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 $Tv = \lambda Sv$, 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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(T, S) is an *unreducible pencil* if $t^2_{i,i+1} + s^2_{i,i+1} \neq 0$ 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
```

Listing 1: T, S as couple of array

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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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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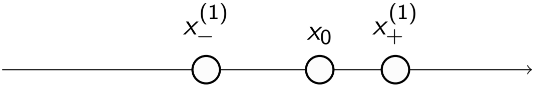

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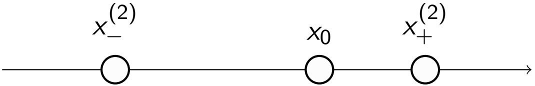

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Fast and secure iterative method

Def (Laguerre's iteration)

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

$$x_+^{(k)} = L_+^k(x) = L_+(L_+(\ldots(x_0)))$$
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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* $\{x_-^{(k)}\}_{k=1,\dots}$ *converge monotonically in asymptotically cubic rate to* λ_m.

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*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 $\{x_+^{(k)}\}_{k=1,\dots}$ conv. mon. cubic to λ_{m+1}

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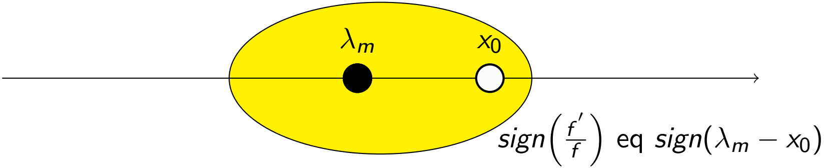

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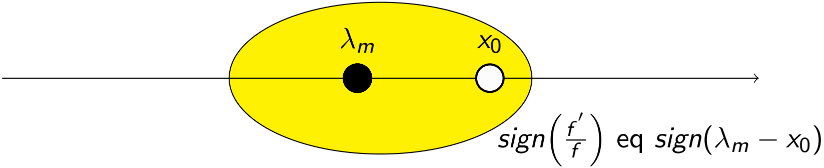

The Laguerre's method is fast.

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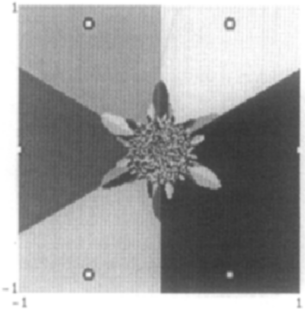
Fast and secure iterative method

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 [**?**]) 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 [?], 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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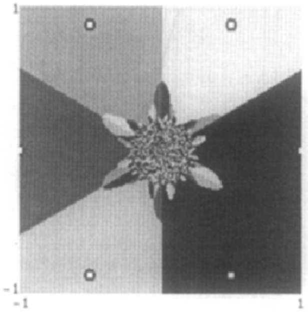

So if we want to solve the Generalized Eigenvalues Problem with $T, S \in \mathbb{C}$ we have great problems to place the starting point if $n > 4$.

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. $n = 4$)

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

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

$$= g \begin{bmatrix} a & b & 0 \\ b & c & d \\ 0 & d & e \end{bmatrix} - f^2 \begin{bmatrix} a & b \\ b & c \end{bmatrix}$$

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Three term recurrence

Remark

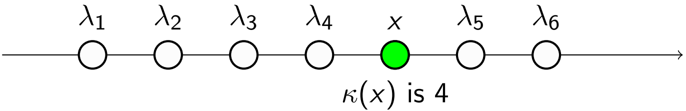
If $x = \lambda$ then $\rho_n(\lambda) = \mathcal{F}_{(T_n, S_n)}(\lambda) = f(\lambda)$

Remark (important results with proof in Appendice)

$\rho_0, \rho_1, \ldots, \rho_n$ is 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 $f^{'} = \rho_{n}^{'}, f^{''} = \rho_{n}^{''}$.

