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Technische Universität Hamburg-Harburg
Institut für Numerische Simulation

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Supported by

- Bundesministerium für Bildung und Forschung
- GAMM

History

- Harrachov 2007
- Düsseldorf 2006
- Dresden 2005
- Hagen 2004
- Braunschweig 2003
- Bielefeld 2002
- Berlin 2001

Welcome to the GAMM Workshop

Applied and Numerical Linear Algebra

with special emphasis on

Regularization of Ill-posed Problems

Date:

September 11-12, 2008
Technische Universität Hamburg-Harburg, Germany

Invited speakers (confirmed):

Lars Eldén (Linköping, Sweden)

Per Christian Hansen (Lyngby, Denmark)

Marielba Rojas (Lyngby, Denmark)

Fiorella Sgallari (Bologna,Italy)

last modified on: 2008-04-14, 15:55

Quasi-Minimal Residual Eigenpairs

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

Institut für Numerische Simulation
Technische Universität Hamburg-Harburg

10.09.2008
9.50 am – 10.15 am

IWASEP 7
June 9-12, 2008
Dubrovnik, Croatia

Outline

Krylov decompositions

We consider a given Krylov decomposition

$$AQ_k = Q_{k+1}\underline{C}_k = Q_kC_k + q_{k+1}c_{k+1,k}e_k^T. \tag{1}$$

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$$A \in \mathbb{C}^{(n,n)}$$ is a general square matrix,

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We do not consider perturbations. We remark that important parts of the results carry over to general rectangular approximations $\underline{C}_k$ of A which not necessarily have to be Hessenberg.

QMR eigenpairs

We proceed similar to the QMR approach often applied to linear systems,

$$\min_{z,y=Q_k v} \frac{\|zy - Ay\|}{\|y\|} \tag{2}$$

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Definition (QMR eigenpair)

The pair $(\grave{\theta}, \grave{y} = Q_k \grave{v})$ is a QMR eigenpair, iff

$$\frac{\|(\grave{\theta}\underline{I}_k - \underline{C}_k)\grave{v}\|}{\|\grave{v}\|} = \operatorname*{min\,loc}_{z\in\mathbb{C}, v\in\mathbb{C}^k, \|v\|=1} \frac{\|(z\underline{I}_k - \underline{C}_k)v\|}{\|v\|}, \tag{3}$$

where “min loc” denotes a (not necessarily strict) local minimum.

QMR eigenpairs: SVD characterization

We denote the SVD of ${}^{z}\underline{C}_k \equiv z\underline{I}_k - \underline{C}_k$ by $U(z)\Sigma(z)V(z)^H = U\,\Sigma(z)V^H$.

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Since for every $z \in \mathbb{C}$

$$\sigma_k(z) = \|\sigma_k(z)u_k\| = \frac{\|{}^z\underline{C}_k v_k\|}{\|v_k\|} = \min_v \frac{\|{}^z\underline{C}_k v\|}{\|v\|},$$

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QMR eigenpairs: SVD steepest descent

Simple singular values $\sigma(z)$ and corresponding singular vectors v_k, u_k of the complex matrices ${}^{z}\underline{C}_k = z\underline{I}_k - \underline{C}_k$ are real analytic (Sun, 1988),

$$\sigma(z+w) = \sigma(z) + \sigma_z(z)w + \sigma_{\bar{z}}(z)\overline{w} + O(|w|^2) \tag{6}$$

$$= \sigma(z) + 2\Re((u_k^H \underline{I}_k v_k)w) + O(|w|^2). \tag{7}$$

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We obtain steepest descent by subtracting the conjugate of the gradient $\sigma_z(z)$:

$$z_{\text{new}} = z - \alpha\, \overline{u_k^H \underline{I}_k v_k} = z - \alpha\, v_k^H \underline{I}_k^H u_k \tag{8}$$

$$= z - \frac{\alpha}{\sigma_k} v_k^H \underline{I}_k^H (z\underline{I}_k - \underline{C}_k) v_k = z - \frac{\alpha}{\sigma_k} v_k^H (zI_k - C_k) v_k. \tag{9}$$

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We note that $\sigma_k(z)$ is the backward error of the approximate eigenvalue z. Setting $\alpha = \sigma_k$ yields alternating projections and is nearly optimal:

$$z_{\text{new}} = v_k^H C_k v_k. \tag{10}$$

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Steepest descent exhibits linear convergence. The real-analyticity of simple singular values can also be used to adopt Newton's method for stationary points.

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Enhancement: Damped Newton's method or simply BFGS.

Remark: Multiple singular values can not occur in the symmetric case due to the unreduced Hessenberg structure, but still may be pathologically close, compare with results by Lehmann and Wilkinson.

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Given an QMR eigenvector $\grave{v}$, we obtain $\grave{\theta}$ by the Rayleigh quotient with C_k, as

$$\grave{\theta} = \frac{\grave{v}^H C_k \grave{v}}{\grave{v}^H \grave{v}} = \operatorname*{arg\,min}_{z \in \mathbb{C}} \frac{\|(z\underline{I}_k - \underline{C}_k)\grave{v}\|}{\|\grave{v}\|}. \tag{11}$$

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It can then be shown that the QMR eigenvectors give minima of the resulting real-analytic function

$$\lambda \,:\, G_1(\mathbb{C}^k) \to \mathbb{R}_{\geqslant 0},$$

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The stationary points of real-analytic λ are always singular vectors.

