Polynomial root-finding using companion matrices

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Outline

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Goal

Compute the roots of (scalar) polynomials

$$p(z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0 \qquad (a_k \in \mathbb{C})$$

using companion forms.

We can restrict ourselves to **monic** polynomials (after dividing by a_n, if necessary)

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$A(a_0, a_1, \ldots, a_{n-1})$ such that

$$p_A(z) = \det(zI - A) = z^n + a_{n-1}z^{n-1} + \cdots + a_1 z + a_0 = p(z)$$

(Only for monic polynomials).

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

Theoretically:

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

But numerically, they are different problems !!!

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Motivation

Frobenius companion matrices:

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

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

Companion forms

Companion form: Valid for non-monic polynomials.

Companion form

$A(a_0, a_1, \ldots, a_{n-1}, a_n) \quad \rightsquigarrow \quad$ May have entries of the form $a + bz$

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Backward stability

Problem:	Algorithm:
$f : \underbrace{X}_{data} \longrightarrow \underbrace{Y}_{solution}$	$\widetilde{f} : \underbrace{X}_{data} \longrightarrow \underbrace{Y}_{solution}$

$\widetilde{f}$ is backward stable if $\widetilde{f}(x) = f(x + \delta x), \quad \|\delta x\| = O(u)\|x\|$

($u =$ unit roundoff)

☞ Different approaches for **poly root-finding** using **companion matrices**:

1. B'stability on the companion matrix (e-vals):

   $\widetilde{f} =$ e-val algorithm, $f =$ e-val problem, $x =$ companion matrix

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2. B'stability on the polynomial (roots):

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Complexity (Computational cost)

- Computation time (number of flops)
- Storage

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👍 In practice, it can be considered b'stable (in the poly sense) $\rightsquigarrow$ balancing!!

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- Many variants of the QR algorithm: [Calvetti-etal'02], [Bini-etal'04, '05, '10], [Gemignani'07], [Chandrasekharan-etal'08], [Van Barel-etal'10], [Aurentz-etal'13]
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Q: B'stability in the polynomial sense ???

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).

Goal:

Analyze $\frac{\|p - \widetilde{p}\|}{\|p\|}$, for A a **Fiedler matrix**.

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Fiedler matrices: definition

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

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

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

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

Fiedler matrix of p associated with the bijection σ

- Introduced by **Fiedler** in 2003.

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Fiedler matrices: some examples

- Frobenius companion matrices:

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$$C_2 = M_0 M_1 \cdots M_{n-1} = C_1^\top$$

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

- $$M_6(M_4 M_5)(M_2 M_3)(M_0 M_1) = \begin{bmatrix} -a_5 & 1 & 0 & 0 & 0 & 0 \\ -a_4 & 0 & -a_3 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -a_2 & 0 & -a_1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a_0 & 0 \end{bmatrix} \qquad (n = 6)$$

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$$C_2 = M_0 M_1 \cdots M_{n-1} = C_1^\top$$

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

- $$M_6(M_4 M_5)(M_2 M_3)(M_0 M_1) = \begin{bmatrix} -a_5 & 1 & 0 & 0 & 0 & 0 \\ -a_4 & 0 & -a_3 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -a_2 & 0 & -a_1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a_0 & 0 \end{bmatrix} \qquad (n = 6)$$

Fiedler matrices: Basic properties

- All M_σ contain the same entries (located in different positions):

$$-a_0, \ldots, -a_{n-1} \quad \& \quad \overbrace{1, \ldots, 1}^{n-1} \quad \& \quad 0's$$

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Outline

Perturbation of the characteristic polynomial: first order term

Using Jacobi's formula:

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

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

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:

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

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- Formula for $[(M_\sigma)_k]_{ij}$: Is a polynomial on a_i with degree ≤ 2

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 $v_{n-j} = 1$:

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

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

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 $a_k(A+E) - a_k(A)$:

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Some particular examples

Frobenius companion matrices:

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

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Some particular examples (II)

