Polynomial root-finding using Fiedler companion matrices

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Joint work with **F. M. Dopico** & **Javier Pérez** (UC3M)

Outline

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1. Framework
2. The adjugate matrix $\mathrm{adj}(zI - M_\sigma)$
3. Backward stability?
4. Numerical experiments

Goal

$$p(z) = z^n + \sum_{k=0}^{n-1} a_k z^k$$

(monic) polynomial ($a_k \in \mathbb{C}$)

Polynomial root-finding: Solve $p(z) = 0$.

- Approach: Compute the eigenvalues of A such that $\det(zI - A) = p(z)$

Roots of $p(z)$ = Eigenvalues of A (i.e.: $p(z) = 0 \Leftrightarrow \det(zI - A) = 0$)

For instance: First and second Frobenius companion matrices:

$$C_1 = \begin{bmatrix} -a_{n-1} & -a_{n-2} & \cdots & -a_0 \\ 1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ 0 & & 1 & 0 \end{bmatrix}, \quad C_2 = C_1^T$$

MATLAB's command `roots`: QR algorithm on C_2

Fast methods available: [Aurentz *et al.* 2013], [Bini *et al.*, 2004, 2005, 2010], [Calvetti *et al.*, 2002], [Gemignani, 2007], [Chandrasekaran *et al*, 2008], [Van Barel *et al*, 2010] ...

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New family of (companion) matrices: Fiedler companion matrices [Fiedler'03] $\rightsquigarrow$ **many interesting features.**

Goal Analyze the numerical behavior of Fiedler matrices in the polynomial root-finding.

Theoretically:

Polynomial root-finding $\overset{\text{Companion matrices}}{\Longleftrightarrow}$ Standard eigenvalue problem

But numerically, they are different problems !!!

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B'err of polynomial root-finding using companion matrices

Given $p(z)$ → Choose A such that $p(z) = \det(zI - A)$ → Compute the e-vals of A = e-vals of $A+E$, $\|E\| = O(u)\|A\|$

(if we use a backward stable algorithm, like QR)

Set $\widetilde{p}(z) = \det(zI - (A+E))$

Question: Is $\widetilde{p}(z)$ close to $p(z)$?

$$\frac{\|p-\widetilde{p}\|}{\|p\|} = O(u) \ ?$$

$\frac{\|p-\widetilde{p}\|}{\|p\|}$: b'err of polynomial root-finding as an eigenvalue problem (using A).

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Fiedler matrices: definition

$p(z) = z^n + \sum_{i=1}^{n-1} a_i z^i$

$$M_0 = \begin{bmatrix} I_{n-1} & \\ & -a_0 \end{bmatrix}, \quad M_k = \begin{bmatrix} I_{n-k-1} & & & \\ & -a_k & 1 & \\ & 1 & 0 & \\ & & & I_{k-1} \end{bmatrix}, \quad \text{for } k = 1, \ldots, n-1.$$

Let $\sigma : \{0, 1, \ldots, n-1\} \to \{1, \ldots, n\}$ be a bijection. Then:

$$M_\sigma := M_{\sigma^{-1}(1)} \cdots M_{\sigma^{-1}(n)}$$

Example: $C_1 = M_{n-1} \cdots M_1 M_0, \quad C_2 = M_0 M_1 \cdots M_{n-1},$

$$F := M_{n-1} \cdots M_2 M_0 M_1 = \begin{bmatrix} -a_{n-1} & -a_{n-2} & \cdots & 1 \\ 1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ 0 & & -a_0 & 0 \end{bmatrix}$$

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Fiedler matrices: Basic properties

- All M_σ contain the same entries (located in different positions): $(-a_0, \ldots, -a_{n-1})$ + $(n-1)$ 1's + (0's).
- M_σ is a companion matrix (in particular, $\det(zI - M_\sigma) = p(z)$)
- There are 2^{n-1} (generically) different Fiedler matrices.

Definition:

σ has a consecution at $i \in \{0, 1, \ldots, n-2\}$ if $\sigma^{-1}(i) < \sigma^{-1}(i+1)$, and σ has an inversion otherwise.

CIS(σ):="CIS(M_σ)"=$(k_0, \ldots, k_{n-2})$, with $k_i = \begin{cases} 1, & \text{if } \sigma \text{ has a consecution at } i, \\ 0, & \text{if } \sigma \text{ has an inversion at } i. \end{cases}$

Example: CIS(C_1)=$(0, \ldots, 0)$, CIS(C_2)=$(1, \ldots, 1)$, CIS(F)=$(1, 0, \ldots, 0)$.

