An Algorithm for the Generalized Symmetric Tridiagonal Eigenvalue Problem

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Generalized Eigenvalue Problem

Def

$T, S \in \mathbb{R}^{n \times n}$. We call (T, S) *pencil*.

We consider *only* $\boxed{\begin{array}{l}\text{symmetric}\\ \text{and}\\ \text{tridiagonal}\end{array}}$ pencil.

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Def (Problem)

Find $\lambda \in \mathbb{R}$ such that $Tv = \lambda S v$, with $v \in \mathbb{C}^n$.
T, S symmetric implies $\lambda \in \mathbb{R}$.

Algorithm philosophy

We find zeros of the polynomial equation

$$\mathcal{F}_{(T,S)}(\lambda) = \det(T - \lambda S) = 0$$

using an iterative method, living on real line.

Brainstorming

We want:	Fast and secure iterative method. Starting points for our method. Scalability.
We have:	Laguerre's method. Cuppen's divide and conquer method. Symmetric tridiagonal matrices.
We add:	Unreducible condition. Dynamic programming (Bottom-up). Efficient matrix storing.

Rapid tour

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Unreducible pencil

Def (as in [MR739278])

(T, S) is an *unreducible pencil* if $t_{i,i+1}^2 + s_{i,i+1}^2 \neq 0$ for $i = 1, 2, \ldots, n-1$.

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exemplum gratie:

Bad

$$\boxed{\begin{array}{l} T = I, S = 0 \\ T = I, S = I \end{array}}$$

Good

$$\boxed{\begin{array}{l} T = I, S = trid(-1, 2, -1) \\ T = trid(-1, 2, -1), S = trid(-1, 2, -1) \\ T = trid(rnd_{sub}, rnd_{diag}, rnd_{sub}), S = I, \\ \text{with } rnd_{sub} \text{ random number} \neq 0. \end{array}}$$

Matrix storin

$$T = trid(sub, diag, super)$$

But T is symmetric, so $sub = super$. We define and use

```
integer, parameter :: dp = kind(1.d0)
real(dp), dimension(1:n,0:1) :: T, S
```

with $T(:,0) = diag$ and $T(:,1) = super$.

Remark

We don't use T(1,1) and S(1,1).

Fast and secure iterative method

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$$g_u(X) = (x - X)^2 \sum_{i=1}^{n} \frac{(u - \lambda_i)^2}{(x - \lambda_i)^2} - (u - X)^2$$

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Bolzano's Theorem tell us that there are two zeros of g_u between λ_m and λ_{m+1}. We call them X_-, X_+.

Fast and secure iterative method

$$\lambda_m < X_- < x < X_+ < \lambda_{m+1}$$

We have one freedom: the u parameter.
Calling $\hat{X}_- = min_u X_-$ and $\hat{X}_+ = max_u X_+$ we can obtain

$$\lambda_m \approx \hat{X}_- < x < \hat{X}_+ \approx \lambda_{m+1}$$

and with algebraic manipulations:

$$\hat{X}_-, \hat{X}_+ = L_\pm(x) = x + \frac{n}{-\frac{f'}{f} \pm \sqrt{(n-1)[(n-1)(-\frac{f'}{f}) - n\frac{f''}{f}]}}$$

with $\frac{f'}{f} = \frac{(\mathcal{F}_{T,S}(\lambda))'}{\mathcal{F}_{T,S}(\lambda)}$.

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We will see that "only" with the symmetric tridiagonal condition we can have derivatives of determinats.

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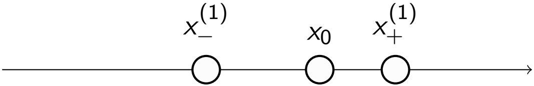

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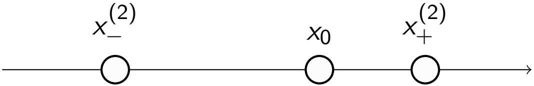

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Fast and secure iterative method

Def (Laguerre's iteration)

If $mlt(\lambda_m) = mlt(\lambda_{m+1}) = 1$ then

$$
\begin{aligned}
x_+^{(k)} &= L_+^k(x) = L_+(L_+(\ldots(x_0))) \\
x_-^{(k)} &= L_-^k(x) = L_-(L_-(\ldots(x_0)))
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else we have a similar expression.

