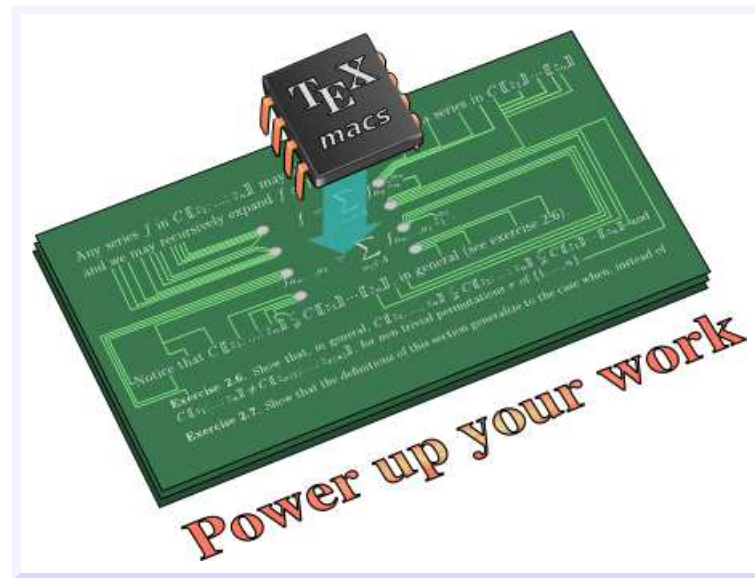


Efficient certification of numeric solutions to eigenproblems

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1 2 3 4 5 6 7 8 9 10 11 12

Single eigenvalues

Given M , find T with

$$T^{-1}MT = D = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$$

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Multiple eigenvalues

Given M , find T with

$$T^{-1}MT = D = \begin{pmatrix} \Lambda_1 & & \\ & \ddots & \\ & & \Lambda_p \end{pmatrix}$$

$$\Lambda_k = \begin{pmatrix} \lambda_{i_k} & * & * \\ & \ddots & * \\ & & \lambda_{i_k} \end{pmatrix}$$

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$$\Lambda_k = \begin{pmatrix} \lambda_{i_k} & & \\ & \ddots & \\ & & \lambda_{i_{k+1}-1} \end{pmatrix} + E_k, \quad \lambda_{i_k} \approx \dots \approx \lambda_{i_{k+1}-1}, \quad E_k \text{ "small"}$$

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Single eigenvalues

$$M = \begin{pmatrix} M_{1,1} & \cdots & M_{1,n} \\ \vdots & & \vdots \\ M_{n,1} & \cdots & M_{n,n} \end{pmatrix} = \begin{pmatrix} \mathcal{B}(c_{1,1}, r_{1,1}) & \cdots & \mathcal{B}(c_{1,n}, r_{1,n}) \\ \vdots & & \vdots \\ \mathcal{B}(c_{n,1}, r_{n,1}) & \cdots & \mathcal{B}(c_{n,n}, r_{n,n}) \end{pmatrix}$$

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Find

$$T = \begin{pmatrix} T_{1,1} & \cdots & T_{1,n} \\ \vdots & & \vdots \\ T_{n,1} & \cdots & T_{n,n} \end{pmatrix} = \begin{pmatrix} \mathcal{B}(c'_{1,1}, r'_{1,1}) & \cdots & \mathcal{B}(c'_{1,n}, r'_{1,n}) \\ \vdots & & \vdots \\ \mathcal{B}(c'_{n,1}, r'_{n,1}) & \cdots & \mathcal{B}(c'_{n,n}, r'_{n,n}) \end{pmatrix},$$

such that for every $M \in \mathcal{M}$ (e.g. $|M_{i,j} - c_{i,j}| \leq r_{i,j}$), there exists a $T \in \mathcal{T}$ with

$$T^{-1} M T = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$$

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Main goal

Given an approximate numerical solution to an eigenproblem, find an efficient algorithm for certifying the solution.

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Ideally speaking

Only use a finite number of matrix multiplications at the current working precision.

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Only use a finite number of matrix multiplications at the current working precision.

Asymptotic complexity

Two $n \times n$ matrices with p -bit integer entries can be multiplied in time

$$\text{MM}(n, p) = O(n^2 I(p) + n^\omega p 2^{O(\lg^* p - \lg^* n)} I(\lg n) / \lg n) \quad [\text{Harvey-vdH 2014}].$$

$I(p)$: cost of p -bit integer multiplication, $O(n^\omega)$: cost of $n \times n$ matrix multiplication

$$I(p) = O(p \lg p K^{\lg^* p}), \quad K \leq \begin{matrix} 6 \\ 4^* \end{matrix} \quad \begin{matrix} [\text{Harvey 2017}] \\ [\text{Harvey-vdH-Lecerf 2014}] \end{matrix}$$

$$\omega < 2.3728639 \quad [\text{LeGall 2014}]$$

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Given an approximate numerical solution to an eigenproblem, find an efficient algorithm for certifying the solution.

Ideally speaking

Only use a finite number of matrix multiplications at the current working precision.