Then: $M_{\sigma_1} = M_{\sigma_2} \Leftrightarrow$ CIS(σ_1)=CIS(σ_2).

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More Fiedler matrices

For $n \geq 3$, there are 4 different **pentadiagonal** Fiedler matrices: $M_{\sigma_1}, M_{\sigma_2}, M_{\sigma_3}, M_{\sigma_4}$, with:

$$\mathrm{CIS}(\sigma_1) = (1,0,1,\ldots) \quad \mathrm{CIS}(\sigma_2) = (1,1,0,1,\ldots)$$
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$$M_{\sigma_1} = \begin{bmatrix} -a_5 & 1 & 0 & 0 & 0 & 0 \\ -a_4 & 0 & -a_3 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -a_2 & 0 & -a_1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a_0 & 0 \end{bmatrix} \qquad (n=6)$$

These are the Fiedler matrices with **lowest bandwidth**.

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Perturbation of the characteristic polynomial: first order term

Using Jacobi's formula:

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

$$\mathrm{adj}(zI - A) = \sum_{k=0}^{n-1} z^k A_k \text{ (matrix polynomial of degree } n-1)$$

Hence, if we set: $\det(zI - X) = z^n + \sum_{k=0}^{n-1} a_k(X) z^k$, then, to **first order** in E:

$$a_k(A+E) - a_k(A) = -\mathrm{tr}(A_k E) = -\mathrm{vec}({A_k}^T)^T \mathrm{vec}(E).$$

$$(\mathrm{vec}(M) := [m_{11} \dots m_{m1}\ m_{12} \dots m_{m2} \dots m_{1n} \dots m_{mn}]^T)$$

- Formula for $\mathrm{adj}(zI - M_\sigma)$: Depends on a_i and:

$\mathfrak{c}_\sigma(i:j) = \#\{\text{consecutions of } \sigma \text{ from } i \text{ to } j\}$, $\mathfrak{i}_\sigma(i:j) = \#\{\text{inversions of } \sigma \text{ from } i \text{ to } j\}$

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Perturbation of the characteristic polynomial: first order term

Using Jacobi's formula:

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

$$\mathrm{adj}(zI - A) = \sum_{k=0}^{n-1} z^k A_k \text{ (matrix polynomial of degree } n-1)$$

Hence, if we set: $\det(zI - X) = z^n + \sum_{k=0}^{n-1} a_k(X) z^k$, then, to **first order** in E:

$$\boxed{a_k(A+E) - a_k(A) = -\mathrm{tr}(A_k E) = -\mathrm{vec}({A_k}^T)^T \mathrm{vec}(E).}$$

$(\mathrm{vec}(M) := [m_{11} \ldots m_{m1}\, m_{12} \ldots m_{m2} \ldots m_{1n} \ldots m_{mn}]^T)$

- Formula for $\mathrm{adj}(zI - M_\sigma)$: Depends on a_i and:

$\mathfrak{c}_\sigma(i:j) = \#\{\text{consecutions of } \sigma \text{ from } i \text{ to } j\}$, $\mathfrak{i}_\sigma(i:j) = \#\{\text{inversions of } \sigma \text{ from } i \text{ to } j\}$

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Outline

Explicit formula for the adjugate matrix

Theorem

$\mathrm{PCIS}(\sigma) = (v_0, v_1, \ldots, v_{n-1})$. The (**nonzero**) kth coefficients of the (j,i) entry of $\mathrm{adj}(zI - M_\sigma)$ are:

(a) if $v_{n-i} = v_{n-j} = 0$:
- $a_{k+\mathfrak{i}_\sigma(n-j:n-i)}$, if $j \geq i$ and $n-k-i+1 \leq \mathfrak{i}_\sigma(n-j:n-i) \leq n-k$;
- $-a_{k+1-\mathfrak{i}_\sigma(n-i:n-j-1)}$, if $j < i$ and $k+1+i-n \leq \mathfrak{i}_\sigma(n-i:n-j-1) \leq k+1$;

(b) if $v_{n-i} = v_{n-j} = 1$:
- $a_{k+\mathfrak{c}_\sigma(n-i:n-j)}$, if $j \leq i$ and $n-k-j+1 \leq \mathfrak{c}_\sigma(n-i:n-j) \leq n-k$;
- $-a_{k+1-\mathfrak{c}_\sigma(n-j:n-i-1)}$, if $j > i$ and $k+1+j-n \leq \mathfrak{c}_\sigma(n-j:n-i-1) \leq k+1$;