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

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So*

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

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

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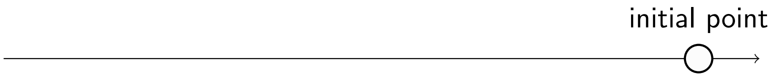
Example



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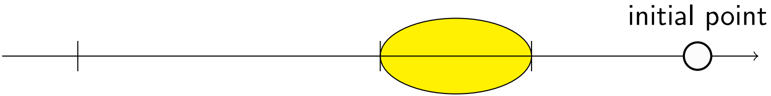
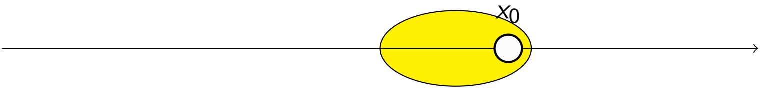


with bisection we can find the neighbourhood of λ_m

Example

we can now use the Laguerre's iteration



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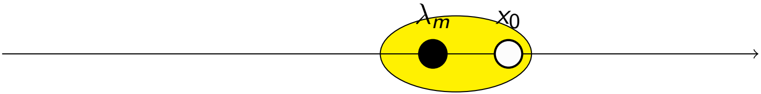

What we really calculate is...

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We also define $\eta_i = \frac{\rho_i^{'}}{\rho_i}, \zeta_i = \frac{\rho_i^{''}}{\rho_i}$ for $i = 0, 1, \ldots, n$ and we finally we have

$$\kappa(x) = \text{ number of negative terms in } \{\xi_i\}_{i=1}^{n}$$

$$-\frac{f^{'}(x)}{f(x)} = \eta_n$$

$$\frac{f^{''}(x)}{f(x)} = \zeta_n$$

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So we have to calculate three three-term-recurrences.

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So we have to calculate three three-term-recurrences.
* Total $\leq 2 + 38n$ multiplications.
For every step in Laguerre's iteration we have to do $2 + 7 + 38n$ (at most) multiplications and 1 square root extraction. Because the convergence is cubic we hope in a small number of iteration.

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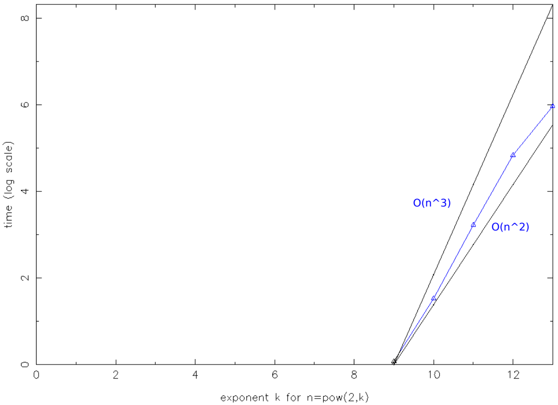
Complexity

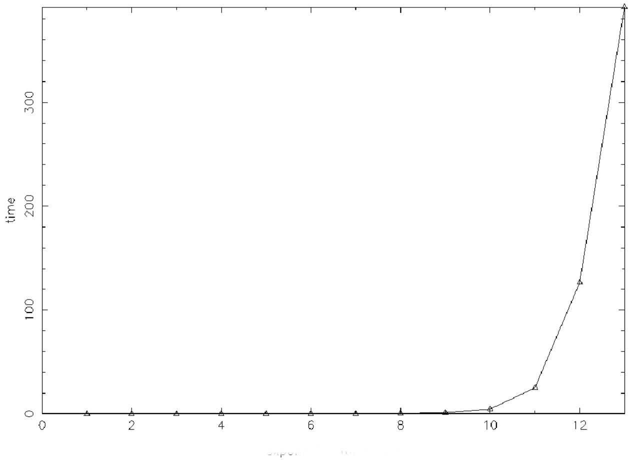
*Author's prevision: $O(n^2)$.
With (I, S) and eigenvalues between 0.5 and 1.5 we have



*They use $n < 100$,
my experiment ends up with $n = 2^{13} = 8192$.