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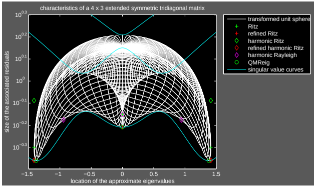
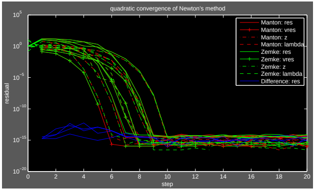
For Newton's method we have to compute the second covariant derivative, i.e., to use the Levi-Civita connection on the Grassmannian. This is simplified if using orthonormal frames, compare with the introductory textbook by Boothby.

QMR eigenpairs: Grassmannian Newton

```
for j = 1:convergence

  [Q,R] = qr(v); W = Q(:,2:k); v = Q(:,1);

  z = v'*Ck*v; zuCk = z*uIk-uCk;
  zuCkW = zuCk*W; zuCkv = zuCk*v;
  slambda = norm(zuCkv);
  y = zuCkW'*zuCkv;
  grad = 2*[real(y);imag(y)];
  res = norm(grad);

  A = zuCkW'*zuCkW; zCk = uIk'*zuCk;
  g1 = (zCk*W)'*v; r1 = real(g1); c1 = imag(g1);
  g2 = W'*(zCk*v); r2 = real(g2); c2 = imag(g2);
  outer1 = [r1+r2;c1+c2];
  outer2 = [c2-c1;r1-r2];
  Hesse = 2*[real(A) imag(A)';...
             imag(A) real(A)]-...
          2*slambda^2*I-...
          2*outer1*outer1'-2*outer2*outer2';
  ab = Hesse\grad;
  u = -W*(ab(1:k-1)+i*ab(k:2*k-2));
  normu = norm(u);
  v = v*cos(normu)+u*sin(normu)/normu;

end
```

(This is to convince you that the code is short enough to fit on one page.)





A graphical representation

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Remark 2: There exist “graphical” bounds for general and “Rayleigh” approximations.

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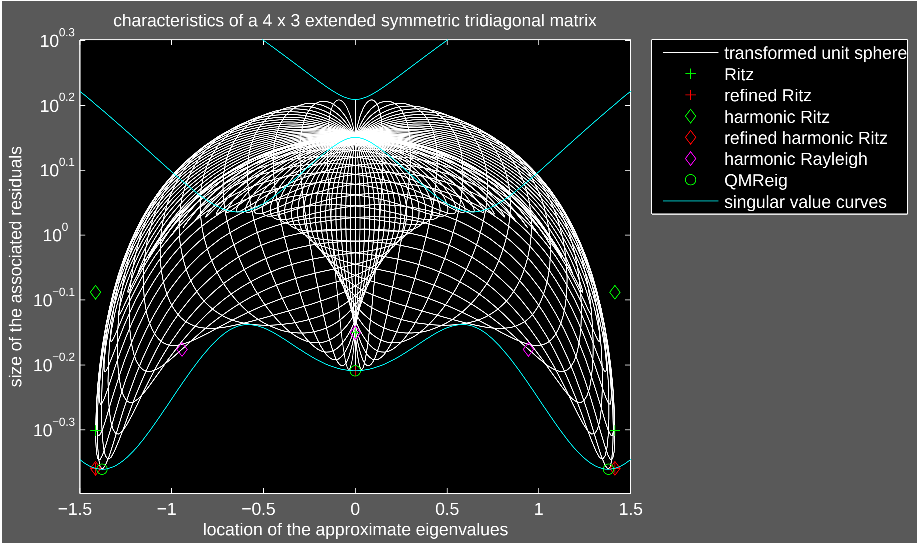

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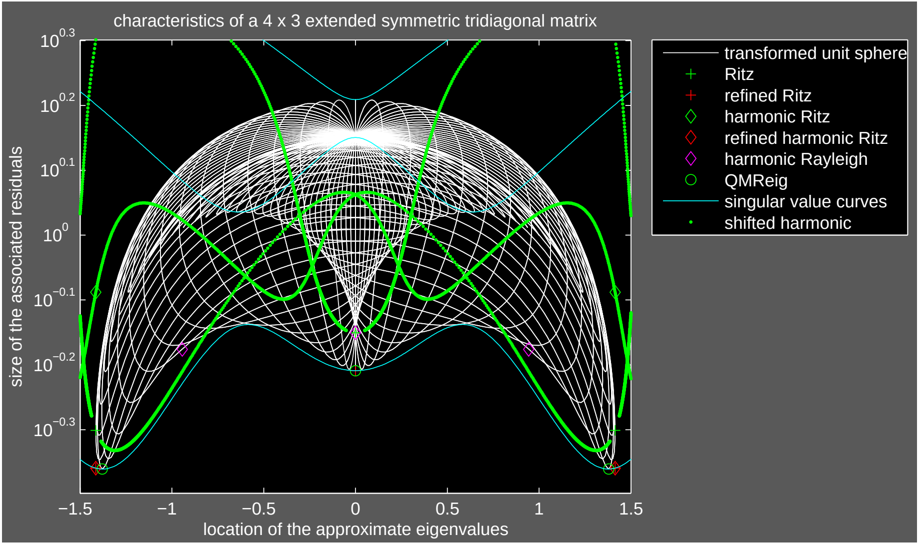

