Inverse Inequality Estimates with Symbolic Computation

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Doctoral Program
Computational Mathematics
Numerical Analysis and Symbolic Computation

RICAM
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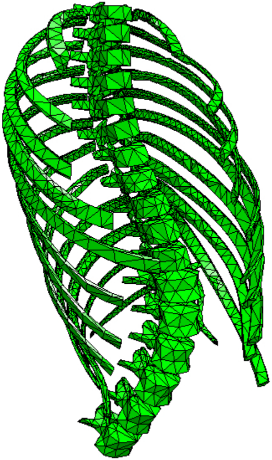
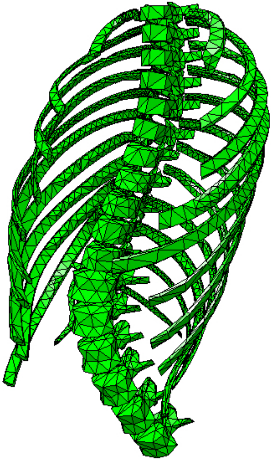
FOR COMPUTATIONAL AND APPLIED MATHEMATICS

Symbolic Computation and Numerical Analysis

"A marriage made in heaven"



Inverse Inequalities
that appear in
Numerical Analysis



Inverse Inequalities

We consider inequalities of the form

$$\|v_n\|_{X(\Omega)} \leqslant c_1(h,n)\,\|v_n\|_{Y(\Omega)} \qquad \text{for all } v_n \in V_n$$
$$\|v_n\|_{Z(\partial\Omega)} \leqslant c_2(h,n)\,\|v_n\|_{Y(\Omega)} \qquad \text{for all } v_n \in V_n$$

- $\Omega \subset \mathbb{R}^d, d \in \mathbb{N}$
- V: some infinite-dimensional space of functions defined on Ω
- $\|\cdot\|_{X(\Omega)}$, $\|\cdot\|_{Y(\Omega)}$, $\|\cdot\|_{Z(\partial\Omega)}$: norms that are used in the analysis of numerical methods
- $(V_n)_{n\in\mathbb{N}}$: finite-dimensional approximation of V
- $h > 0$: finite element diameter

Dependence on h is easily obtained by a scaling argument:
$\longrightarrow$ Transform the problem to a reference element $\hat{\Omega}$.

Inverse Inequalities

We obtain for c_1 (and similarly for c_2):

$$\hat{c}_1(n) = \sup_{v_n \in \hat{V}_n} \frac{||v_n||_{X(\hat{\Omega})}}{||v_n||_{Y(\hat{\Omega})}} = \sqrt{\sup_{v_n \in \hat{V}_n} \frac{(v_n, v_n)_{X(\hat{\Omega})}}{(v_n, v_n)_{Y(\hat{\Omega})}}}$$

Let $(\varphi_k)_{1 \leqslant k \leqslant n}$ be a basis of $\hat{V}_n$. Then:

$$\big(\hat{c}_1(n)\big)^2 = \sup_{\vec{v}_n \in \mathbb{R}^n} \frac{(K_n \vec{v}_n, \vec{v}_n)_{\ell^2}}{(M_n \vec{v}_n, \vec{v}_n)_{\ell^2}}$$

for certain symmetric and positive (semi-) definite matrices

$$K_n(i,j) := (\varphi_j, \varphi_i)_{X(\hat{\Omega})}\,, \text{ and } M_n(i,j) := (\varphi_j, \varphi_i)_{Y(\hat{\Omega})}\,.$$

This can be reformulated as a generalized eigenvalue problem:

$$K_n \vec{x}_n = \lambda_n M_n \vec{x}_n$$

where the largest eigenvalue λ_n gives the desired $\big(\hat{c}_1(n)\big)^2$.

