An Extension of Ostrowski's Two-Sided RQI to Nonlinear Eigenvalue Problems

Hubert Schwetlick
joint work with Kathrin Schreiber
Technical University of Dresden

Hubert.Schwetlick@tu-dresden.de

http://math.tu-dresden.de/~schwetli

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Outline

- The nonlinear eigenproblem: Basic definitions
- Ostrowski's Two-Sided RQI for linear eigenproblems
- Nonlinear Rayleigh functionals
- Nonlinear shifted inverse iteration
- Ostrowski's Two-Sided RQI for nonlinear eigenproblems
- Cubic convergence - a sketch of proof

1. The Nonlinear Eigenvalue Problem

Consider the nonlinear eigenvalue problem

$$T(\lambda)x = 0 \quad \text{with} \quad T(\,.\,) : D \subset \mathbb{C} \mapsto \mathbb{C}^{n\times n} \quad \text{suff. smooth.}$$

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Let $\lambda_* \in \mathbb{C}$ be an algebraically simple eigenvalue of T, i. e.,

- it is geometrically simple: $\operatorname{rank} T(\lambda_*) = n - 1 \quad \Longleftrightarrow$ $\exists\, x_*, y_* \in \mathbb{C}^n$, $\|x_*\| = \|y_*\| = 1$, such that

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  which implies $\quad T(\lambda_*)\, x_* = 0, \qquad y_*^H\, T(\lambda_*) = 0$

- $\dot\delta(\lambda_*) \neq 0$ where $\delta(\lambda) = \det T(\lambda) \iff \alpha_* = y_*^H \dot T(\lambda_*) x_* \neq 0$

Special cases

- $T(\lambda) = A - \lambda I$: special linear evp, $\alpha_* = -y_*^H x_*$
- $T(\lambda) = A - \lambda B$: generalized linear evp, $\alpha_* = -y_*^H B x_*$
- $T(\lambda) = \lambda^2 M + \lambda C + K$: quadratic evp, $\alpha_* = 2\lambda_* y_*^H M x_* + y_*^H C x_*$

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Question

- Is there a reasonable extension of

  Ostrowski's Two-Sided RQI (=: 2sRQI)

  developed for linear eigenproblems to the case of nonlinear eigenvalue problems?
- Can one proof cubic convergence as has been done for the linear case?

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S1: Set $\boxed{\theta = p(u) := u^H A u = u^H A u / u^H u}$

S2: Solve $\boxed{(A - \theta I) u_+^{invit} = u}$ for u_+^{invit}, set $\boxed{u_+ = u_+^{invit} / \|u_+^{invit}\|}$

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Convergence:

- Cubic in case $A = A^H$ (in fact, $AA^H = A^H A$ is enough!)
- Quadratic otherwise (since then $p(u)$ is not stationary at x_*)

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This leads to Ostrowski's two-sided Rayleigh Quotient Iteration:

Given (u, v) with $\|u\| = \|v\| = 1$, Step $(u, v) \mapsto (u_+, v_+)$:

S1: Set $\theta = p(u, v) := v^H A u / v^H u$

S2: Solve $(A - \theta I) u_+^{invit} = u$ for u_+^{invit}, set $u_+ = u_+^{invit} / \|u_+^{invit}\|$

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3. Nonlinear Rayleigh Functionals

The generalized Rayleigh quotient

$$p(u,v) = \frac{v^H A u}{v^H u}, \qquad v^H u \neq 0,$$

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Hence, in case of nonlinear problems $T(\lambda)x = 0$, for given (u,v), the nonlinear Rayleigh functional $p(u,v)$ may be defined as solution $\lambda = p(u,v)$ of the scalar equation

$$g(\lambda, u, v) = v^H T(\lambda) u = 0 \qquad \text{(NRF-EQ)}$$

with respect to λ. Note that (NRF-EQ) is a Galerkin-Petrov orthogonality condition for the residual $T(\lambda)u$.

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What about existence und uniqueness?

