

# An Algorithm for the Generalized Symmetric Tridiagonal Eigenvalue Problem

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# Generalized Eigenvalue Problem

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We consider *only*

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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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*exemplum gratie:*

**Bad**

$$\begin{aligned} T &= I, S = 0 \\ T &= I, S = I \end{aligned}$$

**Good**

$$\begin{aligned} T &= I, S = \text{trid}(-1, 2, -1) \\ T &= \text{trid}(-1, 2, -1), S = \text{trid}(-1, 2, -1) \\ T &= \text{trid}(\text{rnd}_{\text{sub}}, \text{rnd}_{\text{diag}}, \text{rnd}_{\text{sub}}), S = I, \\ &\text{with } \text{rnd}_{\text{sub}} \text{ random number } \neq 0. \end{aligned}$$

# Matrix storin

$$T = \text{trid}(\text{sub}, \text{diag}, \text{super})$$

But  $T$  is symmetric, so  $\text{sub} = \text{super}$ . We define and use

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

Listing 1:  $T, S$  as couple of array

with  $T(:,0) = \text{diag}$  and  $T(:,1) = \text{super}$ .

## Remark

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

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Bolzano's Theorem tell us that there are two zeros of  $g_u$  between  $\lambda_m$  and  $\lambda_{m+1}$ . 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:

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

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

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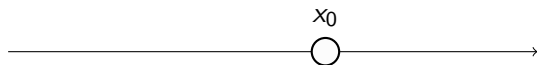
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We will see that “only” with the **symmetric tridiagonal** condition we can have **derivatives of determinats**.

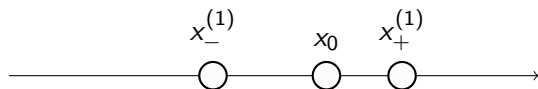
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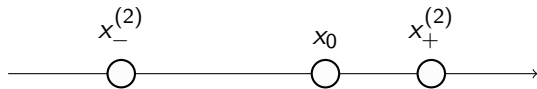
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## Def (Laguerre's iteration)

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

$$x_+^{(k)} = L_+^k(x) = L_+(L_+(\dots(x_0)))$$

$$x_-^{(k)} = L_-^k(x) = L_-(L_-(\dots(x_0)))$$

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

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So Laguerre's method is **secure**.

# Fast and secure iterative method

We also have an important property:

Teo

*If we choose\*  $\lambda_m < x_0$  s.t.  $\text{sign}\left(\frac{f'(x_0)}{f(x_0)}\right) = \text{sign}(\lambda_m - x_0)$  then*

*$\{x_-^{(k)}\}_{k=1,\dots}$  converge monotonically in asymptotically cubic rate to  $\lambda_m$ .*

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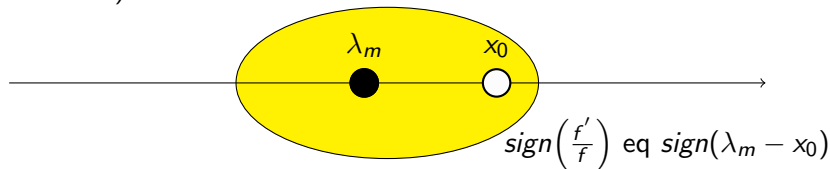
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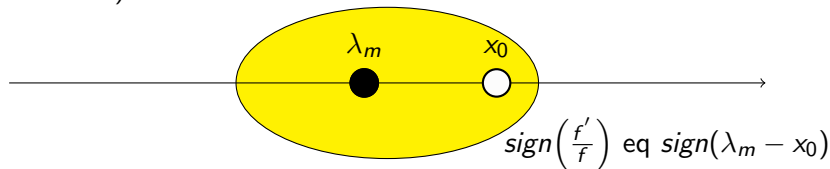
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The Laguerre's method is **fast**.

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# Fast and secure iterative method

It's clear that we need a powerful method to obtain  $x_0$  and an algorithm to estimate  $mlt(\lambda_m)$ .

*Overestimate*  $mlt(\lambda_m)$  (as we can read in [?]) causes no trouble, so the most important aspects of our calculation are:

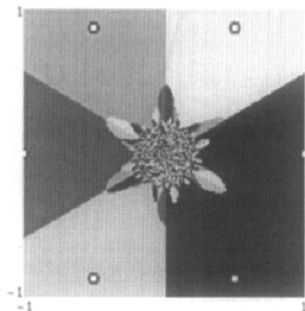
Good  $x_0$ .

Good evaluation of  $L_{\pm}(x)$ .