Practical complexity

Two $n \times n$ matrices with p -bit integer entries can be multiplied in time

$$\text{MM}(n, p) = O(n^3 p).$$

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Individual eigenvectors for single eigenvalues

$O(n^4 p)$

- T. Yamamoto 1980
- Rump 1989

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Individual eigenvectors for single eigenvalues

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Individual eigenvectors for multiple eigenvalues

 $O(n^4 p)$

- Dongarra, Moler, Wilkinson 1983
- Rump 2001
- Graillat, Trébuchet 2009
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All eigenvectors, no multiple eigenvalues

 $O(n^3 p)$

- vdH-Mourrain-Trébuchet 2009
- Miyajima 2010 (eigenvalues only)

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Assume that

$$M = D + H, \quad D = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}.$$

Then the solution is of the form $T = 1 + E$, with

$$(1 + E)^{-1} (D + H) (1 + E) = D + \Delta$$

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$$DE - ED \approx \Delta - H$$

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Now $DE - ED$ equals

$$\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} \begin{pmatrix} E_{1,1} & \cdots & E_{1,n} \\ \vdots & & \vdots \\ E_{n,1} & \cdots & E_{n,n} \end{pmatrix} - \begin{pmatrix} E_{1,1} & \cdots & E_{1,n} \\ \vdots & & \vdots \\ E_{n,1} & \cdots & E_{n,n} \end{pmatrix} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$$

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$$\begin{pmatrix} 0 & (\lambda_1 - \lambda_2) E_{1,2} & & (\lambda_1 - \lambda_n) E_{1,n} \\ (\lambda_2 - \lambda_1) E_{2,1} & 0 & & \\ \vdots & & \ddots & (\lambda_{n-1} - \lambda_n) E_{n-1,n} \\ (\lambda_n - \lambda_1) E_{n,1} & \dots & (\lambda_n - \lambda_{n-1}) E_{n,n-1} & 0 \end{pmatrix}$$

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We thus obtain a simple approximate solution

$$\Delta_{i,i} = H_{i,i}$$

$$E_{i,j} = \frac{H_{i,j}}{\lambda_j - \lambda_i}, \quad (i \neq j)$$

1 2 3 4 5 6 7 8 9 10 11 12

We have reduced our problem

$$T^{-1}(D + H)T = \text{diagonal matrix}$$

$$\downarrow$$

$$(T')^{-1}(D' + H')T' = \text{diagonal matrix}',$$

where

$$E_{i,j} = H_{i,j} / (\lambda_j - \lambda_i)$$

$$M' = (1 + E)^{-1}(D + H)(1 + E)$$

$$D' = \text{diagonal part of } M'$$

$$H' = \text{off-diagonal part of } M'$$

$$T = (1 + E)T'$$

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$$\begin{aligned}
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 &\quad \downarrow \\
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 M' &= (1 + E)^{-1}(D + H)(1 + E) \\
 D' &= \text{diagonal part of } M' \\
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 T &= (1 + E)T'
 \end{aligned}$$

Theorem. *This "Newton iteration" converges quadratically to a solution.*

1 2 3 4 5 6 7 8 9 10 11 12

We have reduced our problem

$$\begin{aligned} T^{-1}(D + H)T &= \text{diagonal matrix} \\ &\downarrow \\ (T')^{-1}(D' + H')T' &= \text{diagonal matrix}' \end{aligned}$$

where

$$\begin{aligned} E_{i,j} &= H_{i,j} / (\lambda_j - \lambda_i) \\ M' &= (1 + E)^{-1}(D + H)(1 + E) \\ D' &= \text{diagonal part of } M' \\ H' &= \text{off-diagonal part of } M' \\ T &= (1 + E)T' \end{aligned}$$

Theorem. This “Newton iteration” converges quadratically to a solution.

Theorem. We can bound $\|T - 1\|$ as a function of $\|D\|$, $\|H\|$ and $\sigma := \max_{i \neq j} |\lambda_i - \lambda_j|^{-1}$.

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Clustering

Partition $\{1, \dots, n\} = I_1 \sqcup \dots \sqcup I_p$ and define $i \sim j \iff (\exists k, \{i, j\} \subseteq I_k)$

Idea: $i \sim j \iff (|\lambda_i - \lambda_j| \text{ is small})$

Block matrices: after a permutation, reduce to the case when $I_1 < \dots < I_p$

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Modified Newton iteration

$$E_{i,j} = \begin{cases} H_{i,j} / (\lambda_j - \lambda_i) & \text{if } i \neq j \\ 0 & \text{if } i \sim j \end{cases}$$

$$M' = (1 + E)^{-1} (D + H) (1 + E)$$

$$D' = \text{block diagonal part of } M'$$

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$$T = (1 + E) T'$$

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$$T = (1 + E) T'$$

Theorem. This "modified Newton iteration" converges linearly to a solution.