Theorem 1: Suppose that $T(\,.\,) : D \in \mathbb{C} \to \mathbb{C}^{n\times n}$, D open, is holomorphic on D, and that $\lambda_* \in D$ is an algebraically simple eigenvalue of T, i.e., there exist eigenvectors x_*, y_* with $\|x_*\| = \|y_*\| = 1$ such that $\ker T(\lambda_*) = \operatorname{span}\{x_*\}$, $\ker T(\lambda_*)^H = \operatorname{span}\{y_*\}$ and $\alpha_* := y_*^H \dot{T}(\lambda_*) x_* \neq 0$. Then there are constants $0 < \tau_0$, $0 < \varepsilon_0 < \pi/2$ such that, for all $(u,v) \in \mathcal{K}(\varepsilon_0)$, there exists a unique $p = p(u,v) \in S_0 := \bar{S}(\lambda_*, \tau_0)$ with $g(p,u,v) = v^H T(p(u,v))u = 0$ and $\dot{g}(p,u,v) = v^H \dot{T}(p(u,v))u \neq 0$. Moreover, one has

$$|p(u,v) - \lambda_*| \leq K_1 \tan\xi \, \tan\eta \quad \text{with} \quad K_1 = \frac{8}{3}\frac{\|T(\lambda_*)\|}{|\alpha_*|}$$

(NRF-EST)

where $\mathcal{K}(\varepsilon) = \{(u,v) \in \mathbb{C}^n \times \mathbb{C}^n : \xi \leq \varepsilon,\ \eta \leq \varepsilon\}$ for any $\varepsilon < \pi/2$

with $\xi = \measuredangle(\operatorname{span}\{u\}, \operatorname{span}\{x_*\}), \eta = \measuredangle(\operatorname{span}\{v\}, \operatorname{span}\{y_*\}).$

Note that $\varepsilon < \pi/2$ implies $u \neq 0$, $v \neq 0$ and that (NRF-EST), as the value of $p(u,v)$, does not depend on the scaling of u, v.

It is also possible to prove a

Perturbation expansion: Assumptions and constants as in the theorem but now suppose $(u,v) \in \mathcal{K}(\varepsilon_0/2)$. Then there exist $\delta_0,\ K_2 > 0$ such that, if s and t satisfy $\delta_u = \|s\|/\|u\| \le \delta_0$, $\delta_v = \|t\|/\|v\| \le \delta_0$, then $(u+s, v+t) \in \mathcal{K}(\varepsilon_0)$, hence, $p(u+s, v+t)$ uniquely exists in $\bar{S}(\lambda_*, \tau_0)$, and one has the first order expansion

$$p(u+s, v+t) = p(u,v) - \frac{v^H T(p(u,v))s}{v^H \dot{T}(p(u,v))u} - \frac{t^H T(p(u,v))u}{v^H \dot{T}(p(u,v))u} + \rho(s,t) \tag{NRF-EXP}$$

with second order remainder

$$|\rho(s,t)| \le K_2(\delta_u + \delta_v)^2 = K_2(\|s\|/\|u\| + \|t\|/\|v\|)^2.$$

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Note that (NRF-EXP) shows for arbitrarily scaled eigenvectors x_*, y_* the stationarity of $p(u,v)$ at (x_*, y_*) in the sense of

$$p(x_* + s, y_* + t) = \lambda_* + \mathcal{O}((\|s\|/\|x_*\| + \|t\|/\|y_*\|)^2).$$

4. Nonlinear Shifted Inverse Iteration

After having found a nonlinear Rayleigh functional, we have to look for a nonlinear analog for the shifted inverse iteration step

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Recall: The Newton step $(u, \theta) \mapsto (u_+^N, \theta_+^N)$ for the extended system $(A - \lambda I)x = 0,\ w^H x = 1$ delivers an x-part $u_+^N = \mu(A - \theta I)^{-1} u$ which is proportional to u_+^{invit}.

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Do the same in the nonlinear case: Consider the extended system

$$\mathbf{F}_w(\mathbf{z}) = \mathbf{F}_w(x, \lambda) = \begin{bmatrix} T(\lambda)x \\ w^H x - 1 \end{bmatrix} = \begin{bmatrix} 0_n \\ 0_1 \end{bmatrix} \qquad \text{(ES)}$$

for $\mathbf{z} = \left[\begin{smallmatrix} x \\ \lambda \end{smallmatrix}\right] \in \mathbb{C}^{n+1}$ where $w \in \mathbb{C}^n$, $\|w\| = 1$, is a normalizing vector such that $w^H x_* \neq 0$, cf. Anselone/Rall [1967].