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$$\lambda_m \leftarrow \ldots x_-^{(2)} < x_-^{(1)} < x_0 < x_+^{(1)} < x_+^{(2)} \cdots \rightarrow \lambda_{m+1}$$

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So Laguerre's method is secure.

Fast and secure iterative method

We also have un important property:

Teo

*If we choose** $\lambda_m < x_0$ *s.t.* $sign\left(\frac{f'(x_0)}{f(x_0)}\right) = sign(\lambda_m - x_0)$ *then* $\{x_-^{(k)}\}_{k=1,\ldots}$ *converge monotonically in asymptotically cubic rate to* λ_m.

*for $x_0 < \lambda_{m+1}$ s.t. $sign\left(\frac{f'(x_0)}{f(x_0)}\right) = sign(\lambda_m - x_0)$ we have $\{x_+^{(k)}\}_{k=1,\ldots}$ conv. mon. cubic to λ_{m+1}

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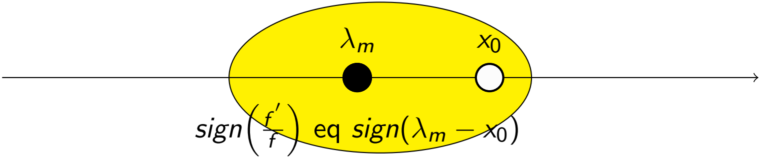

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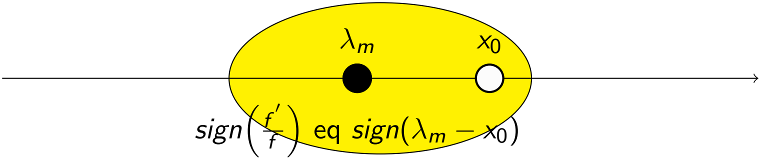

The Laguerre's method is fast.

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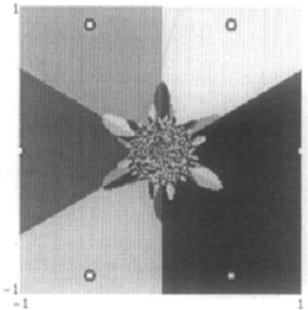
Fast and secure iterative method

It's clear that we need a powerfull method to obtain x_0 and an algorithm to estimate $mlt(\lambda_m)$.
Overstimate $mlt(\lambda_m)$ (as we can read in [**MR1289159**]) causes no trouble, so the most importan aspects of our calculation are:

Good x_0.
Good evaluation of $L_\pm(x)$.

Complex case (little digression)

According to [**MR2019677**], we observe that searching $z \in \mathbb{C}$ such that $z^n - 1 = 0$ for $n > 4$ with Laguerre's method it's difficult because near the origin there is a Julia fractal set for starting point z_0. (figure: $n = 6$)



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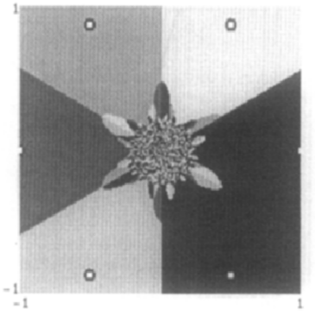

So if we want to solve the Generalized Eigenvalues Problem with $T, S \in \mathbb{C}$ we have great problems to place the starting point if $n > 4$.

Three term recurrence

For a generic $x \in \mathbb{R}$ we call $\rho_n(x) = \det(T_n - xS_n)$, and $\rho_{n-1}(x) = \det(T_{n-1} - xS_{n-1})$, with T_{n-1} leading principal submatrix.
We have

$$\rho_0 := 1\,,\ \rho_1 := t_{1,1} - xs_{1,1}$$
$$\rho_i := (t_{i,i} - xs_{i,i})\rho_{i-1} - (t_{i-1,i} - xs_{i-1,i})^2\rho_{i-2}\,,\ i = 2, 3, \ldots, n$$

Three term recurrence

We can proove it with the *Laplace expansion* (e.g. $n = 4$)

$$T_4 - xS_4 = \begin{pmatrix} a & b & 0 & 0 \\ b & c & d & 0 \\ 0 & d & e & f \\ 0 & 0 & f & g \end{pmatrix}$$

$$\begin{aligned} det\left(T_4 - \lambda S_4\right) &= g \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & d & e \end{bmatrix} - f \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & 0 & f \end{bmatrix} \\ &= g \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & d & e \end{bmatrix} - f^2 \begin{bmatrix} a & b \\ b & c \end{bmatrix} \end{aligned}$$