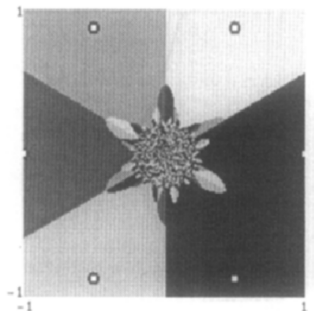
## Complex case (little digression)

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  $z_0$ .  
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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

$$\rho_0 := 1, \rho_1 := t_{1,1} - x s_{1,1}$$

$$\rho_i := (t_{i,i} - x s_{i,i}) \rho_{i-1} - (t_{i-1,i} - x s_{i-1,i})^2 \rho_{i-2}, \quad i = 2, 3, \dots, n$$

# Three term recurrence

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

$$T_4 - \lambda S_4 = \begin{pmatrix} a & b & 0 & 0 \\ b & c & d & 0 \\ 0 & d & e & f \\ 0 & 0 & f & g \end{pmatrix}$$

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

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## Remark

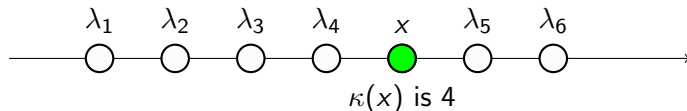
If  $x = \lambda$  then  $\rho_n(\lambda) = \mathcal{F}_{(T_n, S_n)}(\lambda) = f(\lambda)$

Remark ( important results with [▶ proof](#) in Appendice)

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

$\kappa(x) := \#$  eigenvalues less than  $x$

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



# Three term recurrence

Obviously  $f' = \rho'_n, f'' = \rho''_n$ .

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

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

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# Example

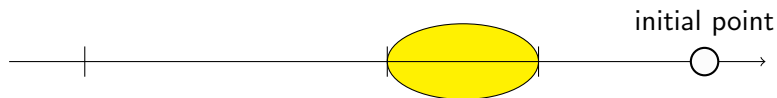
initial point



## Example



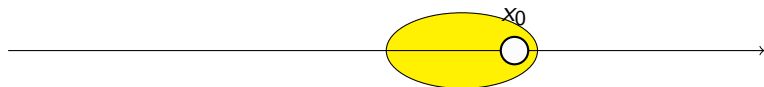
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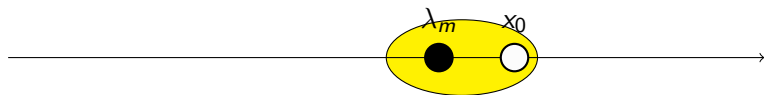
with **bisection** we can find the neighbourhood of  $\lambda_m$

## Example

we can now use the Laguerre's iteration



# Example



## What we really calculate is...

We **define**  $\xi_i = \frac{\rho_i}{\rho_{i-1}}$  for  $i = 2, \dots, n$  and we have  $\rho_i = \prod_{k=1}^n \xi_k$ .

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We also **define**  $\eta_i = \frac{\rho_i'}{\rho_i}$ ,  $\zeta_i = \frac{\rho_i''}{\rho_i}$  for  $i = 0, 1, \dots, n$  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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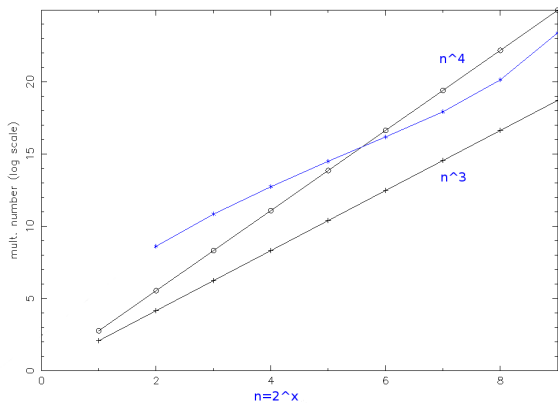
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For every step in Laguerre's iteration we have to do  $2 + 7 + 38n$  multiplications and 1 square root extraction. Because the convergence is cubic we **hope** in a small number of iteration.

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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  $\epsilon$  machine precision, and both  $\delta T$  and  $\delta S$  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  $\epsilon_u$  is the underflow threshold (in double precision is  $10^{-308}$ ).

# Error Analysis

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



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# Searching initial points

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

## Ideas:

If  $n = 1$  we have  $t \cdot v = \lambda \cdot s \cdot v$ .  $s \neq 0$ , so  $\lambda = \frac{t}{s}$ .