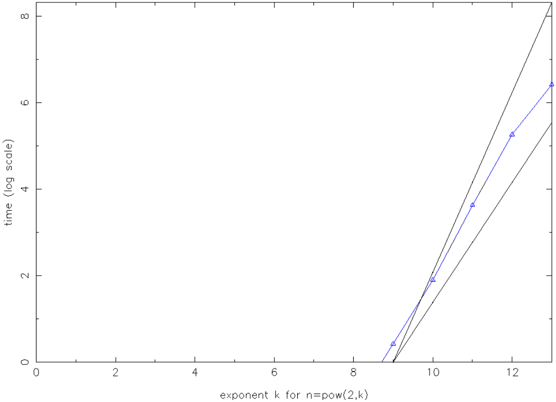
Complexity

And in linear scale:



Complexity

With $T = (a_i, 1, a_i), S = (b_i, c_i, b_i)$ and a_i, b_i random numbers such that $|a_i| \leq 10^{-3}, |b_i| \leq 10^{-1}, c_i = i10^{-1} + |2b_i|$ we have



We can appreciate little differences between $T = (0, 1, 0)$ and $T = (a_i, 1, a_i)$

Error Analysis

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Teo

$$fl[f(x)] = fl[det[T - xS]] = (1+\gamma)det[(T+\delta T) - x(S+\delta S)]$$

where $|\gamma| \leq n\epsilon$*, with* ϵ *machine precision, and both* δT *and* δS *are symmetric tridiagonal matrices satisfying entrywise inequalities* $|\delta T|_\infty \leq 2.51\epsilon|T|_\infty + \sqrt{\epsilon_u}$, $|\delta S|_\infty \leq 3.51\epsilon|S|_\infty$*, where* ϵ_u *is the underflow threshold (in double precision is* 10^{-308}*).*

Error Analysis

We are interested not only in $\mathrm{fl}[f(x)] = \mathrm{fl}\Big[\prod_{i=1}^{n} \mathrm{fl}[\xi_i]\Big]$, but also in $\mathrm{fl}[\eta_n]$ and $\mathrm{fl}[\zeta_n]$, because we use these three value to calculate the Laguerre's iteration.

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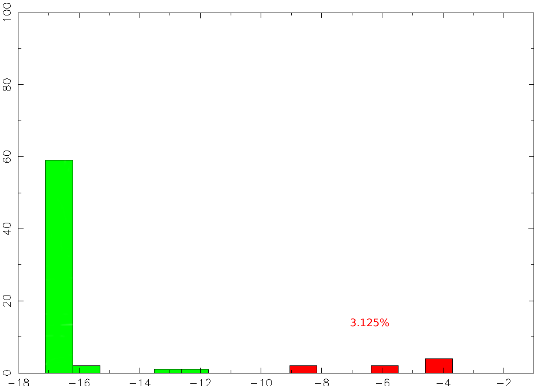
The authors doesn't report this important aspect of analysis.
($\mathrm{fl}[\eta_n], \mathrm{fl}[\zeta_n]$ suffer from similar problems and have similar backward analysis, but they are -in partucular ζ_n- enourmous in magnitude, sometimes this can cause trobles)

Exponent of absolute error ($n = 256$)

With (I, S) and eigenvalue between 0.5 and 1.5 we have



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Laguerre's iteration break the monotonic convergence!
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I think the problem is in κ, η_n, ζ_n.
Sometimes, when $|\lambda_j - x_0| \leq 10^{-4}$ and (T, S) have small elements, we can have troubles.
If we compare $\kappa(x_i)$ and the same number obtained with *inertia* for $|\lambda_j - x_i| \leq 10^{-i}$ and $i = 1, \ldots, 16$ we have

Searching initial points

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.

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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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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

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

$^*\alpha = s_{2,2}t_{1,1} - s_{1,2}t_{1,2}, \beta = -s_{1,2}t_{1,2} + s_{1,1}t_{2,2}$
$\gamma = -s_{1,2}t_{1,2} + s_{1,1}t_{1,2}, \delta = s_{1,1}s_{2,2} - s_{1,2}^2$.

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.

Ideas:

From μ_j we can enter in our "neighbourhood" of λ_j using simple bisection:

---

*This is the most important part of our method.
Authors of [**?**, **?**] doesn't explain this point. ▸ code

Ideas:

From μ_j we can enter in our "neighbourhood" of λ_j using simple bisection:

Speudocode:

set $a_j = 0$ and $b_j = \mu_j$
set $x = \mu_j$
\# IF $\kappa(x) < j$
THEN set $a_j = x$
ELSE set $b_j = x$
*IF $-\frac{f^{'}(x)}{f(x)} = sign(\lambda_j - x)$
THEN stop
ELSE set $x = \frac{b_j - a_j}{2}$ and go to #

*This is the most important part of our method. Authors of [?, ?] doesn't explain this point.

