Backward stability of polynomial root-finding using Fiedler companion matrices

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joint work with Fernando De Terán and Javier Pérez

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Abstract (I)

- Computing the roots of a monic polynomial

$$p(z) = z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0, \quad a_i \in \mathbb{C}$$

as the eigenvalues of a companion matrix is a standard procedure.

- $A \in \mathbb{C}^{n \times n}$ is a companion matrix of $p(z)$ if is easily constructible from $p(z)$ and its characteristic polynomial is $p(z)$.
- This is MATLAB's approach by applying the QR-algorithm to the (balanced) classical Frobenius companion matrix C of $p(z)$.
- Drawbacks of MATLAB: $O(n^3)$ computational cost and $O(n^2)$ storage.
- Advantages of MATLAB: Reliability in several senses. In particular
  1. **Perfect matrix backward stability**: the computed roots of $p(z)$ are the exact eigenvalues of

$$C + E, \quad \text{with} \quad \|E\|_2 = O(u)\|C\|_2,$$

where $u \approx 10^{-16}$ is the unit roundoff.

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- Given $q(z) = b_n\, z^n + b_{n-1}\, z^{n-1} + \cdots + b_1\, z + b_0$,

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so $\|p\|_\infty \geq 1$ and $c_n\, \|C\|_2 \leq \|p\|_\infty \leq d_n\, \|C\|_2$, for c_n, d_n low powers of n.

- So, **MATLAB computed roots of $p(z)$ are** the exact eigenvalues of

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- Van Dooren & DeWilde (1983), Edelman & Murakami (1995), Lemmonier & Van Dooren (2003) proved

$$\widetilde{p}(z) = p(z) + e(z), \quad \text{with} \quad \|e(z)\|_\infty = O(u)\|p(z)\|_\infty^2,$$

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- This **penalty** in the **polynomial** backward error is an **intrinsic matrix perturbation phenomenon**, **independent of the algorithm**, and it is determined by

  1. The particular properties of the Frobenius companion matrix C,
  2. The magnitude of $\|E\|_2 = O(u)\|C\|_2 (= O(u)\|p\|_\infty)$,
  3. and the magnitude of

  $$\|\widetilde{p}(z) - p(z)\|_\infty = \|\det(zI - (C + E)) - \det(zI - C)\|_\infty$$

  A key reason for this penalty is that E is dense and does not respect the structure of C.

- In this talk, we solve a similar perturbation problem for the wider class of **Fiedler companion matrices** of $p(z)$ (the hope was to improve!!) and,

- if M_σ is a Fiedler matrix, we consider more general perturbations of M_σ

  $$\|E\|_2 = O(u)\,\alpha(p)\,\|M_\sigma\|_2,$$

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A fundamental remark

“...a general principle: a numerical process is more likely to be backward stable when the number of outputs is small compared with the number of inputs, so that there is an abundance of data onto which to “throw the backward error”...”

N. Higham, *Accuracy and Stability of Numerical Algorithms*, 2nd ed., p.65.

Outline

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1. Perturbation on characteristic polynomials of general matrices
2. Antecedents: results for Frobenius companion matrices
3. Fiedler matrices: definition and properties
4. Backward errors of poly. root-finding from Fiedler matrices
5. Balancing Fiedler matrices
6. Numerical experiments
7. Conclusions

Jacobi formula and consequences (I)

Theorem (Jacobi)

Let $A, E \in \mathbb{C}^{n \times n}$. *Then*

$$\widetilde{p}(z) - p(z) := \det(zI - (A+E)) - \det(zI - A) = -\mathrm{trace}(\,\mathrm{adj}(zI - A)\,E) + O(\|E\|^2),$$

where $\mathrm{adj}(zI - A)$ *is the adjugate matrix (or classical adjoint) of* $zI - A$*, i.e., the transpose matrix of its cofactors.*

Lemma (Gantmacher, 1959)

Let $A \in \mathbb{C}^{n \times n}$ *and* $p(z) := \det(zI - A) = z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0$. *Then*

$$\mathrm{adj}(zI - A) = \sum_{k=0}^{n-1} z^k A_k, \quad A_k \in \mathbb{C}^{n \times n},$$

and

$$A_{n-1} = I, \quad A_k = A\,A_{k+1} + a_{k+1} I, \quad \text{for } k = n-2, n-3, \ldots, 0$$

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Explicit formulas for $\mathrm{trace}(\, A_k\, E)$ obtained for

- $A =$ Frobenius companion matrix of $p(z)$ by Edelman-Murakami (1995),
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The Frobenius companion matrices