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

(d) if $v_{n-i} = 0$ and $v_{n-j} = 1$:
- $$\sum_{l=\max\{0,k+1+j-\mathfrak{c}_\sigma(n-j:n-i-1)-n\}}^{l=\min\{k+1-\mathfrak{c}_\sigma(n-j:n-i-1),i-1\}} -(a_{n+1-i+l}\, a_{k+1-\mathfrak{c}_\sigma(n-j:n-i-1)-l}),$$
  if $j > i$ and $k+2+j-i-n \leq \mathfrak{c}_\sigma(n-j:n-i-1) \leq k+1$;
- $$\sum_{l=\max\{0,k+1+i-\mathfrak{i}_\sigma(n-i:n-j-1)-n\}}^{l=\min\{k+1-\mathfrak{i}_\sigma(n-i:n-j-1),j-1\}} -(a_{n+1-j+l}\, a_{k+1-\mathfrak{i}_\sigma(n-i:n-j-1)-l}),$$
  if $j < i$ and $k+2+i-j-n \leq \mathfrak{i}_\sigma(n-i:n-j-1) \leq k+1$;

(where we set $a_n := 1$, and $v_{n-1} = v_{n-2}$).

Formula for the adjugate: main features

To first order in E:

$$a_k(A+E) - a_k(A) = -\sum_{i,j=1}^{n} p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})\, E_{ij}, \qquad k = 0, 1, \ldots, n-1,$$

where:

- $p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})$ 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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Recursive formula for the adjugate

$p(z) = z^n + \sum_{k=0}^{n-1} a_k z^k$

Proposition [Gantmacher, 1959]

Set:

$$\begin{cases} A_{n-1} = I, \quad \text{and} \\ A_k = A \cdot A_{k+1} + a_k I, \quad \text{for } k = n-2, \ldots, 1, 0. \end{cases}$$

Then,

$$\mathrm{adj}(zI - A) = \sum_{k=0}^{n-1} z^k A_k.$$

Note:

$$A_{k-1} = p_{n-k}(A) = A^{n-k} + a_{n-1} A^{n-k-1} + \cdots + a_{k+1} A + a_k I.$$

($(n-k)$th Horner shift of $p(z)$ evaluated at A)

Hence: $p_{n-k-1}(A)$ encodes the information on the variation $a_k(A+E) - a_k(A)$:

$$a_k(A+E) - a_k(A) = -\sum_{i,j} (p_{n-k-1}(A))_{ji} E_{ij} + O(\|E\|^2).$$

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Some particular examples

Frobenius companion matrices:

$$p_{n-k-1}(C_1^T) = p_{n-k-1}(C_2) = \left[\begin{array}{ccc|cccc} 0 & \dots & 0 & 1 & & & 0 \\ -a_k & & & a_{n-1} & 1 & & \\ \vdots & \ddots & & \vdots & a_{n-1} & \ddots & \\ -a_1 & \ddots & -a_k & a_{k+1} & \vdots & \ddots & 1 \\ -a_0 & \ddots & \vdots & & a_{k+1} & \ddots & a_{n-1} \\ & \ddots & -a_1 & & & \ddots & \vdots \\ 0 & & -a_0 & 0 & & & a_{k+1} \end{array}\right].$$

These are the **only** Fiedler matrices M_σ for which **all** $p_k(M_\sigma)$ have entries of **degree 1** !!!!

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Some particular examples (II)

$$F = M_{n-1} \cdots M_2 M_0 M_1$$

$$p_{n-k-1}(F) = \left[\begin{array}{cccc|cccc}
0 & & & & 1 & & & 0 \\
-a_k & & & & a_{n-1} & \ddots & & \vdots \\
\vdots & \ddots & & & \vdots & \ddots & 1 & 0 \\
-a_1 & & -a_k & & a_{k+2} & & a_{n-1} & -a_0 \\
-a_0 & \ddots & \vdots & -a_k & a_{k+1} & \ddots & \vdots & -{\color{blue}a_0 a_{n-1}} \\
 & \ddots & -a_1 & \vdots & & \ddots & a_{k+2} & \vdots \\
 & & -a_0 & -a_1 & & & a_{k+1} & -{\color{blue}a_0 a_{k+2}} \\
 & & & 1 & & & & a_{k+1}
\end{array}\right], \quad \text{for } k = 0 : n-3,$$

$$p_1(F) = \begin{bmatrix}
0 & & & & & 0 \\
-a_{n-2} & 1 & & & & \\
-a_{n-3} & a_{n-1} & 1 & & & \\
\vdots & & a_{n-1} & \ddots & & \\
\vdots & & & \ddots & 1 & \\
-a_1 & & & & a_{n-1} & -a_0 \\
1 & & & & 0 & a_{n-1}
\end{bmatrix}, \quad \text{and} \quad p_0(F) = I.$$