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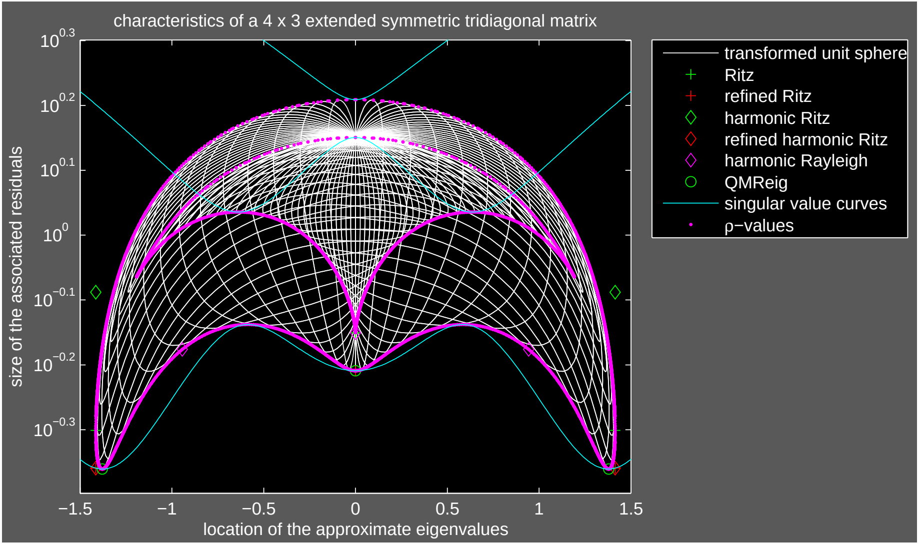

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Thank you for your attention!

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$$\underline{C}_k = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \tag{21}$$

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At zero a stationary point exists which is a maximum of the smallest singular value curve and a saddle point of the transformed sphere.

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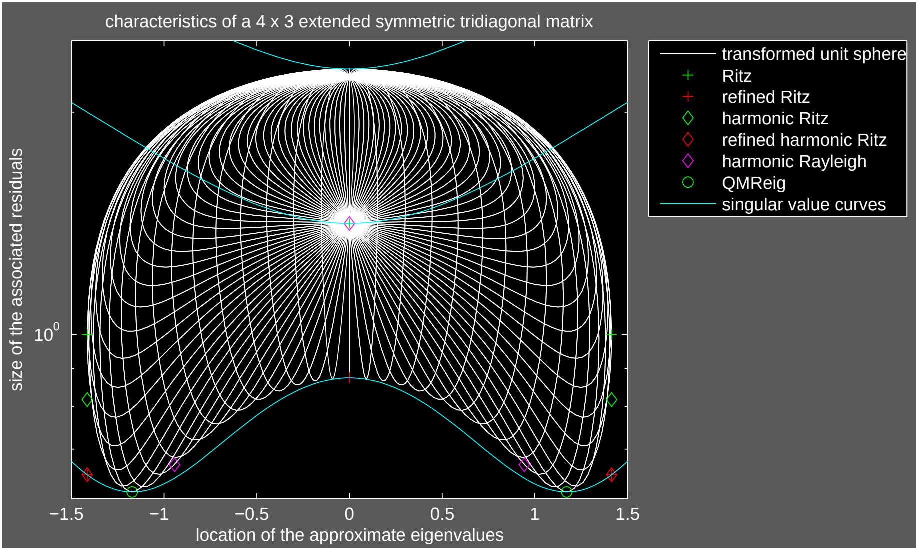

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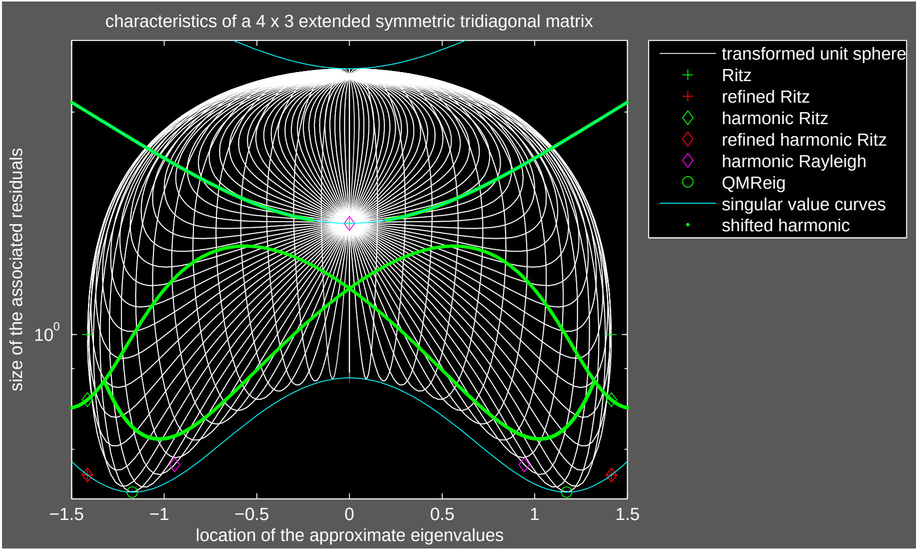