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Case $T(\lambda) = A - \lambda I$: Unger [ZAMM 1950], see also Zurmühl [1953], with coordinate vector $w = e_i$, i. e., $x_i = 1$, cf.
`http://www.math.tu-dresden.de/~schwetli/Unger.html`

Derivatives of $\mathbf{F}_w(x,\lambda) = (T(\lambda)x, w^H x - 1)$

$$\partial \mathbf{F}_w(x,\lambda)\begin{bmatrix} s \\ \mu \end{bmatrix} = \begin{bmatrix} T(\lambda)s + \dot{T}(\lambda)x\mu \\ w^H s \end{bmatrix} = \begin{bmatrix} T(\lambda) & \dot{T}(\lambda)x \\ w^H & 0 \end{bmatrix}\begin{bmatrix} s \\ \mu \end{bmatrix}$$

$$\partial^2 \mathbf{F}_w(x,\lambda)\begin{bmatrix} s \\ \mu \end{bmatrix}\begin{bmatrix} s_1 \\ \mu_1 \end{bmatrix} = \begin{bmatrix} \dot{T}(\lambda)(s\mu_1 + s_1\mu) + \ddot{T}(\lambda)x\mu\mu_1 \\ 0 \end{bmatrix}$$

Obviously $F(x_*^w, \lambda_*) = 0$ for $x_*^w = x_*/(w^H x_*)$, and one has

$$\partial F(x_*^w, \lambda_*) = \left[\begin{array}{c|c} T(\lambda_*) & \dot{T}(\lambda_*)x_*^w \\ \hline w^H & 0 \end{array}\right] \text{ nonsingular}$$

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Now perform for $\mathbf{F}_w(\mathbf{z}) = \mathbf{F}_w(x,\lambda) = 0$ one Newton step

$$\mathbf{z}_k = (u,\theta) \mapsto \mathbf{z}_{k+1}^N = (u_+^N, \theta_+^N) = (u + s, \theta + \mu)$$

This means: Solve the linear system $\mathbf{F}_w(u,\theta) + \partial\mathbf{F}_w(u,\theta)(s,\mu) = 0$ for the Newton correction (s,μ), i.e., solve the block system

$$\begin{bmatrix} T(\theta) & \dot{T}(\theta)u \\ w^H & 0 \end{bmatrix} \begin{bmatrix} s \\ \mu \end{bmatrix} = - \begin{bmatrix} T(\theta)u \\ 0 \end{bmatrix}, \quad \Leftrightarrow \quad \begin{array}{rl} T(\theta)s + \dot{T}(\theta)u\mu & = -T(\theta)u \\ w^H s & = 0 \end{array}$$

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The upper block can be rewritten as

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Hence, the Newton direction $\operatorname{span}\{u_+^N\}$ is identical with the direction $\operatorname{span}\{u_+^{invit}\}$ obtained by one step of the so-called nonlinear inverse iteration with shift θ from u:

$$u_+^{invit} = T(\theta)^{-1}\dot{T}(\theta)u \ (= -(A-\theta I)^{-1}u \text{ for linear problems})$$

Convergence

From general Newton theory it follows that, for fixed w,

$$\left\| \begin{bmatrix} u_+^N - x_*^w \\ \theta_+^N - \lambda_* \end{bmatrix} \right\| \leq K_3 \left\| \begin{bmatrix} u - x_*^w \\ \theta - \lambda_* \end{bmatrix} \right\|^2 = K_3 \sqrt{\|u - x_*^w\|^2 + |\theta - \lambda_*|^2}$$

provided that $\|\mathbf{z} - \mathbf{z}_*^w\| = \left\| \begin{bmatrix} u - x_*^w \\ \theta - \lambda_* \end{bmatrix} \right\|$ is sufficiently small.

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However, taking into account the special product form

$$\partial^2 \mathbf{F}_w(x, \lambda) \begin{bmatrix} s \\ \mu \end{bmatrix}^2 = \begin{bmatrix} 2\,\dot{T}(\lambda) s\mu + \ddot{T}(\lambda) x \mu^2 \\ 0 \end{bmatrix} = \mu \begin{bmatrix} 2\,\dot{T}(\lambda) s + \ddot{T}(\lambda) x \mu \\ 0 \end{bmatrix}$$

of the 2nd derivative as did Unger, we obtain the better estimate

$$\left. \begin{matrix} \|u_+^N - x_*^w\| \\ |\theta_+^N - \lambda_*| \end{matrix} \right\} \leq \left\| \begin{bmatrix} u_+^N - x_*^w \\ \theta_+^N - \lambda_* \end{bmatrix} \right\| \leq K_4\, |\theta - \lambda_*| \,\{\|u - x_*^w\| + |\theta - \lambda_*|\}$$