code

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

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

with T_0, T_1, S_0, S_1 symmetric tridiagonal, and let be

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

eigenvalues of $(\hat{T}, \hat{S})$, they are what we call $\mu_1, \ldots, \mu_n$.

Split

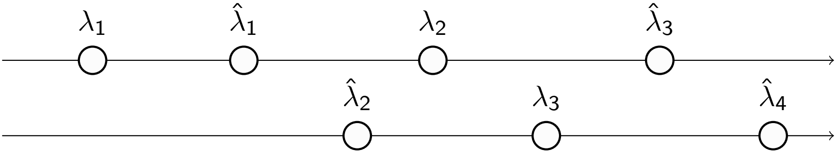
Teo (A sort of “interlacing” with ▸ proof)

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

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

Remark

It’s possible that



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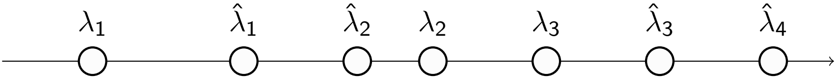

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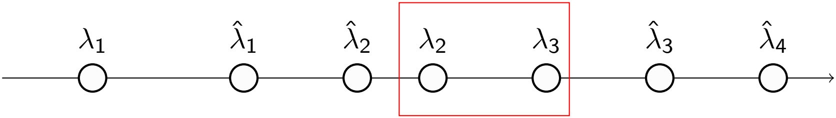

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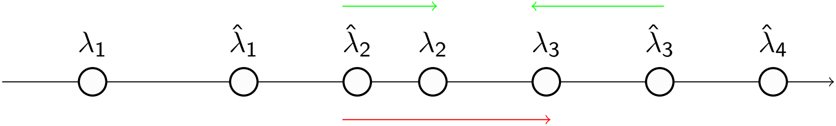
Our method is monotonic



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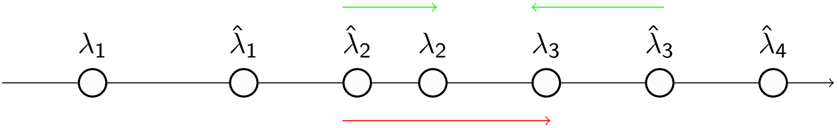

We can reach λ_2 only from $\hat{\lambda}_2$, moving from left to right (and similar λ_3 only from $\hat{\lambda}_3$, moving from right to left).

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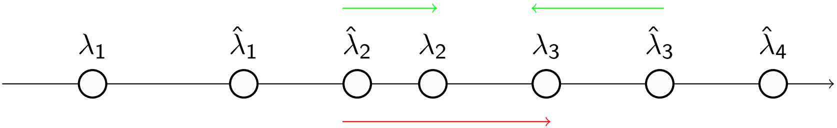

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If $|\lambda_2 - \lambda_3| \leq 10^{-14}$ we can have trobles.

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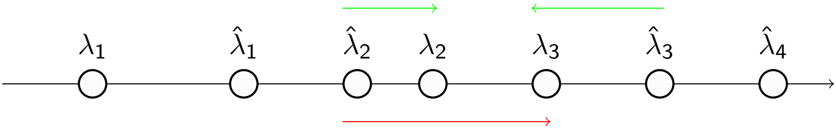

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Luckily we also have a *multiplicity estimator* (called EstMlt) that works only with $\hat{\lambda}_1, \ldots, \hat{\lambda}_n$.

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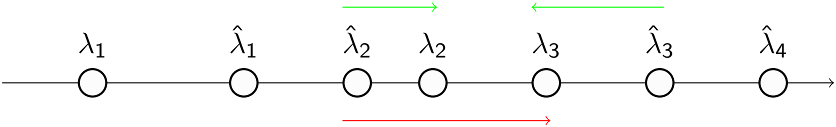

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Luckily we also have a *multiplicity estimator* (called EstMlt) that works only with $\hat{\lambda}_1, \ldots, \hat{\lambda}_n$.
If $mlt = 2$ then we consider $\lambda_2 = \lambda_3$, i.e. we said that λ_2 has multiplicity 2.