Inverse Inequalities

In this work, we consider the reference domain $\hat{\Omega} = (-1,1)^2$ with

$$(u,v)_{X(\hat{\Omega})} = \int_{\hat{\Omega}} \partial_x u(x,y) \partial_x v(x,y) \, \mathrm{d}x \, \mathrm{d}y,$$
$$(u,v)_{Y(\hat{\Omega})} = \int_{\hat{\Omega}} u(x,y) v(x,y) \, \mathrm{d}x \, \mathrm{d}y,$$

for $u, v \in \hat{V}_n$, where $\hat{V}_n$ is the space of polynomials of degree less than n, i.e.

$$\hat{V}_n = \left\{ x^i y^j : 0 \leqslant i, j < n \right\}.$$

Problem Statement

The interest in inverse inequalities leads to the following problem:

Find the largest eigenvalue λ_n of the generalized eigenvalue problem

$$B_n\vec{x}_n = \lambda_n A_n \vec{x}_n$$

where A_n and B_n are certain $n \times n$ matrices.

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Equivalent formulation:

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Relaxed problem: find expressions $b_1(n)$ and $b_2(n)$ such that

$$b_1(n) < \lambda_n < b_2(n)$$

("as accurate as possible").

Problem Statement

$$\boxed{\forall\, n \in \mathbb{N}\colon b_1(n) < \lambda_n < b_2(n)}$$

$$\lambda_n := \max_{\lambda}\ \det(B_n - \lambda A_n) = 0$$

The matrix entries are:

$$a_{i,j} := \frac{1 - (-1)^{i+j-1}}{i+j-1}$$

$$b_{i,j} := (i-1)(j-1)\frac{1 - (-1)^{i+j-3}}{i+j-3}$$

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Automatic DISCOVERY(!) and PROOF(!!)
of Holonomic Determinant Evaluations

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linear recurrences
polynomial coefficients
finitely many initial values

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- $A_n = (a_{i,j})_{1 \leqslant i,j \leqslant n}$ is an $n \times n$ matrix,
- $a_{i,j}$ is a bivariate holonomic sequence, not depending on n,
- $b_n \neq 0$ for all $n \geqslant 1$.

$$
\begin{pmatrix}
a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\
a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\
a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\
\vdots & \vdots & \vdots & & \vdots \\
a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n}
\end{pmatrix}
$$

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (A_n^{-1})_{1,n} \\ (A_n^{-1})_{2,n} \\ (A_n^{-1})_{3,n} \\ \vdots \\ (A_n^{-1})_{n,n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$
\begin{pmatrix}
a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\
a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\
a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\
\vdots & \vdots & \vdots & & \vdots \\
a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n}
\end{pmatrix}
\begin{pmatrix}
(-1)^{n+1} \dfrac{\det A_n^{(n,1)}}{\det A_n} \\
(-1)^{n+2} \dfrac{\det A_n^{(n,2)}}{\det A_n} \\
(-1)^{n+3} \dfrac{\det A_n^{(n,3)}}{\det A_n} \\
\vdots \\
(-1)^{2n} \dfrac{\det A_n^{(n,n)}}{\det A_n}
\end{pmatrix}
=
\begin{pmatrix}
0 \\
0 \\
0 \\
\vdots \\
1
\end{pmatrix}
$$

- $A_n^{(i,j)}$: matrix A_n with row i and column j deleted

$$
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\vdots & \vdots & \vdots & & \vdots \\
a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n}
\end{pmatrix}
\begin{pmatrix}
(-1)^{n+1} \dfrac{M_{n,1}}{\det A_n} \\
(-1)^{n+2} \dfrac{M_{n,2}}{\det A_n} \\
(-1)^{n+3} \dfrac{M_{n,3}}{\det A_n} \\
\vdots \\
\dfrac{M_{n,n}}{\det A_n}
\end{pmatrix}
=
\begin{pmatrix}
0 \\
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0 \\
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1
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- $A_n^{(i,j)}$: matrix A_n with row i and column j deleted
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- Define $c_{n,j} := (-1)^{n+j} M_{n,j} / M_{n,n}$

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- Define $c_{n,j} := (-1)^{n+j} M_{n,j}/M_{n,n}$
- We obtain $\sum_{j=1}^{n} a_{i,j} c_{n,j} = \delta_{i,n} \dfrac{\det A_n}{\det A_{n-1}}$

Determinant Evaluation: Proof by Induction

Problem: Prove that $\det A_n = \det\limits_{1 \leqslant i,j \leqslant n} a_{i,j} = b_n$ for all $n \in \mathbb{N}$.

