I_n)^{-1} \mathbf{v}_k}.
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In both variants also the Rayleigh quotient can be used, the Rayleigh quotient uniquely solves the least squares problem

$$\rho(v_k) = \arg\min_{\rho \in \mathbb{C}} \|Av_k - v_k\rho\|$$

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Both these methods typically exhibit a quadratic convergence behavior.
When automatic computers became available, the combination of inverse iteration with Rayleigh’s original RQI resulted in the locally Q-cubically convergent (symmetric) RQI

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Symmetric RQI

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

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The iteration involves two sequences of vectors,

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\]

\( k = 0, 1, \ldots \)

This trick recovers the cubic convergence of RQI at the price of the solution of an additional system.
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).
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The proofs by Crandall and Ostrowski are beautiful and worth reading.
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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, …
Outline

Classical Root Finding
- Newton’s Method
- The Secant Method
- König’s Method
- The Opitz-Larkin Method

Rayleigh Quotient Iteration
- John William Strutt’s RQI
- Inverse Iteration
- Symmetric RQI
- Two-Sided RQI

The Hessenberg-Matrix Point Of View
Hessenberg matrices are in some sense the closest **computable normal form** of square matrices under **unitary similarity** transformations.
Simplification

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The implicit Q-Theorem gives uniqueness of the upper part of the reduction to Hessenberg form in case of given first column $q$, if we fix the signs of the elements in the lower diagonal, e.g., to be non-negative real.
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We use the implicit Q-Theorem to unitarily transform the pair $(A, q)$ with $\|q\|_2 = 1$ to the pair $(H_n, e_1)$, where $H_n$ is upper Hessenberg and $e_1$ denotes the first standard unit vector.