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Three term recurrence

Remark

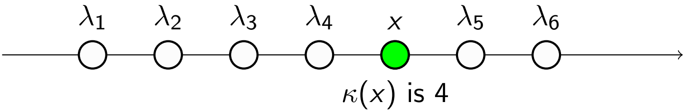
If $x = \lambda$ then $\rho_n(\lambda) = \mathcal{F}_{(T_n, S_n)}(\lambda) = f$

Remark

$\rho_0, \rho_1, \ldots, \rho_n$ i a *Sturm sequence* of polynomials so, $\forall x \in \mathbb{R}$, we have

$$\kappa(x) := \#\text{ eigenvalues less then } x$$

$$\kappa(x) = \#\text{ consecutive sign changes in } \{\rho_i\}_{i=0,\ldots,n}$$



Three term recurrence

Obviusly $f' = \rho_n', f'' = \rho_n''$.

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*$\kappa(x) < m$ implies $sign(\lambda_m - x) = +$

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Obviusly $f^{'} = \rho_n^{'}, f^{''} = \rho_n^{''}$.
So*

$$\text{IF } (\kappa(x_0) \geq m \text{ AND } -\frac{f^{'}}{f} < 0) \text{ OR } (\kappa(x_0) < m \text{ AND } -\frac{f^{'}}{f} \geq 0) \text{ THEN}$$

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We have cubic convergence in Laguerre's method with x_0 as starting point.

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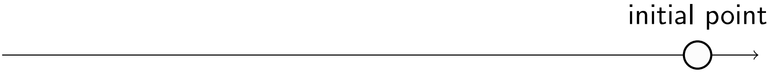
Example



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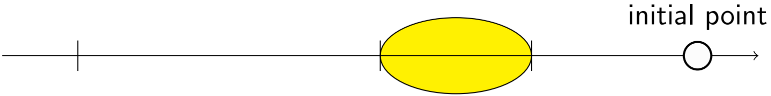

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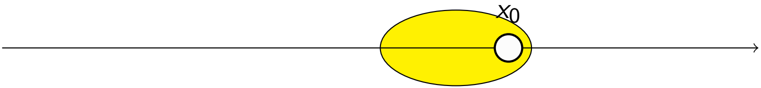

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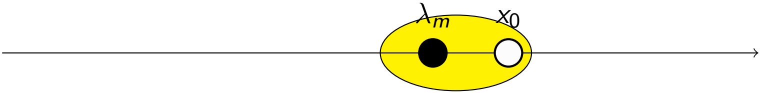

Searching x_0

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We have:	Laguerre's method. Cuppen's divide and conquer method. Symmetric tridiagonal matrices.
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If $n = 1$ we have $t \cdot v = \lambda \cdot s \cdot v$. $s \neq 0$, so $\lambda = \frac{t}{s}$.

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If $n = 2$ we have $\begin{bmatrix} t_{1,1} & t_{1,2} \\ t_{2,1} & t_{2,2} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \lambda \begin{bmatrix} s_{1,1} & s_{1,2} \\ s_{2,1} & s_{2,2} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$

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calling*

$$S^{-1}T = \delta^{-1} \cdot \begin{pmatrix} \alpha & \gamma \\ \gamma & \beta \end{pmatrix}$$

we resolve $det[S^{-1}T - \lambda I] = 0$ with

$$\lambda_{1,2} = \frac{1}{2\delta}\left(\alpha + \beta \pm \sqrt{\alpha^2 + \beta^2 + \gamma^2 - \alpha\beta}\right)$$

$^*\alpha =, \beta =, \gamma =.$

Ideas:

And if $n = 4$?

$$\begin{pmatrix} t_{1,1} & t_{1,2} & 0 & 0 \\ t_{2,1} & t_{2,2} & t_{2,3} & 0 \\ 0 & t_{3,2} & t_{3,3} & t_{3,4} \\ 0 & 0 & t_{4,3} & t_{4,4} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = \lambda \begin{pmatrix} s_{1,1} & s_{1,2} & 0 & 0 \\ s_{2,1} & s_{2,2} & s_{2,3} & 0 \\ 0 & s_{3,2} & s_{3,3} & s_{3,4} \\ 0 & 0 & s_{4,3} & s_{4,4} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix}$$

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We can solve the blue part and obtain μ_1, μ_2, the cyan part and obtain μ_3, μ_4.