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Induction step: the assumption implies that the linear system

$$\begin{pmatrix} a_{1,1} & \cdots & a_{1,n-1} & a_{1,n} \\ \vdots & \ddots & \vdots & \vdots \\ a_{n-1,1} & \cdots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} c_{n,1} \\ \vdots \\ c_{n,n-1} \\ c_{n,n} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

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has a unique solution, namely $c_{n,j} = (-1)^{n+j} M_{n,j} / M_{n,n}$.

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Now use $c_{n,j}$ to do Laplace expansion of A_n w.r.t. the last row:

$$\det A_n = \sum_{j=1}^{n} (-1)^{n+j} M_{n,j} a_{n,j} = \sum_{j=1}^{n} \underbrace{M_{n,n}}_{b_{n-1}} c_{n,j} a_{n,j}.$$

Showing that the sum evaluates to b_n completes the induction step.

Some Examples

$$\det_{1\leqslant i,j\leqslant n} \frac{1}{i+j-1} = \frac{1}{(2n-1)!} \prod_{k=1}^{n-1} \frac{(k!)^2}{(k+1)_{n-1}}$$

$$\det_{0\leqslant i,j\leqslant n-1} \binom{2i+2a}{j+b} = 2^{n(n-1)/2} \prod_{k=0}^{n-1} \frac{(2k+2a)!k!}{(k+b)!(2k+2a-b)!}$$

$$\det_{0\leqslant i,j\leqslant n-1} \sum_k \binom{i}{k}\binom{j}{k} 2^k = 2^{n(n-1)/2}$$

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Toy Example (Hilbert Matrix)

$$A_n := (a_{i,j})_{1 \leqslant i,j \leqslant n} = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{n+1} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \cdots & \frac{1}{n+2} \\ \vdots & \vdots & \vdots & & \vdots \\ \frac{1}{n} & \frac{1}{n+1} & \frac{1}{n+2} & \cdots & \frac{1}{2n-1} \end{pmatrix}$$

with $a_{i,j} := \dfrac{1}{i+j-1}$.

Toy Example

We can explicitly compute the numbers $c_{n,j}$:

$$
\begin{array}{ccccccc}
n=1 & n=2 & n=3 & n=4 & n=5 & n=6 & n=7 \\
\begin{pmatrix} 1 \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix} &
\begin{pmatrix} \frac{1}{6} \\ -1 \\ 1 \end{pmatrix} &
\begin{pmatrix} -\frac{1}{20} \\ \frac{3}{5} \\ -\frac{3}{2} \\ 1 \end{pmatrix} &
\begin{pmatrix} \frac{1}{70} \\ -\frac{2}{7} \\ \frac{9}{7} \\ -2 \\ 1 \end{pmatrix} &
\begin{pmatrix} -\frac{1}{252} \\ \frac{5}{42} \\ -\frac{5}{6} \\ \frac{20}{9} \\ -\frac{5}{2} \\ 1 \end{pmatrix} &
\begin{pmatrix} \frac{1}{924} \\ -\frac{1}{22} \\ \frac{5}{11} \\ -\frac{20}{11} \\ \frac{75}{22} \\ -3 \\ 1 \end{pmatrix}
\end{array}
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From this we **guess** that

$$c_{n,j} = (-1)^{j+n} \binom{n-1}{j-1} \binom{j+n-2}{j-1} \binom{2n-2}{n-1}^{-1},$$

and then prove (symbolically!) that this guess is correct.

Toy Example

Then we evaluate the sum (e.g., using Zeilberger's algorithm)

$$\sum_{j=1}^{n} a_{n,j} c_{n,j} = \sum_{j=1}^{n} \frac{(-1)^{j+n}}{n+j-1} \binom{n-1}{j-1} \binom{j+n-2}{j-1} \binom{2n-2}{n-1}^{-1}$$

$$= \frac{1}{2n-1} \binom{2n-2}{n-1}^{-2} = \frac{\det A_n}{\det A_{n-1}}.$$

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$$= \frac{1}{2n-1} \binom{2n-2}{n-1}^{-2} = \frac{\det A_n}{\det A_{n-1}}.$$