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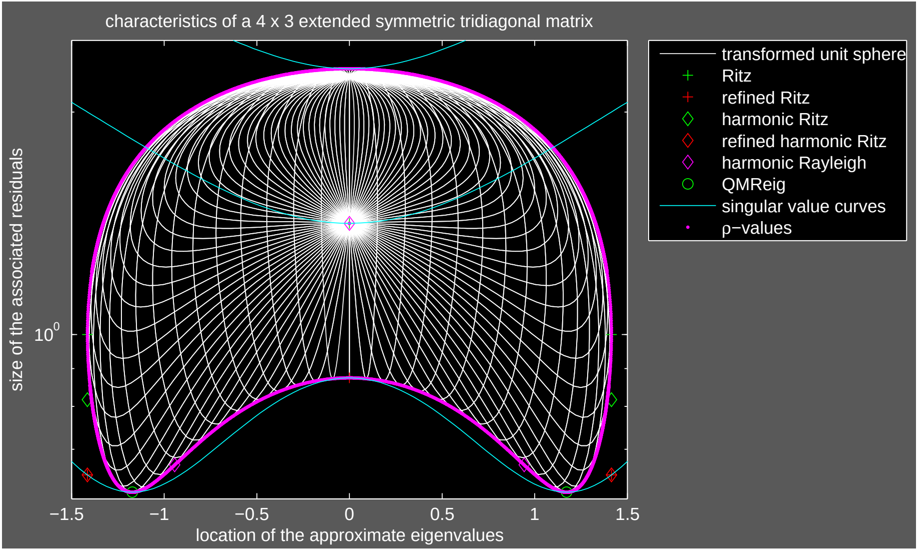

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An interesting example is extended symmetric and generated using MATLAB's `randn` and `hess` functions and is approximately given by

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$$\begin{aligned} \theta_1 &\approx -1.490413407713866, & n(\theta_1, v_1) &\approx 0.185432088955641 7, \\ \underline{\theta}_1 &\approx -1.509143602001304, & n(\underline{\theta}_1, \underline{v}_1) &\approx 0.181039457164899 5, \\ \rho_1 &\approx -1.487425797938723, & n(\rho_1, \underline{v}_1) &\approx 0.179732084050847 2, \\ \grave{\theta}_1 &\approx -1.489367749116040, & n(\grave{\theta}_1, \grave{v}_1) &\approx 0.174658339265659 0. \end{aligned}$$

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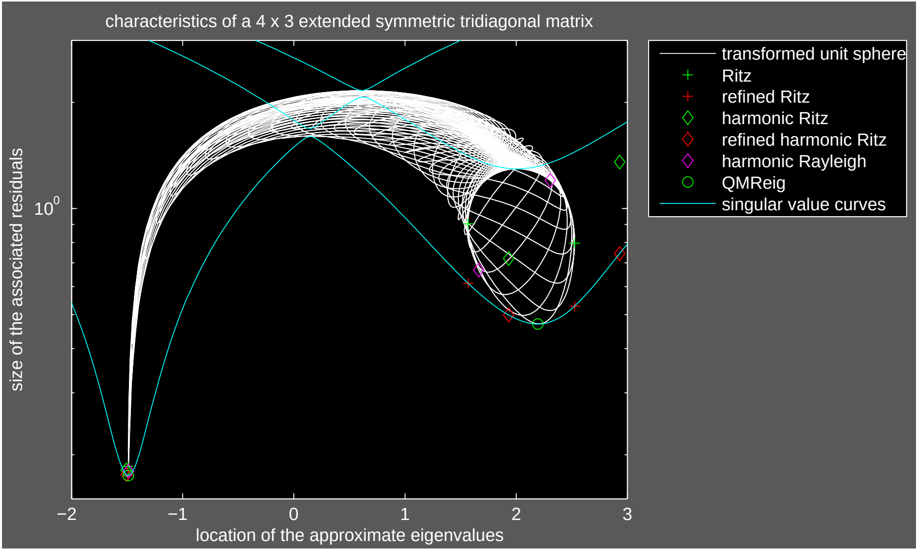