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For $j = 1, 2, 3, 4$, from μ_j we can enter in our "best neighborhood" of λ_j using bisection:

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set $a_j = 0$ and $b_j = \mu_j$

$\#$ Start bisection

set $x = \mu_j$

IF $\kappa(x) < j$

THEN set $a_j = x$

ELSE set $b_j = x$

IF THEN

ELSE go to $\#$

Ideas:

Hopefully we have

$$\begin{aligned} &x_0^1, L(x_0^1), L(L(x_0^1)), \cdots \rightsquigarrow \lambda_1 \\ &x_0^2, L(x_0^2), L(L(x_0^2)), \cdots \rightsquigarrow \lambda_2 \\ &x_0^3, L(x_0^3), L(L(x_0^3)), \cdots \rightsquigarrow \lambda_3 \\ &x_0^4, L(x_0^4), L(L(x_0^4)), \cdots \rightsquigarrow \lambda_4 \end{aligned}$$

Split

Consider $(\hat{T}, \hat{S})$ with

$$\hat{T} = \begin{bmatrix} T_0 & 0 \\ 0 & T_1 \end{bmatrix}$$
$$\hat{S} = \begin{bmatrix} S_0 & 0 \\ 0 & S_1 \end{bmatrix}$$

and let be

$$\hat{\lambda}_1 \leq \hat{\lambda}_2 \leq \cdots \leq \hat{\lambda}_n$$

eigenvalues of $(\hat{T}, \hat{S})$, then

Split

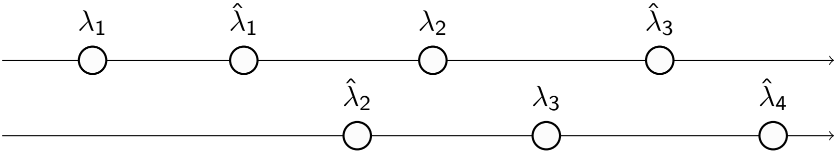
Teo (A sort of "interlacing")

$$\begin{aligned} -\infty < &\lambda_1 \leq \hat{\lambda}_1 \\ \hat{\lambda}_{i-1} \leq &\lambda_i \leq \hat{\lambda}_{i+1} \\ \hat{\lambda}_n \leq &\lambda_n < \infty \end{aligned}$$

with $i = 2, 3, \ldots, n-1$.

Remark

It's possible that



Split

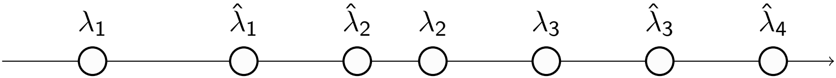
Teo (A sort of "interlacing")

$$\begin{aligned} -\infty &< \lambda_1 \leq \hat{\lambda}_1 \\ \hat{\lambda}_{i-1} &\leq \lambda_i \leq \hat{\lambda}_{i+1} \\ \hat{\lambda}_n &\leq \lambda_n < \infty \end{aligned}$$

with $i = 2, 3, \ldots, n-1$.

Remark

It's possible that



Split

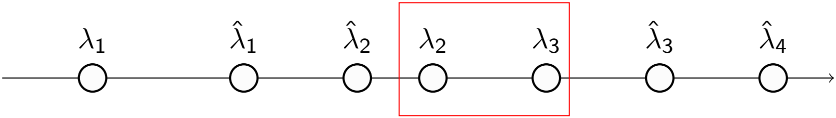
Teo (A sort of "interlacing")

$$
\begin{aligned}
-\infty <& \lambda_1 \leq \hat{\lambda}_1 \\
\hat{\lambda}_{i-1} \leq& \lambda_i \leq \hat{\lambda}_{i+1} \\
\hat{\lambda}_n \leq& \lambda_n < \infty
\end{aligned}
$$

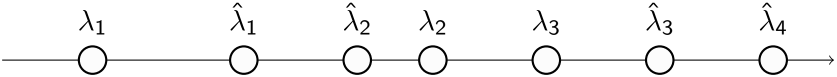
with $i = 2, 3, \ldots, n-1$.

Remark

It's possible that



Split



So we can't

Grazie per l'attenzione.