Therefore:

$$\det A_n = \prod_{k=1}^{n} \frac{1}{2k-1} \binom{2k-2}{k-1}^{-2} = \frac{1}{(2n-1)!} \prod_{k=1}^{n-1} \frac{(k!)^2}{(k+1)_{n-1}}.$$

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$$= \frac{1}{2n-1} \binom{2n-2}{n-1}^{-2} = \frac{\det A_n}{\det A_{n-1}}.$$

Therefore:

$$\det A_n = \prod_{k=1}^{n} \frac{1}{2k-1} \binom{2k-2}{k-1}^{-2} = \frac{1}{(2n-1)!} \prod_{k=1}^{n-1} \frac{(k!)^2}{(k+1)_{n-1}}.$$

Problem: What if there is no such nice closed form for $c_{n,j}$?

Toy Example

Then we evaluate the sum (e.g., using Zeilberger's algorithm)

$$\sum_{j=1}^{n} a_{n,j} c_{n,j} = \sum_{j=1}^{n} \frac{(-1)^{j+n}}{n+j-1} \binom{n-1}{j-1} \binom{j+n-2}{j-1} \binom{2n-2}{n-1}^{-1}$$
$$= \frac{1}{2n-1} \binom{2n-2}{n-1}^{-2} = \frac{\det A_n}{\det A_{n-1}}.$$

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Problem: What if there is no such nice closed form for $c_{n,j}$?
$\longrightarrow$ Use holonomic functions!

Principia Holonomica

1. Sequences are represented by a set (Gröbner basis) of recurrence equations (and initial values).

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Implementations are available in F. Chyzak's Maple package `Mgfun` and our Mathematica package `HolonomicFunctions`; here we will use the latter one.

Toy Example

We can explicitly compute the numbers $c_{n,j}$:

$$
\begin{array}{ccccccc}
n=1 & n=2 & n=3 & n=4 & n=5 & n=6 & n=7 \\
\begin{pmatrix}1\end{pmatrix} &
\begin{pmatrix}-\frac{1}{2}\\ 1\end{pmatrix} &
\begin{pmatrix}\frac{1}{6}\\ -1\\ 1\end{pmatrix} &
\begin{pmatrix}-\frac{1}{20}\\ \frac{3}{5}\\ -\frac{3}{2}\\ 1\end{pmatrix} &
\begin{pmatrix}\frac{1}{70}\\ -\frac{2}{7}\\ \frac{9}{7}\\ -2\\ 1\end{pmatrix} &
\begin{pmatrix}-\frac{1}{252}\\ \frac{5}{42}\\ -\frac{5}{6}\\ \frac{20}{9}\\ -\frac{5}{2}\\ 1\end{pmatrix} &
\begin{pmatrix}\frac{1}{924}\\ -\frac{1}{22}\\ \frac{5}{11}\\ -\frac{20}{11}\\ \frac{75}{22}\\ -3\\ 1\end{pmatrix}
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\end{array}
$$

From this we **guess** that

$$
c_{n,j} = \frac{(j-n-1)(j+n-2)}{(j-1)^2}\, c_{n,j-1},
$$

$$
c_{n,j} = \frac{(n-1)(j+n-2)}{2(2n-3)(j-n)}\, c_{n-1,j}.
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- The values of $c_{n,j}$ can be computed for concrete $n, j \in \mathbb{N}$.
- If recurrences exist they can be guessed automatically (e.g. with M. Kauers's Mathematica package `Guess`)

Toy Example

Guessed holonomic definition for $c_{n,j}$:

$$c_{n,j} = \frac{(j-n-1)(j+n-2)}{(j-1)^2}\, c_{n,j-1},$$
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Show that the definition implies $c_{n,n} = 1$ for all n:

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Prove $\sum_{j=1}^{n} a_{i,j} c_{n,j} = 0$ for all $n \in \mathbb{N}$ and $1 \leqslant i < n$. [skip]

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Use closure properties to get a holonomic representation of $a_{n,j}c_{n,j}$.