The best known companion matrices of a monic polynomial

$$p(z) = z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0,$$

are the first and second Frobenius companion matrices of $p(z)$:

$$C_1 = \begin{bmatrix} -a_{n-1} & \cdots & -a_1 & -a_0 \\ 1 & & & \\ & \ddots & & \\ & & 1 & \end{bmatrix}, \quad C_2 = \begin{bmatrix} -a_{n-1} & 1 & & \\ \vdots & & \ddots & \\ -a_1 & & & 1 \\ -a_0 & & & \end{bmatrix},$$

which have the property that

$$\det(zI - C_1) = \det(zI - C_2) = p(z)$$

Theorem (Edelman, Murakami, 1995)

Let $C_1 \in \mathbb{C}^{n\times n}$ be the first Frobenius companion matrix of $p(z)$, $E \in \mathbb{C}^{n\times n}$, and

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$$\widetilde{p}(z) := \det(zI - (C_1 + E)) = z^n + \widetilde{a}_{n-1}\, z^{n-1} + \cdots + \widetilde{a}_1\, z + \widetilde{a}_0.$$

Then, to first order in E:

$$\widetilde{a}_k - a_k = \sum_{s=0}^{k} \sum_{j=1}^{n-k-1} a_s E_{j-s+k+1,j} - \sum_{s=k+1}^{n} \sum_{j=n-k}^{n} a_s E_{j-s+k+1,j}.$$

Theorem (Edelman, Murakami, 1995)

Let $C_1 \in \mathbb{C}^{n\times n}$ *be the first Frobenius companion matrix of* $p(z)$, $E \in \mathbb{C}^{n\times n}$, *and*

$$p(z) := \det(zI - C_1) = z^n + a_{n-1}\, z^{n-1} + \cdots + a_1\, z + \, a_0,$$
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If $\|E\|_2 = O(u)\,\alpha(p)\,\|C_1\|_2$, then

$$\|\widetilde{p}(z) - p(z)\|_\infty = O(u)\,\alpha(p)\,\|p(z)\|_\infty^{\mathbf{2}}.$$

- Even the "superstable" QR-algorithm applied to C_1 does not lead to a backward stable polynomial root-finding method. Yes if $\|p(z)\|_\infty \approx 1$
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Penalty in polynomial backward errors from C_1

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Definition of Fiedler matrices (Fiedler, LAA, 2003)

Given $p(z) = z^n + a_{n-1}z^{n-1} + \cdots + a_1 z + a_0$, we define the following matrices

$$M_i := \begin{bmatrix} I_{n-i-1} & & & \\ & -a_i & 1 & \\ & 1 & 0 & \\ & & & I_{i-1} \end{bmatrix} \in \mathbb{C}^{n\times n}, \qquad i = 1, 2, \ldots, n-1$$

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For any permutation $\sigma = (i_0, i_1, \ldots, i_{n-1})$ of $(0, 1, \ldots, n-1)$, the Fiedler companion matrix of $p(z)$ associated to σ is

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Theorem (Fiedler, LAA, 2003)

For any monic polynomial $p(z)$, all associated Fiedler matrices are similar to each other, and their characteristic polynomials are equal to $p(z)$.

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Examples of Fiedler matrices

$$p(z) = z^6 + a_5 z^5 + a_4 z^4 + a_3 z^3 + a_2 z^2 + a_1 z + a_0$$

First Frobenius companion matrix: $C_1 = M_5 M_4 M_3 M_2 M_1 M_0$

$$= \begin{bmatrix} -a_5 & -a_4 & -a_3 & -a_2 & -a_1 & -a_0 \\ 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \end{bmatrix}$$

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Every Fiedler matrix has exactly the **same entries** as the first Frobenius companion matrix (in different positions).

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Special Fiedler matrices: **Pentadiagonal matrices** (there are 4 for each degree n).

$$P_1 = (M_0 M_2 M_4)(M_1 M_3 M_5) = \begin{bmatrix} -a_5 & 1 & 0 & 0 & 0 & 0 \\ -a_4 & 0 & -a_3 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -a_2 & 0 & -a_1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a_0 & 0 \end{bmatrix}$$

Structural property 2 of Fiedler matrices

Frobenius companion matrices are the Fiedler matrices with largest bandwidth and pentadiagonal Fiedler matrices are the ones with smallest bandwidth.

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Recall that the Fiedler matrix M_σ associated with a permutation σ of $(0, 1, \ldots, n-1)$ is

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But $M_i M_j = M_j M_i$, for $|i - j| \neq 1$, and many permutations lead to the same matrix.

This allows us to prove:

Lemma

There exist 2^{n-1} different Fiedler matrices associated with a monic polynomial $p(z)$ of degree n.