(N-EST)

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Nonlinear Two-Sided RFI (=N2sRFI)

Given (u, v) with $\|u\| = \|v\| = 1$, Step $(u, v) \mapsto (u_+, v_+)$:

S1: Solve $v^H T(p) u = 0$ for $p = p(u, v)$, set $\theta = p(u, v)$

S2: Solve $T(\theta) u_+^{invit} = \dot{T}(\theta) u$ for u_+^{invit}, set $u_+ = u_+^{invit} / \|u_+^{invit}\|$

S3: Solve $T(\theta)^H v_+^{invit} = \dot{T}(\theta) v$ for v_+^{invit}, set $v_+ = v_+^{invit} / \|v_+^{invit}\|$

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In case of convergence the matrices $T(\theta_k)$ become more and more singular which is not a problem when using a backward stable linear solver as Gaussian LR-factorization, cf. Peters/Wilkinson 1979 for the linear case, but may cause trouble when using iterative Krylov-Solvers when n is large.

Then an alternative implementation based on the bordered block Newton systems is preferable. In order to have for the dual problem $T(\lambda)^H y = 0$, $w_{dual}^H y = 1$ a block Jacobian that is the Hermitian transposed of the Jacobian for the primal problem, we use $w = \dot{T}(\theta)^H v$ and $w_{dual} = \dot{T}(\theta) u$ which is admissible since $w^H x_* = v^H \dot{T}(\theta) x_* \approx \alpha_* \neq 0$, $w_{dual}^H y_* = u^H \dot{T}(\theta)^H y_* \approx \bar{\alpha}_* \neq 0$.

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Therefore, replace the Steps S2, S3 of N2sRFI by

S2': Solve $\begin{bmatrix} T(\theta) & \dot{T}(\theta)u \\ v^H \dot{T}(\theta) & 0 \end{bmatrix} \begin{bmatrix} s \\ \mu \end{bmatrix} = - \begin{bmatrix} T(\theta)u \\ 0 \end{bmatrix}$ for (s, μ)

Set $u_+ = (u + s)/\|u + s\|$

S3': Solve $\begin{bmatrix} T(\theta) & \dot{T}(\theta)u \\ v^H \dot{T}(\theta) & 0 \end{bmatrix}^H \begin{bmatrix} t \\ \nu \end{bmatrix} = - \begin{bmatrix} T(\theta)^H v \\ 0 \end{bmatrix}$ for (t, ν)

Set $v_+ = (v + t)/\|v + t\|$

Remarks

- The directions $\operatorname{span}\{u_+^N\}$ and $\operatorname{span}\{v_+^N\}$ does not depend on the bordering vectors w and w_{dual} used in the Newton step!
- Unlike the $T(\theta_k)$, the bordered matrices

$$\begin{bmatrix} T(\theta_k) & \dot{T}(\theta_k)u_k \\ v_k^H \dot{T}(\theta_k) & 0 \end{bmatrix}$$

  have uniformly bounded inverses for $\theta_k, \xi_k, \eta_k \to 0$ where

$$\xi_k = \measuredangle(\operatorname{span}\{u_k\}, \operatorname{span}\{x_*\}), \ \eta_k = \measuredangle(\operatorname{span}\{v_k\}, \operatorname{span}\{y_*\}).$$

- When, e.g., for GMRES as iterative solver an `ilu`-preconditioner is used, the same preconditioner can be used for both the primal und dual system. Moreover, both systems can be solved in parallel.

6. Cubic Convergence of N2sNRF

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As the basic 2sRQI for linear problems, the new Nonlinear Two-Sided Rayleigh Functional Iteration N2sNRF converges for general T cubically in the following sense:

Theorem 2 Under the assumptions of Theorem 1, there are constants $0 < \tau_0$, $0 < \varepsilon_0 < \pi/2$ such that, for all $\theta_0 \in \bar{S}(x_*, \tau_0)$ and for all $(u_0, v_0) \in \mathcal{K}(\varepsilon_0)$, the algorithm N2sRFI is well defined and converges:

$$\lim_{k\to\infty} \theta_k = \lambda_*, \qquad \lim_{k\to\infty} \xi_k = \lim_{k\to\infty} \eta_k = 0.$$