Creative telescoping yields a recurrence for $S(n) := \sum_{j=1}^{n} a_{n,j}c_{n,j}$:

$$4(4n^2-1)S(n+1) = n^2 S(n), \quad S(1) = 1.$$

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Unique solution of this recurrence: $S(n) = \dfrac{1}{2n-1}\dbinom{2n-2}{n-1}^{-2}$.

Zeilberger's Holonomic Ansatz

1. Compute many values of $c_{n,j}$ (e.g. for $1 \leqslant j \leqslant n \leqslant 100$).
2. Guess linear recurrences for $c_{n,j}$ from that data.
3. Prove the following identities using holonomic closure properties and creative telescoping:

$$c_{n,n} = 1 \qquad (n \geqslant 1), \tag{1}$$

$$\sum_{j=1}^{n} c_{n,j} a_{i,j} = 0 \qquad (1 \leqslant i < n), \tag{2}$$

$$\sum_{j=1}^{n} c_{n,j} a_{n,j} = \frac{b_n}{b_{n-1}} \qquad (n \geqslant 1). \tag{3}$$

Note: all these steps can be executed automatically!

Back to Inverse Inequalities

Recall: We are interested in evaluating $\det(B_n - \lambda A_n)$ for symbolic λ and for symbolic n.

The entries of the matrices A_n and B_n in our case are:

$$a_{i,j} := \frac{1-(-1)^{i+j-1}}{i+j-1}$$

$$b_{i,j} := (i-1)(j-1)\frac{1-(-1)^{i+j-3}}{i+j-3}$$

Back to Inverse Inequalities

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$$|B_6 - \lambda A_6| = \begin{vmatrix} -2\lambda & 0 & -\frac{2}{3}\lambda & 0 & -\frac{2}{5}\lambda & 0 \\ 0 & 2-\frac{2}{3}\lambda & 0 & 2-\frac{2}{5}\lambda & 0 & 2-\frac{2}{7}\lambda \\ -\frac{2}{3}\lambda & 0 & \frac{8}{3}-\frac{2}{5}\lambda & 0 & \frac{16}{5}-\frac{2}{7}\lambda & 0 \\ 0 & 2-\frac{2}{5}\lambda & 0 & \frac{18}{5}-\frac{2}{7}\lambda & 0 & \frac{30}{7}-\frac{2}{9}\lambda \\ -\frac{2}{5}\lambda & 0 & \frac{16}{5}-\frac{2}{7}\lambda & 0 & \frac{32}{7}-\frac{2}{9}\lambda & 0 \\ 0 & 2-\frac{2}{7}\lambda & 0 & \frac{30}{7}-\frac{2}{9}\lambda & 0 & \frac{50}{9}-\frac{2}{11}\lambda \end{vmatrix}$$

Back to Inverse Inequalities

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Hence we get: $\det(B_n - \lambda A_n) = 2^n \det\left(A^{(1)}_{\lceil n/2 \rceil}\right) \cdot \det\left(A^{(0)}_{\lfloor n/2 \rfloor}\right).$

$$A_n^{(0)} = (a_{i,j}^{(0)})_{1 \leqslant i,j \leqslant n} \quad \text{with} \quad a_{i,j}^{(0)} := \frac{(2i-1)(2j-1)}{2i+2j-3} - \frac{\lambda}{2i+2j-1}$$

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$$\det A_1^{(0)} = 1 - \frac{\lambda}{3}$$

$$\det A_2^{(0)} = \frac{4\lambda^2}{525} - \frac{12\lambda}{35} + \frac{4}{5}$$

$$\det A_3^{(0)} = -\frac{256\lambda^3}{22920975} + \frac{512\lambda^2}{218295} - \frac{256\lambda}{4851} + \frac{256}{2205}$$

$$\det A_4^{(0)} = \frac{65536\lambda^4}{63275987399625} - \frac{131072\lambda^3}{200876150475} + \frac{65536\lambda^2}{1217431215} - \frac{65536\lambda}{6689182}$$

$$\det A_5^{(0)} = -\frac{1073741824\lambda^5}{177624332221127738821875} + \frac{1073741824\lambda^4}{1196123449300523493 75} -$$