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

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

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): $|\widetilde{a}_k - a_k| = \left|\sum_{i,j=1}^n p_{ij}^{(\sigma,k)}(a_0,a_1,\ldots,a_{n-1})E_{ij}\right| \leq \sum_{i,j=1}^n \left|p_{ij}^{(\sigma,k)}(a_0,a_1,\ldots,a_{n-1})\right| \cdot |E_{ij}| \leq (\max_{1\leq i,j\leq n}|E_{ij}|)\cdot\left(\sum_{i,j=1}^n |p_{ij}^{(\sigma,k)}(a_0,a_1,\ldots,a_{n-1})|\right)$. 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, Pérez, 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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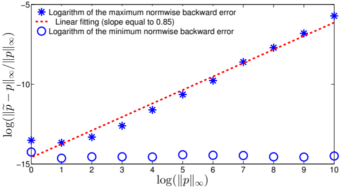
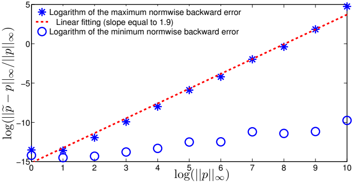
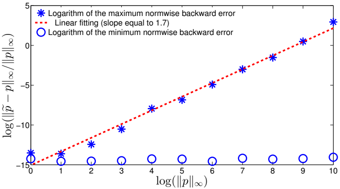
Random polynomials, $n = 20$



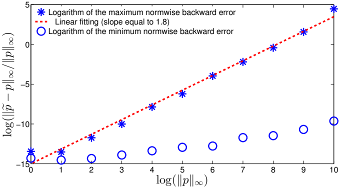
(a) C_2



(b) Pentadiagonal



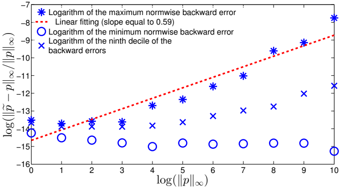
(c) F



(d) M_σ

Figure: 11 samples, 500 random polys, $\|p\|_\infty = 10^k$ ($k = 0:10$), $a_i = a \cdot 10^c$, $a \in [-1,1]$, $c \in [-k,k]$, $a_0 = 10^k$.

Random polynomials, $n = 20$ (with balancing)



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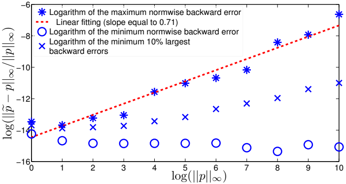
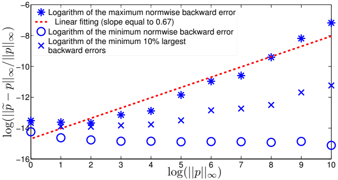
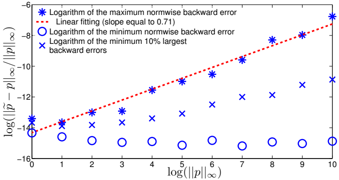


(b) Pentadiagonal



(c) F



(d) M_σ

Figure: 11 samples, 500 random polys, $\|p\|_\infty = 10^k$ $(k = 0:10)$, $a_i = a \cdot 10^c$, $a \in [-1,1]$, $c \in [-k,k]$, $a_0 = 10^k$.

Outline

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Just multiply: $PM_\sigma P^{-1}$ (P invertible)$\rightsquigarrow$ In general, not sparse (**exception**: P is a **permutation** matrix)

☞ We look for sparse companion matrices

Sparse companion matrices (I)

Sparse: It has the smallest number of nonzero entries

☞ For companion matrices, this number is $2n - 1$ [Ma-Zhan'13]

(we focus on: $\underbrace{1, \ldots, 1}_{n-1}, a_0, \ldots, a_{n-1}$)

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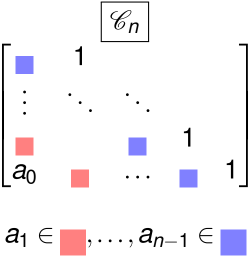

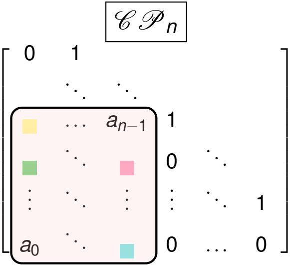

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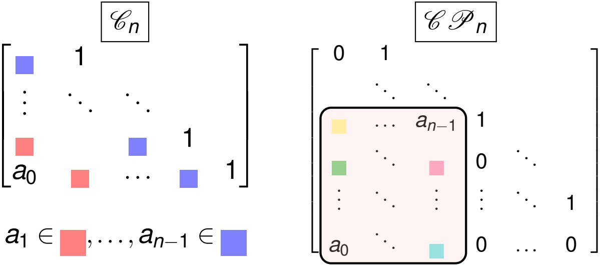

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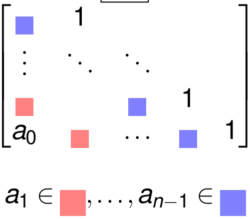

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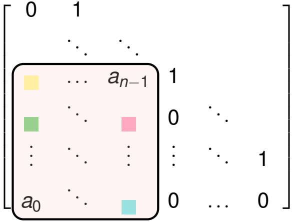