Moreover, there exist constants $K_5, K_6 > 0$ such that

(i) $$|\theta_{k+1} - \lambda_*| \le K_5\, |\theta_k - \lambda_*|^2 \sin\xi_k \sin\eta_k$$

(ii) $$\sin\xi_{k+1} \;\le\; K_6\, \sin^2\xi_k \sin\eta_k, \qquad \sin\eta_{k+1} \;\le\; K_6\, \sin^2\eta_k \sin\xi_k$$

Remarks

- Inequalities (ii) mean that the angles $\{\xi_k\}, \{\eta_k\}$ converge *alternating Q-cubically* toward 0.
- A deeper analysis using some results of J.W.Schmidt 1981 *On the R-order of coupled sequences* shows that the angles $\{\xi_k\}, \{\eta_k\}$ converge both with R-order 3.

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Sketch of the proof

In what follows we omit the index k.

For $\theta = \theta_k$ computed in S1 we get from (NRF-EST) the bound

$$|\theta - \lambda_*| = |p(u,v) - \lambda_*| \le K_1 \tan\xi \tan\eta. \qquad \text{(a)}$$

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For investigating the improvement in the direction of u, v caused by the inverse iteration steps in S2 and S3, we exploit that u_+^N defined by one Newton step for (NS) and u_+^{invit} defined in S2 span the same direction, i.e., they have the same angle ξ_+ with $\operatorname{span}\{x_*\}$. In the proof we chose $w = u$ for normalizing u_+.

Analogously, v_+^N obtained from one Newton step $(v, \theta) \mapsto (v_+^N, \theta_+^N)$ for $T(\lambda)^H y = 0$, $v^H y = 1$ and v_+^{invit} from S3 span the same direction which has the angle η_+ with $\operatorname{span}\{y_*\}$.

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At first one has to show that the Jacobians $\partial \mathbf{F}_u(u,\theta)$ have uniformly bounded inverses w.r.t. (u,θ) with $\xi \leq \varepsilon_0$ and $\|\theta - \lambda_*\| \leq \tau_0$.

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The Newton estimate (N-EST) for the x-part with $w = u$ was

$$\|u_+^N - x_*^u\| \leq K_4 \, |\theta - \lambda_*| \, \{\|u - x_*^u\| + |\theta - \lambda_*|\}. \qquad \text{(b')}$$

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For introducing ξ on the right hand side we use that

$$\|u - x_*^u\|^2 = \|u - \frac{x*}{u^H x_*}\|^2 = \underbrace{\|u\|^2}_{=1} - 2\,\underbrace{\text{Re}(u^H \frac{x*}{u^H x_*})}_{=1} + \underbrace{\|\frac{x*}{u^H x_*}\|^2}_{=1/\cos^2 \xi} = \tan^2 \xi$$

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For introducing ξ_+ on the left hand side, we use the fact that

$$\sin\xi_+ \le \left\| \frac{u_+^N}{\|x_*^u\|} - \frac{x_*^u}{\|x_*^u\|} \right\| = \frac{\|u_+^N - x_*^u\|}{\|x_*^u\|} = \cos\xi\,\|u_+^N - x_*^u\| \le \|u_+^N - x_*^u\|$$

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$$|\theta - \lambda_*| \leq K_1 \tan \xi \tan \eta \qquad \text{(a)}$$

from above yields

$$\sin \xi_+ \leq K \underbrace{\tan \xi}_{\leq K \sin \xi} \; \underbrace{\tan \eta}_{\leq K \sin \eta} \; \{\underbrace{\tan \xi + K \tan \xi \tan \eta}_{\leq K \tan \xi \leq K \sin \xi}\} \leq K \sin^2 \xi \sin \eta,$$

hence, the first inequality in (ii). Here K is a generic constant.

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The bound for $\sin\eta_+$ is obtained considering $T(\lambda)^H y = 0,\ v^H y = 1$.

The bound (i) is obtained from (a) and (b) as follows:

$$|\theta_+-\lambda_*| \le K_1 \underbrace{\tan\xi_+}_{\le K|\theta-\lambda_*|\tan\xi} \underbrace{\tan\eta_+}_{\le K|\theta-\lambda_*|\tan\eta} \le K\,|\theta-\lambda_*|^2 \sin\xi\sin\eta.$$

The end — thanks for your attention!

Greetings from Dresden – the Frauenkirche