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- These polynomials are irreducible.
- Hence $\det\left(A_n^{(0)}\right) / \det\left(A_{n-1}^{(0)}\right)$ is (probably) not holonomic.
- Neither is $\det\left(A_n^{(0)}\right)$ a holonomic sequence.

$$
\begin{pmatrix}
a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\
a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\
a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\
\vdots & \vdots & \vdots & & \vdots \\
a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n}
\end{pmatrix}
\begin{pmatrix}
(-1)^{n+1} \dfrac{M_{n,1}}{M_{n,n}} \\
(-1)^{n+2} \dfrac{M_{n,2}}{M_{n,n}} \\
(-1)^{n+3} \dfrac{M_{n,3}}{M_{n,n}} \\
\vdots \\
1
\end{pmatrix}
=
\begin{pmatrix}
0 \\
0 \\
0 \\
\vdots \\
\dfrac{\det A_n^{(0)}}{\det A_{n-1}^{(0)}}
\end{pmatrix}
$$

$$
\begin{pmatrix}
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\vdots & \vdots & \vdots & & \vdots \\
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\end{pmatrix}
\begin{pmatrix}
(-1)^{n+1}\dfrac{M_{n,1}}{M_{n,n}} \\
(-1)^{n+2}\dfrac{M_{n,2}}{M_{n,n}} \\
(-1)^{n+3}\dfrac{M_{n,3}}{M_{n,n}} \\
\vdots \\
1
\end{pmatrix}
=
\begin{pmatrix}
0 \\
0 \\
0 \\
\vdots \\
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\end{pmatrix}
$$

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- This normalization could be used if $\det A^{(0)}$ was holonomic.

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (-1)^{n+1}\dfrac{M_{n,1}}{\ell_n} \\ (-1)^{n+2}\dfrac{M_{n,2}}{\ell_n} \\ (-1)^{n+3}\dfrac{M_{n,3}}{\ell_n} \\ \vdots \\ \dfrac{M_{n,n}}{\ell_n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \dfrac{\det A_n^{(0)}}{\ell_n} \end{pmatrix}$$

- ℓ_n is the leading coefficient of $\det A_n^{(0)}$.

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} c_{n,1}^{(0)} \\ c_{n,2}^{(0)} \\ c_{n,3}^{(0)} \\ \vdots \\ c_{n,n}^{(0)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \dfrac{\det A_n^{(0)}}{\ell_n} \end{pmatrix}$$

- ℓ_n is the leading coefficient of $\det A_n^{(0)}$.
- Define $c_{n,j}^{(0)} := (-1)^{n+j} \dfrac{M_{n,j}}{\ell_n}$.

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- Define $c_{n,j}^{(0)} := (-1)^{n+j} \dfrac{M_{n,j}}{\ell_n}$.
- Thanks to the parameter λ this normalization is easy to achieve.

We conjecture

$$c_{n,j}^{(0)} = \frac{2^{2n+2j-3}\left(\frac{3}{2}\right)_{2n-1}\left(n+\frac{1}{2}\right)_{j-1}}{(n-1)!\,(2j-1)!} \times \sum_{m=0}^{n-1}\sum_{k=0}^{2n-2m-2} \frac{(-1)^{j+m}\,(2m+1)_{2k}\,\lambda^m}{4^{m+k}k!\,(2m+k-n-j+2)!}$$

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Then we prove

$$\sum_{j=1}^{n} a_{i,j}^{(0)} c_{n,j}^{(0)} = \delta_{i,n} \sum_{j=0}^{n} (-4)^{j-n} \frac{(2n-2j+1)_{2n}}{(2j)!} \lambda^j$$

from which we can conclude that

$$\det A_n^{(0)} = c_n \cdot \sum_{j=0}^{n} (-4)^{j-n} \frac{(2n-2j+1)_{2n}}{(2j)!} \lambda^j$$

for some (yet unknown) constant c_n.