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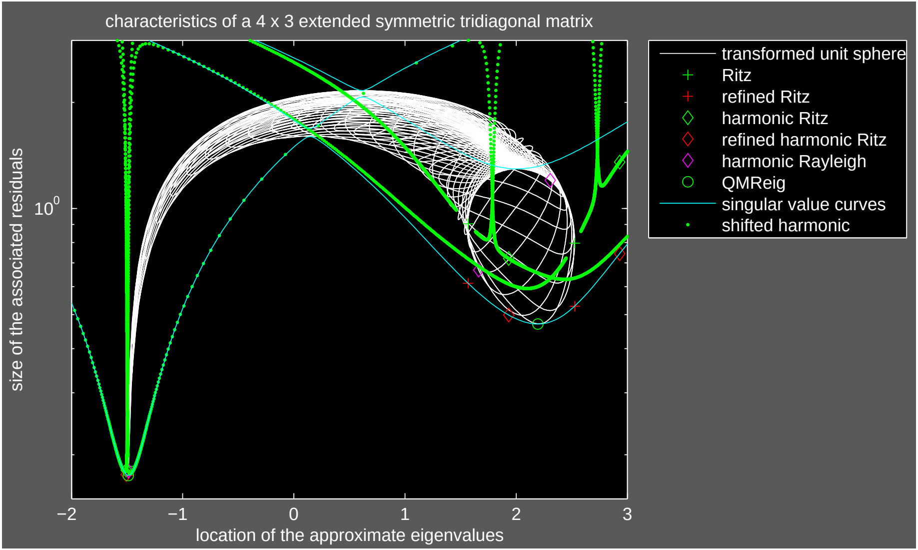

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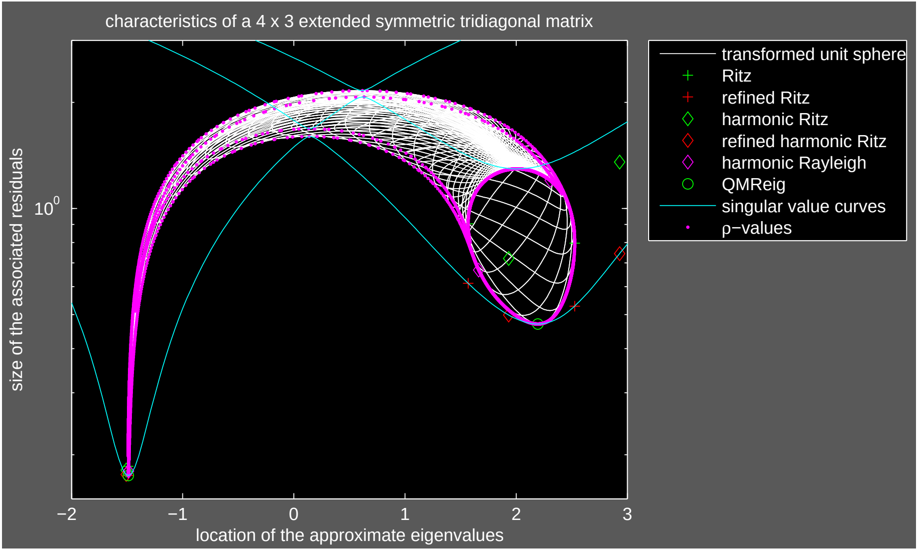

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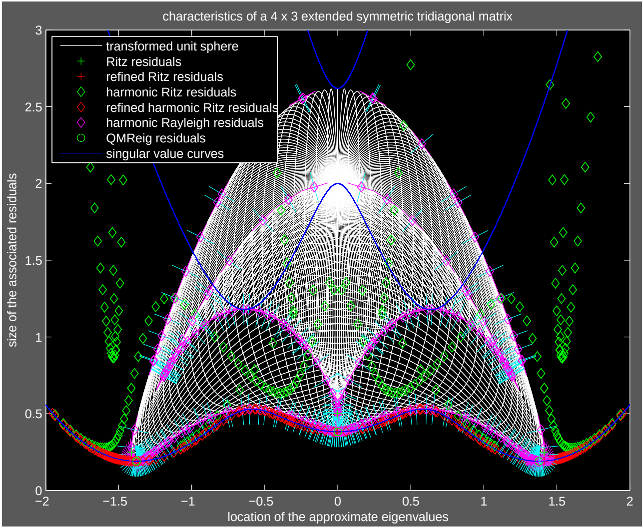

Shifted harmonic Ritz values and the SVD

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As the harmonic Ritz values are not shift-invariant (in contrast to Ritz and QMR eigenvalues), and by interlacing of singular values and the connection of the pseudoinverse to the singular value decomposition we might expect to see relations between shifted harmonic Ritz and the SVD in the pictures.