EstMlt

We have $j, x,$ $\text{sgn}\left(-\frac{f^{'}(x)}{f(x)}\right)$ and $\hat{\lambda}_1, \ldots, \hat{\lambda}_n$ as *INPUT*.

Speudocode:

```
mlt = 1
do k = 1, ...
m = j + k sgn( - f'(x)/f(x) )
if m ≤ 0 then
something goes wrong
go to #
end if
if |λ̂_j − λ̂_m| ≤ 0.01|λ̂_j − x| then
mlt = mlt + 1
else go to #
end if
end do
# stop
```

Appendice A: proof of Laguerre's convergence

According to [**?**, p.444] we can write

$$x_{\pm}^{(k+1)} = x_{\pm}^{(k)} - \frac{nf}{f' \pm H^{\frac{1}{2}}}$$

$$H = (n-1)^2 (f')^2 - n(n-1) f f''$$

If we choose the sign so that the $|f' \pm H^{\frac{1}{2}}|$ has the larger absolute value then we can approx $x_{\pm}^{(k+1)} - \lambda_m$ as

$$x_{\pm}^{(k+1)} - \lambda_m \approx \frac{1}{2}(x_{\pm}^{(k)} - \lambda_m)^3 \frac{(n-1)\Sigma_2' - (\Sigma_1')^2}{n-1}$$

$$\Sigma_2' = \sum_{i \neq n} \frac{1}{(\lambda_m - \lambda_i)^2}$$

$$\Sigma_1' = \sum_{i \neq n} \frac{1}{\lambda_m - \lambda_i}$$

Appendice A: proof of Laguerre's convergence

So we have convergence and $x_{\pm}^{(k+1)} - \lambda_m \approx$ number $(x_{\pm}^{(k)} - \lambda_m)^3$ tell us that the convergence is cubic.

back

Appendice B: proof of property about Sturm sequence

back

Appendice B: interlacing

Def

For $\alpha \in [0,1]$ we define the pencil
$\big(T(\alpha), S(\alpha)\big) := \big((1-\alpha)\hat{T} + \alpha T, (1-\alpha)\hat{S} + \alpha S\big)$.

Lemm

$\big(T(\alpha), S(\alpha)\big)$ is a symmetric definite pencil for each $\alpha \in [0,1]$.

Calling $\lambda_1(\alpha) \le \lambda_2(\alpha) \le \cdots \le \lambda_n(\alpha)$ the n real eigenvalues of the pencil $\big(T(\alpha), S(\alpha)\big)$ we have

Lemm

Each $\lambda_i(\alpha)$ is a continuous function of $\alpha \in [0,1]$.

Appendice B: interlacing

Teo (A sort of "interlacing")

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\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
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$$

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

Appendice B: interlacing

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Classic interlacing still works for $-\infty < \lambda_1 \leq \hat{\lambda}_1$ and for $\hat{\lambda}_n \leq \lambda_n < \infty$.

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Classic interlacing still works for $-\infty < \lambda_1 \leq \hat{\lambda}_1$ and for $\hat{\lambda}_n \leq \lambda_n < \infty$.

We have to proove that $\lambda_i \geq \hat{\lambda}_{i-1}$ (and similar $\lambda_i \leq \hat{\lambda}_{i+1}$).

Appendice B: interlacing

(Proof by contradiction) if we consider $\lambda_i < \hat{\lambda}_{i-1}$ for some $i \in \{2, 3, \ldots, n-1\}$ (that, in our new writing, is $\lambda_i(1) < \lambda_{i-1}(0)$ because all $\lambda_j(1)$ are eigenvalues of (T, S) and all $\lambda_j(0)$ are eigenvalues of $(\hat{T}, \hat{S})$) then

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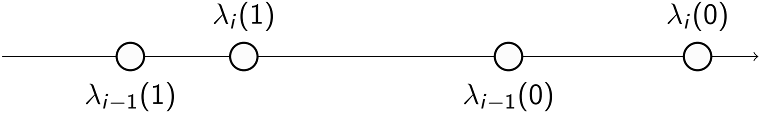

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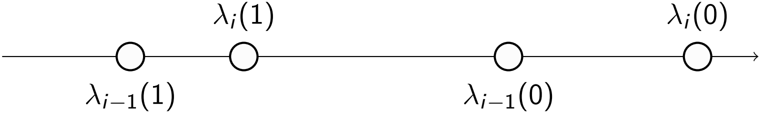

in symbols: $\lambda_{i-1}(1) \leq \lambda_i(1) < \lambda_{i-1}(0) \leq \lambda_i(0)$.