With the original version of the holonomic ansatz, we prove

$$c_n = \det\Bigl(\lim_{\lambda\to\infty} \tfrac{1}{\lambda} A_n^{(0)}\Bigr) = \bigl(-\tfrac{1}{2}\bigr)^n \prod_{i=1}^{n} \frac{\bigl((i-1)!\bigr)^2}{\bigl(i+\frac{1}{2}\bigr)_n}$$

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And hence we obtain:

Theorem.

$$\det A_n^{(0)} = \underbrace{\big(-\tfrac{1}{2}\big)^n \prod_{i=1}^{n} \frac{\big((i-1)!\big)^2}{\big(i+\frac{1}{2}\big)_n}}_{\text{“hyperholonomic” part}} \underbrace{\sum_{j=0}^{n} (-4)^{j-n} \frac{(2n-2j+1)_{2n}}{(2j)!} \lambda^j}_{\text{holonomic part}},$$

$$\det A_n^{(1)} = \big(-\tfrac{1}{2}\big)^n \prod_{i=1}^{n} \frac{\big((i-1)!\big)^2}{\big(i-1+\frac{1}{2}\big)_n} \sum_{j=0}^{n-1} \frac{(2n-2j-1)_{2n-1}}{(-4)^{n-j-1}(2j+1)!} \lambda^j.$$

Part II: Estimation of the Largest Eigenvalue

Let $F_n(\lambda) := \det(B_n - \lambda A_n)$ and $\nu(n) := \left\lfloor \frac{n}{2} \right\rfloor$.

We have to estimate the largest root of the polynomial

$$\begin{aligned} F_n(\lambda) &= \sum_{j=0}^{\nu(n)} (-1)^j f_j(n) \lambda^{\nu(n)-j} \\ &= \lambda^{\nu(n)} - f_1(n)\lambda^{\nu(n)-1} + f_2(n)\lambda^{\nu(n)-2} - \dots \end{aligned}$$

where

$$f_j(n) := \frac{(n-2j+1)_{4j}}{4^j (2j)!}.$$

We prove a series of lemmas concerning the properties of this family of polynomials...

Monotonicity of the Largest Root

Lemma. Let $n \in \mathbb{N}$ with $n \geqslant 2$. If $\lambda \in \mathbb{R}$ is a root of F_n with $\lambda > \frac{1}{2} f_1(n)$ then $F_{n+1}(\lambda) < 0$.

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Proof. Case $n = 2k+2$. We have that $\nu(n) = \nu(n+1) = k+1$. Define

$$\begin{aligned} G_n(x) &:= F_{n+1}(x) - F_n(x) \\ &= \sum_{j=0}^{k} (-4)^{j-k} \frac{(2k-2j+3)_{2k+2}}{(2j+1)!} (j-k-1) x^j, \end{aligned}$$

and denote by $g_j(n)$ the absolute value of the j-th coefficient:

$$g_j(n) = 4^{j-k} \frac{(2k-2j+3)_{2k+2}}{(2j+1)!} (k-j+1).$$

Our goal is to show that $G_n(x) < 0$ for $x > \frac{1}{2} f_1(n)$.

Subgoal: Show $\lambda\, g_j(n) > g_{j-1}(n)$ for $1 \leqslant j \leqslant k$ and $\lambda > \frac{1}{2} f_1(n)$.
Next: Show that $\frac{1}{2} f_1(n)\, g_j(n) > g_{j-1}(n)$ for $1 \leqslant j \leqslant k$.
Substituting for $g_j(n)$ we obtain

$$\tfrac{1}{2} f_1(n) 4^{j-k} \tfrac{(k-j+1)(2k-2j+3)_{2k+2}}{(2j+1)!} > 4^{j-1-k} \tfrac{(k-j+2)(2k-2j+5)_{2k+2}}{(2j-1)!}.$$

Multiply by $(2j-1)!$ and divide by $4^{j-1-k}(2k-2j+5)_{2k}$:

$$2 f_1(n) \tfrac{(k-j+1)(2k-2j+3)(2k-2j+4)}{2j(2j+1)} > (k-j+2)(4k-2j+5)(4k-2j+6).$$

Plugging in $f_1(n) = \frac{1}{8}(2k+1)(2k+2)(2k+3)(2k+4)$ and substituting $j \to k-j$ leads to

$$\begin{aligned} &(16j^3 + 72j^2 + 88j + 16)k^4 + (80j^3 + 360j^2 + 424j + 48)k^3 \\ &+ (172j^3 + 774j^2 + 906j + 92)k^2 + (196j^3 + 882j^2 + 1070j + 180)k \\ &\qquad - 16j^5 - 112j^4 - 212j^3 + 16j^2 + 276j + 72 > 0 \end{aligned}$$

for $0 \leqslant j \leqslant k-1$. Since $k > j$, the above inequality is true if it is true for $k = j$. Substituting $k = j$ yields

$$16j^7 + 152j^6 + 604j^5 + 1298j^4 + 1624j^3 + 1178j^2 + 456j + 72 > 0,$$

which is obviously true for all $j \geqslant 0$.