The following Matlab-code gives the transformed pair:

```matlab
[Q,R] = qr(q);
[P,H] = hess(Q'*A*Q);
signs = sign(diag(H,-1));
S = diag(cumprod([1;signs]));
P = P*S;
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$$zH_n := (zI_n - H_n).$$
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The first resolvent identity (Chatelin, 1993, Lemma 2.2.1, p. 63), valid for $z_1 \neq z_2$ from the resolvent set, gives

$$\begin{align}
(z_1 H_n)^{-1} (z_2 H_n)^{-1} &= (z_1 I_n - H_n)^{-1} (z_2 I_n - H_n)^{-1} \\
&= (z_1 H_n)^{-1} - (z_2 H_n)^{-1} \\
&= \frac{z_1 H_n}{z_2 - z_1} = -[z_1, z_2] (zH_n)^{-1}.
\end{align}$$

(1a) (1b)
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\]

\[
= \frac{(z_1 H_n)^{-1} - (z_2 H_n)^{-1}}{z_2 - z_1} = -[z_1, z_2](zH_n)^{-1}.
\]

The first resolvent identity is based on the trivial observation that

\[
(z_2 I_n - H_n) - (z_1 I_n - H_n) = (z_2 - z_1)I_n.
\]
This identity can be generalized to $k$ distinct points of evaluation:

$$
\prod_{i=1}^{k} (z_i H_n)^{-1} = (-1)^{k-1} [z_1, \ldots, z_k] (z H_n)^{-1}.
$$

(2)
Simplification

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

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The inverse of the characteristic matrix \( z H_n \) is the rational function

\[
(z H_n)^{-1} = \frac{\text{adj}(z H_n)}{\chi(z)} =: \frac{P_n(z)}{\chi(z)}, \quad \chi(z) := \det(z H_n),
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$$\left(\frac{z}{H_n}\right)^{-1} = \frac{\text{adj}(z H_n)}{\chi(z)} =: \frac{P_n(z)}{\chi(z)}, \quad \chi(z) := \det(z H_n),$$  \hspace{1cm} (3)

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

Thus, confluent divided differences are well-defined and we do not need to restrict the points \( \{z_i\}^k_{i=1} \) from the resolvent set.
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).
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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** \((Schweins, \ 1825, \ Erste Abtheilung, \ IV. Abschnitt, \ § \ 154, \ Seite \ 361, \ Gleichung \ 560))\).
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There exist short proofs based on Laplace expansion and Cramer’s rule.
Simplification

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

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Polynomial vectors $\nu$ and $\tilde{\nu}$ are defined by

$$\nu(z) := \left( \frac{\chi_{j+1:n}(z)}{h_{j:n-1}} \right)_{j=1}^{n}$$

and

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

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

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

$$\chi_{i:j}(z) := \det (zH_{i:j}) = \det (zI_{j-i+1} - H_{i:j}).$$
By (Z, 2006, Lemma 3.1, Eqn. (3.5)) for $z$ in the resolvent set

$$
(zH_n)\nu(z) = \frac{\chi(z)}{h_{1:n-1}} e_1 \iff \frac{\nu(z) h_{1:n-1}}{\chi(z)} = (zH_n)^{-1} e_1,
$$

(5a)

$$
\tilde{\nu}(z)^T(zH_n) = e_n^T \frac{\chi(z)}{h_{1:n-1}} \iff \frac{h_{1:n-1} \tilde{\nu}(z)}{\chi(z)} = e_n^T (zH_n)^{-1}.
$$

(5b)
By (Z, 2006, Lemma 3.1, Eqn. (3.5)) for \( z \) in the resolvent set

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

\[
\hat{\nu}(z)^T (\mathbf{z} \mathbf{H}_n) = \mathbf{e}_n^T \frac{\chi(z)}{h_{1:n-1}} \quad \iff \quad \frac{h_{1:n-1} \hat{\nu}(z)}{\chi(z)} = \mathbf{e}_n^T (\mathbf{z} \mathbf{H}_n)^{-1}. \quad (5b)
\]

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

\[
\left( \prod_{i=1}^{k} (\mathbf{z}_i \mathbf{H}_n)^{-1} \right) \mathbf{e}_1 = (-1)^{k-1} [z_1, \ldots, z_k] (\mathbf{z} \mathbf{H}_n)^{-1} \mathbf{e}_1 \quad (6)
\]

\[
= (-1)^{k-1} [z_1, \ldots, z_k] \frac{\nu(z) h_{1:n-1}}{\chi(z)}. \quad (7)
\]
The Hessenberg-Matrix Point Of View

Simplification

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

\[
(zH_n)\nu(z) = \frac{\chi(z)}{h_{1:n-1}} e_1 \quad \Leftrightarrow \quad \frac{\nu(z)h_{1:n-1}}{\chi(z)} = (zH_n)^{-1} e_1,
\]

\[
\nu(z)^T(zH_n) = e_n^T \frac{\chi(z)}{h_{1:n-1}} \quad \Leftrightarrow \quad \frac{h_{1:n-1}\nu(z)}{\chi(z)} = e_n^T(zH_n)^{-1}.
\]

The repeated application of resolvents to \( e_1 \) results in

\[
\left( \prod_{i=1}^k (z_i H_n)^{-1} \right) e_1 = (-1)^{k-1} [z_1, \ldots, z_k] (zH_n)^{-1} e_1
\]

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

We note that \( zI_n - zH_n = zI_n - (zI_n - H_n) = H_n \).
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 $e_n^T$. 

$$v_{k+1} = \left( \prod_{i=1}^{k} (z_i H_n) \right)^{-1} e_1,$$

$$x_{k+1} = e_n^T H_n v_{k+1} e_n^T (z_k I_n - (z_k H_n)) \left( \prod_{i=1}^{k} (z_i H_n) \right)^{-1} e_1$$

(8a)

$$z_k = e_n^T (z_k I_n - (z_k H_n)) \left( \prod_{i=1}^{k-1} (z_i H_n) \right)^{-1} e_1$$

(8b)

$$z_k = \left[ z_1, ..., z_{k-1}, z_k \right] \left( 1/\chi \right) \left[ z_1, ..., z_{k-1}, z_k \right]$$

(8c)
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 \( e_n^T \). For this method we have the iterates

\[
v_{k+1} = \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1, \quad x_{k+1} = \frac{e_n^T H_n v_{k+1}}{e_n^T v_{k+1}},
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and thus the approximate eigenvalues are given by the Opitz-Larkin method:

$$x_{k+1} = \frac{e_n^T H_n \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1}{e_n^T \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1} = \frac{e_n^T (z_k I_n - (z_k H_n)) \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1}{e_n^T \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1}$$

$$(8a)$$

$$= z_k - \frac{e_n^T z_k H_n \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1}{e_n^T \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1} = z_k - \frac{e_n^T \left( \prod_{i=1}^{k-1} (z_i H_n)^{-1} \right) e_1}{e_n^T \left( \prod_{i=1}^{k} (z_i H_n)^{-1} \right) e_1}$$

$$(8b)$$

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

$$(8c)$$