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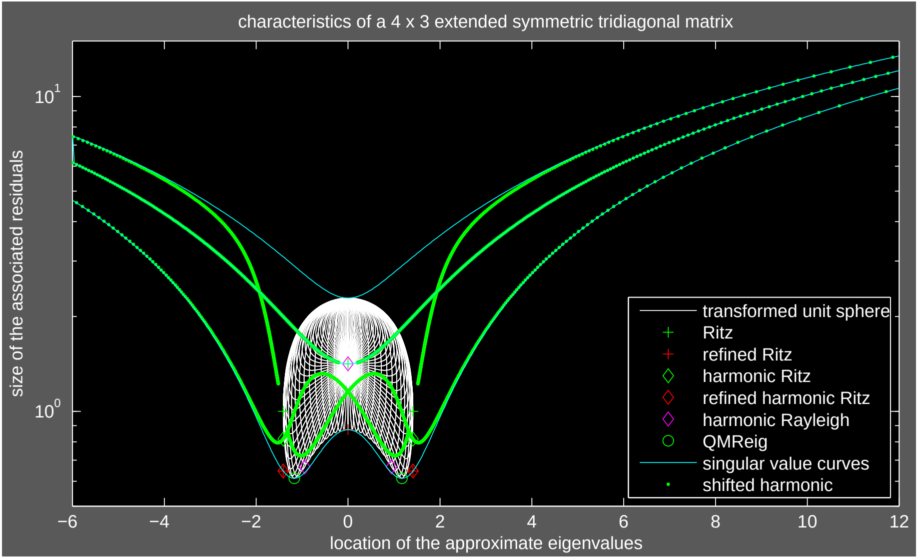

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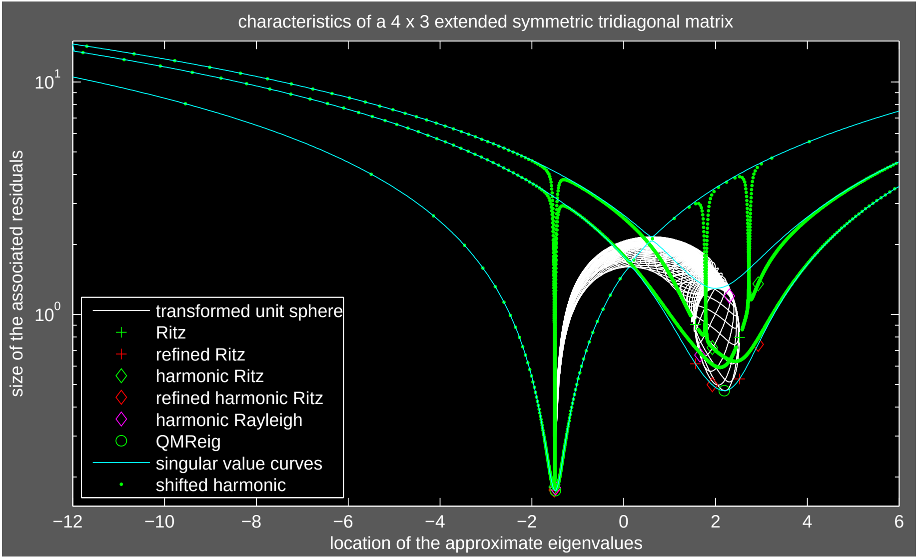

A Jordan block: infinitely many QMR eigenvalues

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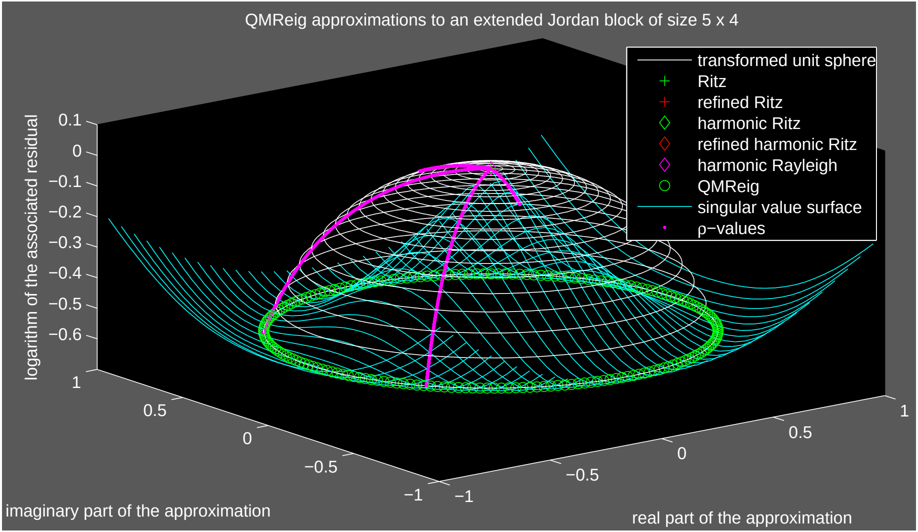
$$\grave{\theta}_\phi = \cos\left(\frac{\pi}{k+1}\right) e^{i\phi}, \quad \phi \in [0, 2\pi). \tag{26}$$