Finally note that if k is even then

$$G_n(\lambda) = \underbrace{-g_0}_{<0} + \sum_{j=1}^{k/2} \underbrace{\big(-g_{2j}(n)\lambda + g_{2j-1}(n)\big)}_{<0} \lambda^{2j-1} < 0,$$

and if k is odd then

$$G_n(\lambda) = \sum_{j=0}^{(k-1)/2} \underbrace{\big(-g_{2j+1}(n)\lambda + g_{2j}(n)\big)}_{<0} \lambda^{2j} < 0.$$

Lesson learned: Don't do that! Use computer algebra!

Case $n = 2k + 1$. Use the same argument as before, which leads to the rational function inequality

$$\frac{k(2k+1)(2k+2)(2k+3)(k-j+1)(2k-2j+3)(k-j+2)}{4j(2j-1)(k-j+2)(2k-j+2)(4k-2j+5)} > 1.$$

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```
CylindricalDecomposition[
  Implies[1 <= j <= k, ineq], {j, k}]
```

yields `True` in a fraction of a second.

Upper and Lower Bounds

Main idea:

$$F_n(\lambda) = \underbrace{\lambda^{\nu(n)} - f_1(n)\lambda^{\nu(n)-1} + f_2(n)\lambda^{\nu(n)-2}}_{\text{head polynomial}} \underbrace{-f_3(n)\lambda^{\nu(n)-3} + \dots}_{\text{tail}}$$

1. Define $m(n)$, the largest root of the head polynomial:

$$m(n) := \frac{1}{2}\Big(f_1(n) + \sqrt{f_1(n)^2 - 4f_2(n)}\Big)$$
$$= \frac{f_1(n)}{2}\left(1 + \sqrt{1 - \frac{2}{3}\frac{(n-2)(n-3)(n+3)(n+4)}{n(n-1)(n+1)(n+2)}}\right).$$

2. Use the lemmas to show that the tail is positive for all $\lambda > m(n)$.

$\longrightarrow m(n)$ is an upper bound for the largest root of $F_n(\lambda)$.

For all $n \in \mathbb{N}$ we have the estimate $b_1(n) < \lambda_n < b_2(n)$ with

$$b_1(n) := \frac{m_1(n)}{2} \left(1 + \sqrt{1 - \frac{2}{3}\frac{(n-2)(n-3)(n+3)(n+4)}{n(n-1)(n+1)(n+2)}}\right),$$

$$b_2(n) := m_1(n) \left(\frac{1}{3} + \left(r_1(n) + \sqrt{r_2(n)}\right)^{1/3} + \left(r_1(n) - \sqrt{r_2(n)}\right)^{1/3}\right),$$

where m_1, r_1, and r_2 are given by

$$m_1(n) := \frac{n(n-1)(n+1)(n+2)}{8},$$

$$r_1(n) := \frac{2(n^8 + 4n^7 + 8n^6 + \cdots - 4733n^2 - 5130n + 16200)}{135n^2(n-1)^2(n+1)^2(n+2)^2},$$

$$r_2(n) := \frac{(n-2)(n-3)(n+4)(n+3)\,q(n)}{145800n^4(n-1)^4(n+1)^4(n+2)^4},$$

and the polynomial q in r_2 is given by

$$7n^{12} + 42n^{11} - 641n^{10} + \cdots - 44971200n + 116640000.$$

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Conclusion

1. Our results improve previously known bounds by a large factor.
2. By putting more and more terms into the head polynomial, one get more and more precise bounds, at the cost of more complicated algebraic expressions.
3. The numerical analysts were very excited about these results.