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Outline

Perturbation of the characteristic polynomial of a Fiedler matrix (I)

Theorem

Let $M_\sigma \in \mathbb{C}^{n\times n}$ be a Fiedler matrix of $p(z)$, $E \in \mathbb{C}^{n\times n}$, and

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Then, to first order in E:

$$\widetilde{a}_k - a_k = -\sum_{i,j=1}^{n} p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})\, E_{ij} \quad \text{for } k = 0, 1, \ldots, n-1,$$

where the functions $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ are **multivariable polynomials in the coefficients of $p(z)$ given by...**

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...the horror!!

(a) if $v_{n-i} = v_{n-j} = 0$:

- $a_{k+\mathfrak{i}_\sigma(n-j:n-i)}$,

  if $j \geq i$ and $n-k-i+1 \leq \mathfrak{i}_\sigma(n-j:n-i) \leq n-k$;
- $-a_{k+1-\mathfrak{i}_\sigma(n-i:n-j-1)}$,

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- 0, otherwise;

(b) if $v_{n-i} = v_{n-j} = 1$:

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- 0, otherwise;

(c) if $v_{n-i} = 1$ and $v_{n-j} = 0$:

- 1, if $\mathfrak{i}_\sigma(0:n-j-1) + \mathfrak{c}_\sigma(0:n-i-1) = k$,
- 0, otherwise;

(d) if $v_{n-i} = 0$ and $v_{n-j} = 1$:

- $$\sum_{l=\max\{0,k+1+j-\mathfrak{c}_\sigma(n-j:n-i-1)-n\}}^{l=\min\{k+1-\mathfrak{c}_\sigma(n-j:n-i-1),i-1\}} -\left(a_{n+1-i+l}\, a_{k+1-\mathfrak{c}_\sigma(n-j:n-i-1)-l}\right),$$

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Perturbation of the characteristic polynomial of a Fiedler matrix (II)

Theorem (Soft version)

Let $M_\sigma \in \mathbb{C}^{n\times n}$ *be a Fiedler matrix of* $p(z)$, $E \in \mathbb{C}^{n\times n}$, *and*

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where $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ *are* **multivariable polynomials such that**

- $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ *is a polynomial in* a_i *with* **degree at most** 2.
- *If* $M_\sigma = C_1, C_2$, *then all* $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ *have* **degree** 1.
- *If* $M_\sigma \neq C_1, C_2$, *then there is at least one* k *and some* (i,j) *such that* $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ *has* **degree** 2.

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- *If $M_\sigma = C_1, C_2$, then all $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ have* **degree** 1.
- *If $M_\sigma \neq C_1, C_2$, then there is at least one k and some (i,j) such that $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ has* **degree** 2.

Corollary

Let $M_\sigma \in \mathbb{C}^{n\times n}$ *be a Fiedler matrix of* $p(z)$, $E \in \mathbb{C}^{n\times n}$, *and*

$$p(z) := \det(zI - M_\sigma) = z^n + a_{n-1}\, z^{n-1} + \cdots + a_1\, z + a_0,$$
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If $\|E\|_2 = O(u)\,\alpha(p)\,\|M_\sigma\|_2$, *then*

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$$\|\widetilde{p}(z) - p(z)\|_\infty = O(u)\,\alpha(p)\,\|p(z)\|_\infty^{\mathbf{2}}.$$

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Scaling does not work: a key remark by V. Noferini

- Let $p(z) = z^n + \sum_{i=0}^{n-1} a_i \, z^i$.
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$$q(z_0) = 0 \Longleftrightarrow p\left(\frac{z_0}{\beta}\right) = 0$$
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Outline

- **Balancing any Fiedler matrix of $p(z)$ before applying QR yields** (very often) **perfect polynomial backward stability**:

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- However, it is always possible to find $p(z)$ for which balancing does not improve backward stability.
- The theoretical treatment of “balancing” Fiedler matrices from the point of view of polynomial backward errors is trivial from our results, but
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- Balancing a Fiedler matrix M_σ of $p(z)$ consists in

$$M_\sigma \longrightarrow D M_\sigma D^{-1}, \quad \text{with } D = \text{diag}(2^{t_1}, \dots, 2^{t_n})$$

such that $\|\text{row}_i(D M_\sigma D^{-1})\|_\infty \approx \|\text{col}_i(D M_\sigma D^{-1})\|_\infty$ for all i.

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Theorem

Let M_σ be a Fiedler matrix of $p(z)$, D its diagonal balancing matrix, $\widetilde{E} \in \mathbb{C}^{n\times n}$, and

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Then, to first order in $\widetilde{E}$:

$$\widetilde{a}_k - a_k = -\sum_{i,j=1}^{n} p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})\, \frac{d_j}{d_i}\, \widetilde{E}_{ij} \quad \text{for } k = 0, 1, \ldots, n-1,$$

where $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ are the previous multivariable polynomials.