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Outline

Backward error

Theorem

If the roots of $p(z)$ are computed as the e-vals of M_σ with a backward stable algorithm, the computed roots are the exact roots of a polynomial $\widetilde{p}(z)$ with:

(a) If $M_\sigma = C_1, C_2$:

$$\frac{\|\widetilde{p} - p\|_\infty}{\|p\|_\infty} = O(u)\|p\|_\infty,$$

(b) if $M_\sigma \neq C_1, C_2$:

$$\frac{\|\widetilde{p} - p\|_\infty}{\|p\|_\infty} = O(u)\|p\|_\infty^2.$$

(u is the machine precision)

Proof (idea): $|\widetilde{a}_k - a_k| = \left|\sum_{i,j=1}^n p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})E_{ij}\right| \leq \sum_{i,j=1}^n \left|p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})\right| \cdot |E_{ij}| \leq \left(\max_{1\leq i,j\leq n}|E_{ij}|\right) \cdot \left(\sum_{i,j=1}^n |p_{ij}^{(\sigma,k)}(a_0, a_1, \ldots, a_{n-1})|\right)$. Therefore,

$$\|\widetilde{p} - p\|_\infty = \max_{k=0,1,\ldots,n-1} |\widetilde{a}_k - a_k| = O(u)\|M_\sigma\|_\infty \|p\|_\infty^2 = O(u)\|p\|_\infty^3,$$

using: $\max_{i,j=1,2,\ldots,n}|E_{ij}| = O(u)\|M_\sigma\|_\infty$ and $\|M_\sigma\|_\infty = O(1)\|p\|_\infty$ [D., Dopico, PÃ©rez, 2013]

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Some remarks

(Recall: $\|p\|_\infty \geq 1$, since p is monic).

- For $\|p\|_\infty$ moderate, backward stability of polynomial root-finding is guaranteed using **any Fiedler matrix**.
- Then, particular features of some Fiedler matrices (like low bandwidth) can make them preferable than C_1 and C_2.
- When $\|p\|_\infty$ is large, C_1 and C_2 are expected to give smaller b'err than any other Fiedler.
- Coefficient-wise backward stability is not guaranteed for any Fiedler matrix, even when $\|p\|_\infty = 1$.
- However, when all $|a_i| = \Theta(1)$ (i.e: moderate and not too close to zero), then: $\max_{k=0,1,\ldots,n-1} \frac{|\widetilde{a}_k - a_k|}{|a_k|} = O(u)$.

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Outline

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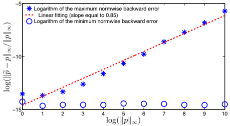
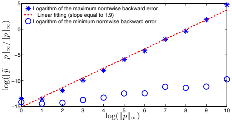
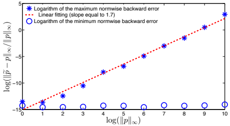
Random polynomials, $n = 20$



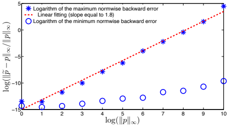
(a) C_2



(b) Pentadiagonal



(c) F



(d) M_σ

Figure: 11 samples of 500 random polys with $\|p\|_\infty = 10^k$ ($k = 0, 1, \ldots, 10$) and $a_i = a \cdot 10^c$, where a is drawn from the uniform distribution on $[-1, 1]$ and c is drawn from the uniform distribution on $[-k, k]$, and where $a_0 = 10^k$.

Conclusions

- We have analyzed the b'err of the polynomial root-finding solved as an e-val problem using Fiedler companion matrices.
- When $\|p\|_\infty$ is moderate, the procedure is **backward stable** for any Fiedler matrix.
- When $\|p\|_\infty$ is large, Frobenius companion matrices are expected to give less b'err than any other Fiedlers.
- Further work: Take advantage of the structure of some Fiedlers (like pentadiagonal) to develop faster methods?

THANK YOU!!!!!

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