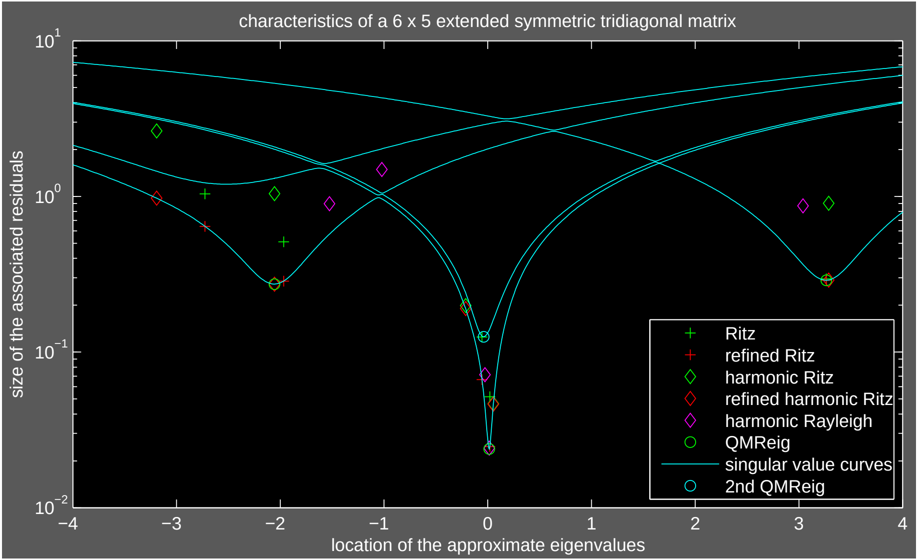
The residual of the corresponding QMR eigenpairs is given by

$$\|(\grave{\theta}_\phi \underline{I}_k - \underline{C}_k)\grave{s}_\phi\| = \sin\left(\frac{\pi}{k+1}\right) \quad \forall\ \phi. \tag{27}$$

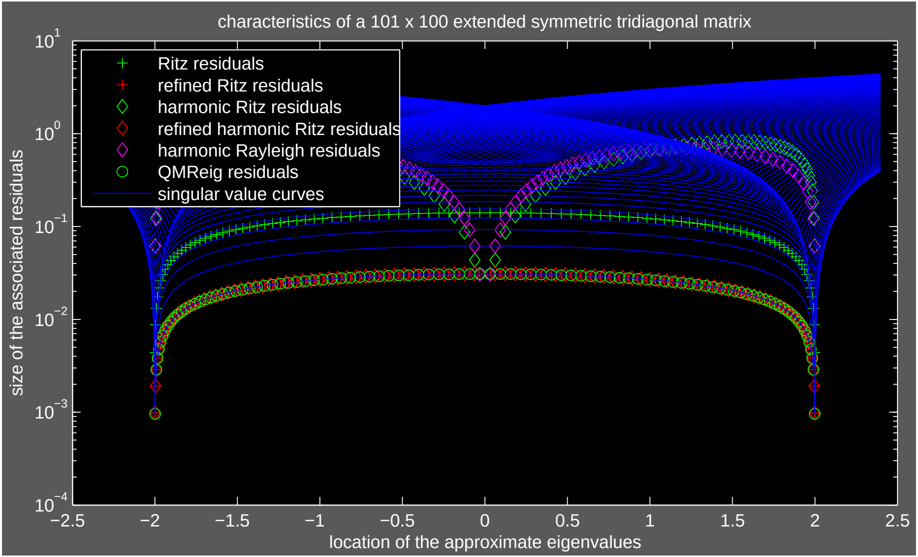
A Jordan block: infinitely many QMR eigenvalues



Always remember: It's only locally optimal . . .



Large matrices and harmonic Ritz



Lehmann's work on eigenvalues

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We have extended his approach to general complex square matrices by replacing "Lehmann optimality" by "backward error". Thus, we have extended his work to normal matrices (Q_{k+1} orthonormal; Arnoldi's method).

Lehmann's results summarized

Lehmann used the information included in $Q \in \mathbb{C}^{(n,k)}$ and $W = AQ \in \mathbb{C}^{(n,k)}$, where $A \in \mathbb{C}^{(n,n)}$ is selfadjoint. We used a generic $x = Qv \in \mathbb{C}^n$.

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Lehmann was interested in optimal shifts, i.e., shifts z resulting in a minimal radius $\sigma(z)$ of the inclusion. These are [Satz 4, 1963] among the stationary points of $\sigma^2(z)$,

$$\frac{\partial \sigma^2(z)}{\partial z} = 0.$$

Lehmann's little-known results

Differentiating an expression involving the Temple quotient $T_\tau(x)$, he obtained the shifted harmonic Ritz values [(20a)+(28), 1963] of Morgan (1991) and Freund (1992),

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He (defined and) noted certain interesting symmetries/properties, namely

$$\tau = z \mp \sigma(z), \qquad \underline{\theta}(\tau) = z \pm \sigma(z), \qquad \text{[(Seite 251),1963]}$$

$$\underline{\theta}(\tau) = T_\tau(\underline{x}), \qquad T_\tau(\underline{x}) = \frac{\underline{x}^H(A-\tau I)^H(A-\tau I)\underline{x}}{\underline{x}^H(A-\tau I)^H\underline{x}} + \tau, \qquad \text{[(15),1963]}$$

$$2z = \tau + \underline{\theta}(\tau), \qquad z^2 - \sigma^2(z) = \tau \cdot \underline{\theta}(\tau). \qquad \text{[(8b)+(21),1963]}$$

QMR eigenpairs: Grassmann Newton

The function λ is stationary only for singular vectors for $z = v^H C_k v$. If the corresponding singular value is simple, we have found a stationary point on the corresponding singular value surface.