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1 2 3 4 5 6 7 8 9 10 11 12

$$\begin{pmatrix} 1.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.000 \\ 0.000 & 0.000 & 1.000 \end{pmatrix} \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix} \begin{pmatrix} 1.000 & 0.000 & 0.000 \\ 0.000 & 1.000 & 0.000 \\ 0.000 & 0.000 & 1.000 \end{pmatrix} \\ = \\ \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix}$$

1 2 3 4 5 6 7 8 9 10 11 12

$$\begin{pmatrix} 0.993 & -0.001 & -0.025 \\ -0.020 & 0.998 & -0.068 \\ 0.296 & 0.028 & 0.991 \end{pmatrix} \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix} \begin{pmatrix} 1.000 & 0.000 & 0.025 \\ 0.000 & 1.000 & 0.068 \\ -0.299 & -0.028 & 1.000 \end{pmatrix}$$

=

$$\begin{pmatrix} 2.323 & 0.456 & 0.031 \\ 0.326 & 2.105 & 0.007 \\ 0.002 & 0.136 & 5.599 \end{pmatrix}$$

1 2 3 4 5 6 7 8 9 10 11 12

$$\begin{pmatrix} 0.990 & -0.001 & -0.034 \\ -0.021 & 0.998 & -0.070 \\ 0.296 & 0.067 & 0.988 \end{pmatrix} \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix} \begin{pmatrix} 1.000 & -0.001 & 0.036 \\ -0.000 & 0.997 & 0.070 \\ -0.299 & -0.067 & 0.997 \end{pmatrix}$$

=

$$\begin{pmatrix} 2.3226 & 0.4551 & 0.0009 \\ 0.3263 & 2.1049 & 0.0030 \\ 0.0127 & 0.0003 & 5.5990 \end{pmatrix}$$

1 2 3 4 5 6 7 8 9 10 11 12

$$\begin{pmatrix} 0.990 & -0.001 & -0.035 \\ -0.021 & 0.998 & -0.071 \\ 0.299 & 0.067 & 0.988 \end{pmatrix} \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix} \begin{pmatrix} 1.000 & -0.001 & 0.035 \\ -0.000 & 0.997 & 0.071 \\ -0.303 & -0.067 & 0.997 \end{pmatrix}$$

=

$$\begin{pmatrix} 2.32259 & 0.45513 & 0.00040 \\ 0.32627 & 2.10488 & 0.00009 \\ 0.00003 & 0.00176 & 5.59903 \end{pmatrix}$$

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$$\begin{pmatrix} 0.990 & -0.001 & -0.035 \\ -0.021 & 0.998 & -0.071 \\ 0.299 & 0.068 & 0.988 \end{pmatrix} \begin{pmatrix} 2.347 & 0.462 & 0.081 \\ 0.397 & 2.121 & 0.235 \\ 0.959 & 0.097 & 5.559 \end{pmatrix} \begin{pmatrix} 1.000 & -0.001 & 0.035 \\ -0.000 & 0.997 & 0.071 \\ -0.303 & -0.068 & 0.997 \end{pmatrix}$$

=

$$\begin{pmatrix} 2.322594 & 0.455127 & 0.000012 \\ 0.326266 & 2.104883 & 0.000039 \\ 0.000165 & 0.000003 & 5.599032 \end{pmatrix}$$

1 2 3 4 5 6 7 8 9 10 11 12**Given**

$$M = \mathcal{B}(M, r)$$
$$T^{-1} M T \approx D$$

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Consider

$$D = T^{-1} M T$$
$$H = D - D$$

1 2 3 4 5 6 7 8 9 10 11 12**Given**

$$M = \mathcal{B}(M, r)$$
$$T^{-1} M T \approx D$$

Consider

$$D = T^{-1} M T$$
$$H = D - D$$

Apply theorem \implies bound $\rho > 0$ such that $\forall H \in \mathcal{H}, \exists E$ with $\|E\| \leq \rho$ and

$$(1 + E)^{-1} (D + H) (1 + E) = \text{block diagonal matrix.}$$

Let $\mathcal{E} = \mathcal{B}(0, \rho)$ be the corresponding ball enclosure for E .

1 2 3 4 5 6 7 8 9 10 11 12

Given

$$\begin{aligned} M &= \mathcal{B}(M, r) \\ T^{-1} M T &\approx D \end{aligned}$$

Consider

$$\begin{aligned} D &= T^{-1} M T \\ H &= D - D \end{aligned}$$

Apply theorem \implies bound $\rho > 0$ such that $\forall H \in \mathcal{H}, \exists E$ with $\|E\| \leq \rho$ and

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Conclude

$$T = T(1 + E)$$

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High precision

It would be more efficient to have quadratic convergence.

This can be achieved by solving the commutation equations exactly:

$$\begin{aligned} DE - ED &\approx \Delta - H \\ &\Downarrow \\ D_{[i]} E_{[i,j]} - E_{[i,j]} D_{[j]} &= -H_{[i,j]} \end{aligned}$$

Certification

We already assume an approximate numeric solution with full precision.

⇒ linear convergence sufficient for certification

⇒ more efficient iteration