Moreover, if $\|\widetilde{E}\|_2 = O(u)\, \|DM_\sigma D^{-1}\|_2$, then

$$\|\widetilde{p}(z) - p(z)\|_\infty = O(u)\, \max_{i,j,k} \left(\left| p_{ij}^{(\sigma,k)}(a_0, \ldots, a_{n-1}) \frac{d_j}{d_i} \right| \right) \|DM_\sigma D^{-1}\|_2.$$

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Outline

- The goals of the numerical experiments are
  1. to show that our bounds correctly predict the dependence on the norm of $p(z)$ of the polynomial backward errors when the roots are computed as the eigenvalues of a Fiedler matrix with QR, and
  2. to study the effect of balancing the Fiedler companion matrices.
- We proceed as follows:
  1. We generate 500 random monic polys for each fixed value $\|p\|_\infty$.
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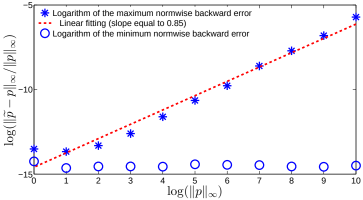
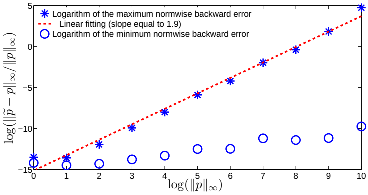
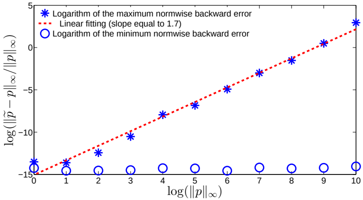
  1. to show that our bounds correctly predict the dependence on the norm of $p(z)$ of the polynomial backward errors when the roots are computed as the eigenvalues of a Fiedler matrix with QR, and
  2. to study the effect of balancing the Fiedler companion matrices.
- We proceed as follows:
  1. We generate 500 random monic polys for each fixed value $\|p\|_\infty$.
  2. We compute exactly (in quadruple precision) the polynomial backward error corresponding to the roots computed by QR.
  3. We do this for four different Fiedler matrices
     - M_{σ_1} = second classical Frobenius,
     - M_{σ_2} = a pentadiagonal,
     - M_{σ_3} = the second F-matrix,
     - M_{σ_4} = “another one”.



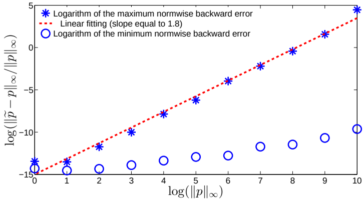
(a) M_{σ_1}



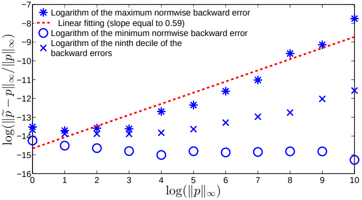
(b) M_{σ_2}



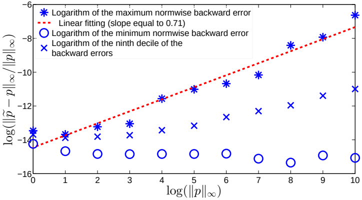
(c) M_{σ_3}



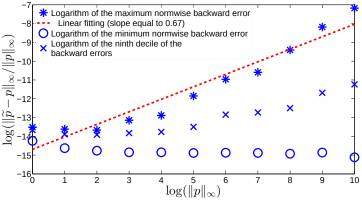
(d) M_{σ_4}



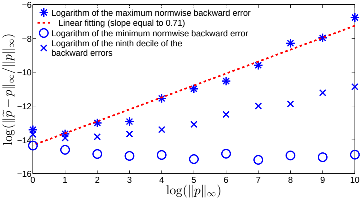
(e) M_{σ_1}



(f) M_{σ_2}



(g) M_{σ_3}



(h) M_{σ_4}

Outline

- Assume that we apply to Fiedler and classical Frobenius companion matrices of a monic polynomial $p(z)$ the "same eigenvalue algorithm" (or algorithms with similar matrix backward stability properties) for computing its roots.
- Then, from the point of view of polynomial backward errors:
- Proved: Unbalanced Fiedler matrices are as good as classical Frobenius companion matrices if $\|p(z)\|_\infty$ is moderate.
- Proved: Unbalanced Fiedler matrices are worse than classical Frobenius companion matrices if $\|p(z)\|_\infty \gg 1$, but both are bad.
- From numerical experiments: Balanced Fiedler matrices are as good as classical Frobenius companion matrices always.

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