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

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

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

---

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

## Ideas:

And if  $n = 4$ ?

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

# Ideas:

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# Ideas:

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We can solve the blue part and obtain  $\mu_1, \mu_2$ , the cyan part and obtain  $\mu_3, \mu_4$ .

# Ideas:

From  $\mu_j$  we can enter in our “neighbourhood” of  $\lambda_j$  using simple [bisection](#):

---

\*This is the most important part of our method.

Authors of [?, ?] doesn't explain this point.

▶ code

# Ideas:

From  $\mu_j$  we can enter in our “neighbourhood” of  $\lambda_j$  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  $-\frac{f'(x)}{f(x)} = \text{sign}(\lambda_j - x)$   
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:

$$x_0^1, L(x_0^1), L(L(x_0^1)), \dots \rightsquigarrow \lambda_1$$

$$x_0^2, L(x_0^2), L(L(x_0^2)), \dots \rightsquigarrow \lambda_2$$

Hopefully we have

$$x_0^3, L(x_0^3), L(L(x_0^3)), \dots \rightsquigarrow \lambda_3$$

$$x_0^4, L(x_0^4), L(L(x_0^4)), \dots \rightsquigarrow \lambda_4$$

# 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

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

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

# Split

Teo (A sort of “interlacing” with [proof](#))

$$-\infty < \lambda_1 \leq \hat{\lambda}_1$$

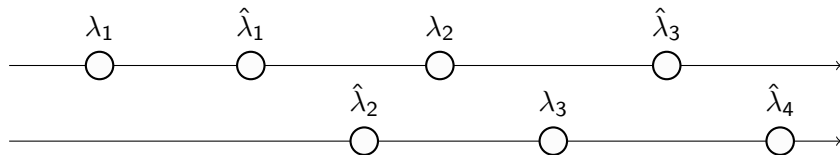
$$\hat{\lambda}_{i-1} \leq \lambda_i \leq \hat{\lambda}_{i+1}$$

$$\hat{\lambda}_n \leq \lambda_n < \infty$$

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

## Remark

It's possible that



# Split

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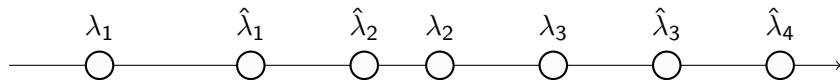
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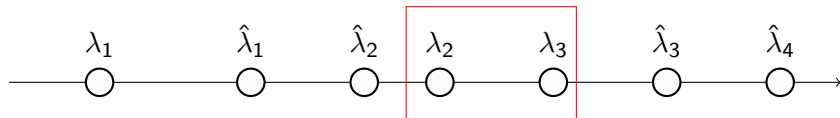
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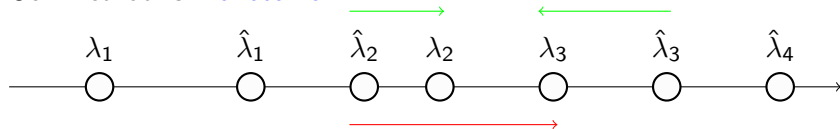
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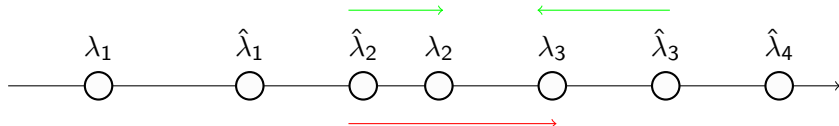
Our method is **monotonic**



# Split

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Our method is **monotonic**

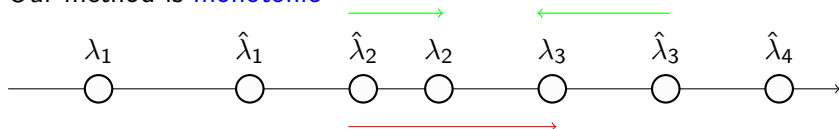


We can reach  $\lambda_2$  only from  $\hat{\lambda}_2$ , moving from left to right (and similar  $\lambda_3$  only from  $\hat{\lambda}_3$ , moving from right to left).

# Split

## Remark

Our method is **monotonic**



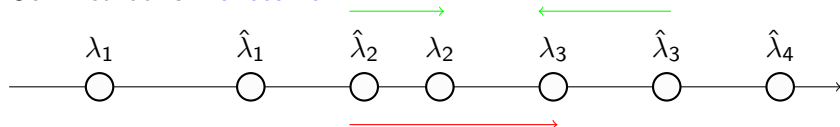
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If  $|\lambda_2 - \lambda_3| \leq 10^{-14}$  we can have troubles.