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$$A(z) = W^H ({}^z\underline{C}_k^H {}^z\underline{C}_k - \sigma_j(z)^2 I_k) W, \qquad W = v_j^\perp.$$

The Hermitean matrix $A(z)$ has the eigenvalues $\sigma_i^2 - \sigma_j^2$, $i \neq j$. The smallest eigenvalue of the Hesse matrix is bounded from above by Weyl's Lemma by $\lambda_{\min} \leqslant \sigma_{\min}^2 - \sigma_j^2 < 0$.

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Is every QMR eigenpair obtained through SVD minimization also obtained by Grassmannian optimization with SPD Hessean and vice versa? How to prove this?

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One direction is quite simple: As any QMR eigenpair $(\grave{\theta}, \grave{v})$ from the SVD minimization satisfies

$$\grave{\theta} = \frac{\grave{v}^H C_k \grave{v}}{\grave{v}^H \grave{v}} = z(\grave{v}),$$

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There can be no smaller function value nearby, since this would result in a sequence of $v(\epsilon_i)$, $\|v(\epsilon_i)\| = 1$, arbitrarily close to $v = \grave{v}$, $\|v\| = 1$, with

$$\sigma_k(z(v)) = \|(z(v)\underline{I}_k - \underline{C}_k)v\| > \|(z(v(\epsilon_i))\underline{I}_k - \underline{C}_k)v(\epsilon_i)\| \geqslant \sigma_k(z(v(\epsilon_i))),$$

thus, there would be a sequence $z_i = z(v(\epsilon_i)) \to z = \grave{\theta}$ with

$$\sigma_k(\grave{\theta}) > \sigma_k(z_i),$$

which gives with the continuity of the functions involved a contradiction.

QMR eigenpairs: Grassmann Newton

If the singular vector to the smallest singular values as a function of the parameter ϵ is continuous, which is at least the case if the singular value is simple and thus real analytic by Sun's results, we can prove that a minimum of the vector-valued function is indeed also a minimum of the singular value surface.

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Denote the "smallest" singular vector of ${}^{(z+\epsilon)}\underline{C}_k$ by $v(\epsilon) = v_k(z+\epsilon)$, i.e.,

$$((z+\epsilon)\underline{I}_k - \underline{C}_k)v(\epsilon) = u_k(z+\epsilon)\sigma_k(z+\epsilon),$$

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Then, obviously,

$$\sigma_k^2(z+\epsilon) \geqslant \|{}^{z(\epsilon)}\underline{C}_k v(\epsilon)\|_2^2 \geqslant \sigma_k^2(z(\epsilon)). \tag{28}$$

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We now use the "closeness" of the functions σ_k^2 and λ, i.e.,

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$$\forall N_z \quad \exists w \in N_z \, : \, \sigma_k(w) < \sigma_k(z), \tag{30}$$

or, by the Axiom of Choice, a sequence of points $\{\epsilon_i \in \mathbb{C}\}_{i=1}^{\infty}$ such that

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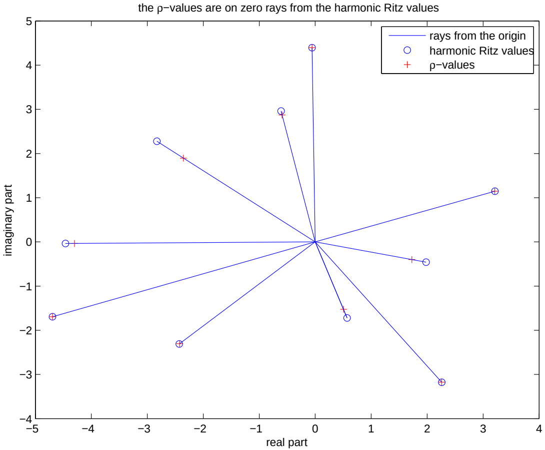

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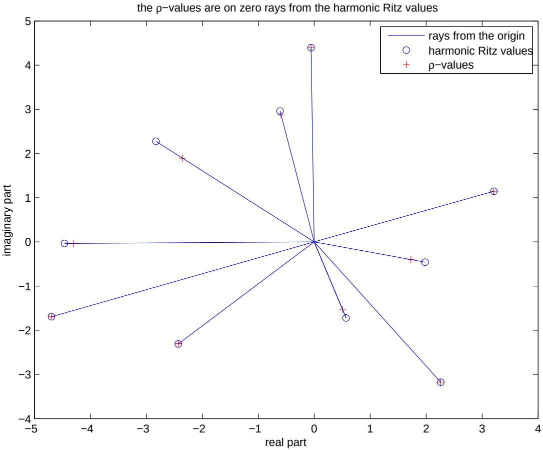

In the general setting the ρ-values and the harmonic Ritz values $\underline{\theta}$ are, again, on the same rays, but now originating from the target $\tau \in \mathbb{C}$.