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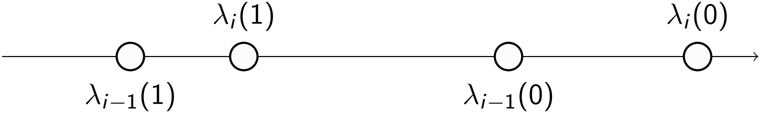
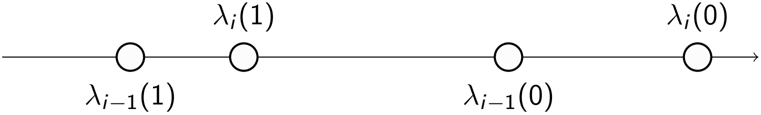


in symbols: $\lambda_{i-1}(1) \leq \lambda_i(1) < \lambda_{i-1}(0) \leq \lambda_i(0)$.
For all $\tilde{\lambda} \in [\lambda_i(1), \lambda_{i-1}(0)]$ we can find α_i, α_{i-1} such as $\tilde{\lambda} = \lambda_i(\alpha_i) = \lambda_{i-1}(\alpha_{i-1})$.

Appendice B: interlacing



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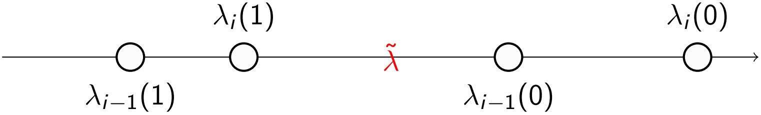

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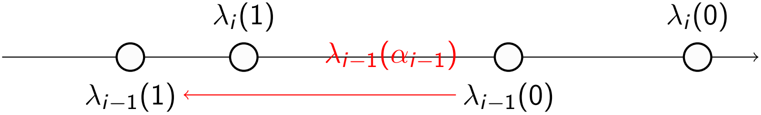

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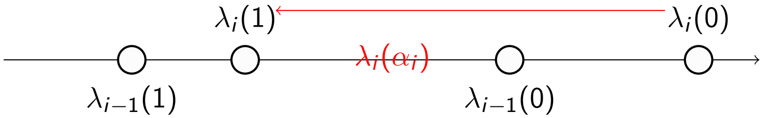

Appendice B: interlacing

$$H(\alpha, \lambda) := det[T(\alpha) - \lambda S(\alpha)] =$$

$$\begin{bmatrix} \ddots & \ddots & & \\ \ddots & t_{k,k} - \lambda s_{k,k} & \alpha(t_{k,k+1} - s_{k,k+1}) & \\ & \alpha(t_{k,k+1} - s_{k,k+1}) & t_{k+1,k+1} - \lambda s_{k+1,k+1} & \ddots \\ & & \ddots & \ddots \end{bmatrix}$$

Appendice B: interlacing

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So

$$H(\alpha, \lambda) = p(\lambda) + \alpha^2 q(\lambda)$$

Appendice B: interlacing

If $q(\tilde{\lambda}) \neq 0$ then $\tilde{\alpha} = +\sqrt{H(\tilde{\alpha}, \tilde{\lambda}) - \frac{p(\tilde{\lambda})}{q(\tilde{\lambda})}} \in [0, 1]$.

only one solution in α.

Appendice B: interlacing

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But we have, for all $\tilde{\lambda}$, two solution in α, named α_i and α_{i-1}.

Appendice B: interlacing

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But we have, for all $\tilde{\lambda}$, two solution in α, named α_i and α_{i-1}.
Then $q(\lambda) = 0$ for all $\tilde{\lambda}$.
We have $\tilde{\lambda}$ eigenvalue of $(\hat{T}, \hat{S})$, for all $\tilde{\lambda}$ and $(\hat{T}, \hat{S})$ have exactly n eigenvalues.

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conctraddiction

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Appendice D: code

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Grazie per l'attenzione.