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 $\chi$. 

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

$$x_{k+1} = \tau + \left[ \tau, \ldots, \tau \right] \left( \frac{1}{\chi} \right) \left[ \tau, \ldots, \tau, \tau \right] \left( \frac{1}{\chi} \right) = \tau + k \left( \frac{1}{\chi} \right) \left( k - 1 \right) \left( \tau \right) \left( \frac{1}{\chi} \right) \left( k \right) \left( \tau \right).$$

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

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

(9)
Simplification

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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.
The original Rayleigh quotient iteration (Strutt, 1894) with the symmetric Rayleigh quotient and, because of the symmetry, a tridiagonal Hermitean Hessenberg matrix \( H_n \), gives the update

\[
\begin{align*}
    z_{k+1} &= \frac{e_1^T (z_k H_n)^{-1} H_n (z_k H_n)^{-1} e_1}{e_1^T (z_k H_n)^{-1} e_1} = \frac{e_1^T H_n (z_k H_n)^{-2} e_1}{e_1^T (z_k H_n)^{-2} e_1} \\
    &= \frac{e_1^T (z_k I_n - z_k H_n) (z_k H_n)^{-2} e_1}{e_1^T (z_k H_n)^{-2} e_1} = z_k - \frac{e_1^T (z_k H_n)^{-1} e_1}{e_1^T (z_k H_n)^{-2} e_1} \\
    &= z_k - \frac{r(z_k)}{r'(z_k)}, \quad r(z) := \frac{\chi(z)}{\chi_2:n(z)}.
\end{align*}
\]

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.
The original Rayleigh quotient iteration (Strutt, 1894) with the symmetric Rayleigh quotient and, because of the symmetry, a tridiagonal Hermitean Hessenberg matrix $H_n$, gives the update

$$z_{k+1} = \frac{e_1^T(z_k H_n)^{-1} e_1}{e_1^T(z_k H_n)^{-1} e_1} = \frac{e_1^T H_n(z_k H_n)^{-2} e_1}{e_1^T(z_k H_n)^{-2} e_1}$$  \hspace{1cm} (10a)$$

$$= \frac{e_1^T(z_k I_n - z_k H_n)(z_k H_n)^{-2} e_1}{e_1^T(z_k H_n)^{-2} e_1}$$  \hspace{1cm} (10b)$$

$$= z_k - \frac{e_1^T(z_k H_n)^{-1} e_1}{e_1^T(z_k H_n)^{-2} e_1} = z_k + \frac{[z_k] (\chi_{2:n}/\chi)}{[z_k, z_k] (\chi_{2:n}/\chi)}$$  \hspace{1cm} (10c)$$

$$= z_k - \frac{r(z_k)}{r'(z_k)} , \hspace{1cm} r(z) := \frac{\chi(z)}{\chi_{2:n}(z)}$$  \hspace{1cm} (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.
Symmetric RQI for Hermitean matrices gives the update

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

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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

\[ x^k - 2x^{k-1} - 2x^{k-2} - \cdots - 2 = 0, \]
Symmetric RQI for Hermitean matrices gives the update

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

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.
The picture changes if we apply the special inverse iteration to a **general unreduced Hessenberg matrix**, not necessarily Hermitean or symmetric.
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 $e_\ell$ as left vector, we obtain the Opitz-Larkin method applied to the meromorphic function

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

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

$$r(z; y) = \chi(z) \sum_{n=1}^n y_n h_{1:1} - 1 \chi_{1+\ell:n}(z) = \chi(z) p(z; y),$$

with $p(z; y) \in P_{<n}$. The polynomials $\chi_{1+\ell:n}$ have degree $\deg(\chi_{1+\ell:n}) = n - \ell$ and leading coefficient one, thus they form a basis of the space of polynomials of degree less than $n$. 

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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 $n$. 
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).
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.
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The best choice is the starting vector \( y \) that represents the derivative of \( \chi \), i.e., the vector \( \bar{y} \) such that

\[
p(z; \bar{y}) = \chi'(z). \tag{14}
\]
Simplification

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\[
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\]

(14)

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

\[
r(z; \bar{y}) = \frac{\chi(z)}{\chi'(z)}
\]

(15)

which has only simple zeros and poles between the eigenvalues.
The Academic Example: The matrix $H_4 = \text{triu}(\text{ones}(4), -1)$ has the eigenvalues $0$ (double), $1$, and $3$, and the vector

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

picks the derivative of the characteristic polynomial.
The Academic Example: The matrix $H_4 = \text{triu}(\text{ones}(4), -1)$ has the eigenvalues $0$ (double), $1$, and $3$, and the vector

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The two-sided RQI with left-hand vector $e_1$ and right-hand vector $y$ performs confluent Opitz-Larkin with double nodes on the Newton’s update $\chi/\chi'$. 
The Hessenberg-Matrix Point Of View

Simplification

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(16)

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The two-sided RQI with left-hand vector $e_1$ and right-hand vector $y$ performs confluent Opitz-Larkin with double nodes on the Newton’s update $\chi/\chi'$.

A variant of original RQI with starting vector $e_1$ and test vector $y$ and updated shifts performs Newton’s method on the Newton’s update $\chi/\chi'$. 
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.
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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.
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 $y$ that determines the denominator polynomial of the rational function

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

in every step and apply one step of the Opitz-Larkin method without confluent nodes. This gives second order convergence.
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.
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Much remains to be done . . .
Thank you very much for your attention!

Hartelijk dank!


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