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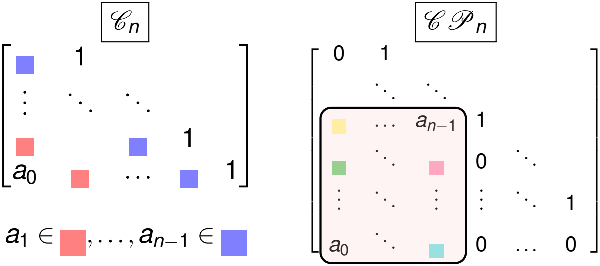

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Theorem [Eastman-etal'14]

$A(a_0, \ldots, a_{n-1}) \in \mathcal{C}_n$ is a sparse companion matrix $\Leftrightarrow A(a_0, \ldots, a_{n-1}) \in \mathcal{CP}_n$.

Why monic polynomials?

If $q(z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0$ (not necessarily monic) $(a_n \neq 0)$

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$\Rightarrow$ It is enough to prove b'stability for monic polys

However...

- B'stability (in the poly sense) is only guaranteed if $\|p\|$ is moderate.
- The QZ algorithm on the Frobenius companion form (non-monic) gives b'stability if $\|p\|_\infty \approx 1$ ([Van Dooren-Dewilde'83]).
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Examples: $F_1 = \begin{bmatrix} a_n z + a_{n-1} & a_{n-2} & \cdots & a_0 \\ -1 & z & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ 0 & & -1 & z \end{bmatrix} \qquad F_2 = F_1^\top$

$$F = \begin{bmatrix} a_6 z + a_5 & -1 & 0 & 0 & 0 & 0 \\ a_4 & z & a_3 & -1 & 0 & 0 \\ -1 & 0 & z & 0 & 0 & 0 \\ 0 & 0 & a_2 & z & a_1 & -1 \\ 0 & 0 & -1 & 0 & z & 0 \\ 0 & 0 & 0 & 0 & a_0 & z \end{bmatrix} \qquad (n = 6)$$

Other companion forms

Companion form

A matrix $A(a_0, a_1, \ldots, a_{n-1}, a_n; z)$ such that:

- The entries are linear polynomials in z.
- $\det A(a_0, a_1, \ldots, a_{n-1}, a_n; z) = a_n z^n + a_{n-1} z^{n-1} + \cdots + a_1 z + a_0$

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Fiedler-like:
$$\begin{bmatrix} 0 & 0 & 0 & z & a_0 + za_1 \\ 0 & 0 & 1 & 0 & -z \\ 0 & z & a_2 + za_3 & -1 & 0 \\ 1 & 0 & -z & 0 & 0 \\ a_4 + za_5 & -1 & 0 & 0 & 0 \end{bmatrix} \qquad (n = 5)$$

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☞ There are many others [Dopico-Lawrence-Pérez-VanDooren]:

- Permutationally equivalent to companion forms in some "extended $\mathscr{C}\mathscr{P}_n$".
- Most of them are not sparse.

Open questions for companion forms

- How many non-permutationally similar companion matrices are there in $\mathscr{C}\mathscr{P}_n$?
- Which is the smallest number of nonzero entries (sparse)?

Open questions for companion forms

- How many non-permutationally similar companion matrices are there in $\mathcal{CP}_n$?
- Which is the smallest number of nonzero entries (sparse)?

$$\begin{bmatrix} 0 & 0 & 0 & z & a_0+za_1 \\ 0 & 0 & 1 & 0 & -z \\ 0 & z & a_2+za_3 & -1 & 0 \\ 1 & 0 & -z & 0 & 0 \\ a_4+za_5 & -1 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{matrix} (n=5, \\ \#(nonzero)=11) \end{matrix}$$

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- Do all sparse companion forms in this $\mathscr{C}_n$ belong to an “extended $\mathscr{CP}_n$"?
- Is there any companion form that provides a smaller b’err than Frobenius ones?

Outline

Conclusions

- B'stability on the e-val problem $\not\Rightarrow$ B'stability on the poly root-finding problem.
- When $\|p\|_\infty$ is moderate, a b'stable e-val algorithm implies poly b'stability for any Fiedler matrix.
- When $\|p\|_\infty$ is large, Frobenius companion matrices are expected to give **less b'err** than any other Fiedlers.
- Though `roots` is b'stable in practice, it could give non-satisfactory results.
- Characterization of all sparse companion **matrices** is known (only for monic polynomials!).
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- Still more room to look for other companion **forms** and to describe all sparse ones.

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DANKE !!