# Split

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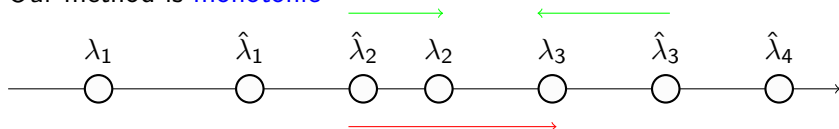
If  $|\lambda_2 - \lambda_3| \leq 10^{-14}$  we can have troubles.

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

# Split

## Remark

Our method is **monotonic**



We can reach  $\lambda_2$  only from  $\hat{\lambda}_2$ , moving from left to right (and similar  $\lambda_3$  only from  $\hat{\lambda}_3$ , moving from right to left).

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

If  $m/t = 2$  then we consider  $\lambda_2 = \lambda_3$ , i.e. we said that  $\lambda_2$  has multiplicity 2.

# EstMlt

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

**Speudocode:**

```
mlt = 1
do k = 1, ...
  m = j + k  $\operatorname{sgn}\left(-\frac{f'(x)}{f(x)}\right)$ 
  if m ≤ 0 then
    something goes wrong
  go to #
end if
if  $|\hat{\lambda}_j - \hat{\lambda}_m| \leq 0.01|\hat{\lambda}_j - x|$  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

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

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  $x_{\pm}^{(k+1)} - \lambda_m \approx \text{number } (x_{\pm}^{(k)} - \lambda_m)^3$   
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

$$(T(\alpha), S(\alpha)) := ((1 - \alpha)\hat{T} + \alpha T, (1 - \alpha)\hat{S} + \alpha S).$$

### Lemm

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

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

### Lemm

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

## Appendice B: interlacing

Teo (A sort of “interlacing”)

$$-\infty < \lambda_1 \leq \hat{\lambda}_1$$

$$\hat{\lambda}_{i-1} \leq \lambda_i \leq \hat{\lambda}_{i+1}$$

$$\hat{\lambda}_n \leq \lambda_n < \infty$$

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

## 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 prove 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  $i \in \{2, 3, \dots, n-1\}$  (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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## Appendix B: interlacing

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

## Appendix B: interlacing

(Proof by contradiction) if we consider  $\lambda_i < \hat{\lambda}_{i-1}$  for some  $i \in \{2, 3, \dots, n-1\}$  (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



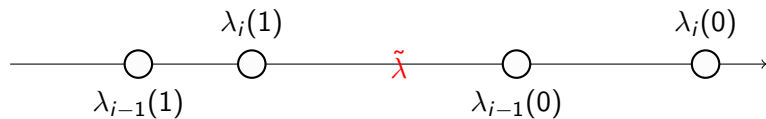
in symbols:  $\lambda_{i-1}(1) \leq \lambda_i(1) < \lambda_{i-1}(0) \leq \lambda_i(0)$ .

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

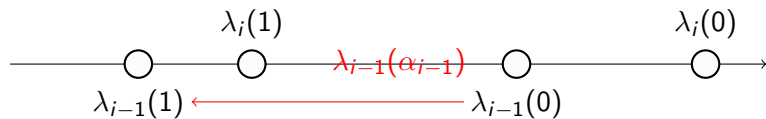
## Appendice B: interlacing



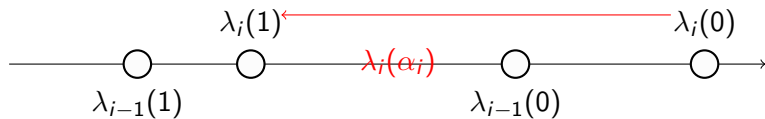
## Appendice B: interlacing



## Appendice B: interlacing



## Appendice B: interlacing



## Appendix B: interlacing

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

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

## Appendice B: interlacing

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

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

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  $\alpha$ .

## Appendice B: interlacing

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

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But we have, **for all**  $\tilde{\lambda}$ , **two** solution in  $\alpha$ , named  $\alpha_j$  and  $\alpha_{j-1}$ .

## Appendice B: interlacing

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But we have, **for all**  $\tilde{\lambda}$ , **two** solution in  $\alpha$ , named  $\alpha_j$  and  $\alpha_{j-1}$ .

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.

## Appendice B: interlacing

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**contradiction**

▶ back

# Appendice D: code

► back



Grazie per l'attenzione.