

Inverse Inequality Estimates with Symbolic Computation (Part II)

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(joint work with Martin Neumüller and Silviu Radu)

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FOR COMPUTATIONAL AND APPLIED MATHEMATICS

Problem Statement

The interest in numerical analysis in so-called inverse inequalities yields 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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$$\lambda_n := \max_{\lambda} \det(B_n - \lambda A_n) = 0.$$

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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").

Overview

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

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

The matrix entries are:

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

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

Part II: With symbolic computations, evaluate $\det(B_n - \lambda A_n)$ in a (complicated) closed form.

Part III: Using the closed form, derive very accurate bounds $b_1(n)$ and $b_2(n)$.

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Automatic DISCOVERY(!) and PROOF(!!)
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- ▶ $a_{i,j}$ is a bivariate **holonomic** sequence, not depending on n ,

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- ▶ $a_{i,j}$ is a bivariate holonomic sequence, not depending on n ,
- ▶ $b_n \neq 0$ for all $n \geq 1$.

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

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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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- ▶ We obtain $\sum_{j=1}^n a_{i,j} c_{n,j} = \delta_{i,n} \frac{\det A_n}{\det A_{n-1}}$

Determinant Evaluation: Proof by Induction

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

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Induction step: the assumption implies that the linear system

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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)

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

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

Toy Example

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

$$n = 1 \quad n = 2 \quad n = 3 \quad n = 4 \quad n = 5 \quad n = 6 \quad n = 7$$

$$(1) \quad \begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{6} \\ -1 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -\frac{1}{20} \\ \frac{3}{5} \\ -\frac{3}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{70} \\ -\frac{2}{7} \\ \frac{9}{7} \\ -2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -\frac{1}{252} \\ \frac{5}{42} \\ -\frac{5}{6} \\ \frac{20}{9} \\ -\frac{5}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{924} \\ -\frac{1}{22} \\ \frac{5}{11} \\ -\frac{20}{11} \\ \frac{75}{22} \\ -3 \\ 1 \end{pmatrix}$$

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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)

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

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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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→ Use holonomic functions!

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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.

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

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$$(1) \quad \begin{pmatrix} -\frac{1}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{6} \\ -1 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -\frac{1}{20} \\ \frac{3}{5} \\ -\frac{3}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{70} \\ -\frac{2}{7} \\ \frac{9}{7} \\ -2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -\frac{1}{252} \\ \frac{5}{42} \\ -\frac{5}{6} \\ \frac{20}{9} \\ -\frac{5}{2} \\ 1 \end{pmatrix} \quad \begin{pmatrix} \frac{1}{924} \\ -\frac{1}{22} \\ \frac{5}{11} \\ -\frac{20}{11} \\ \frac{75}{22} \\ -3 \\ 1 \end{pmatrix}$$

Toy Example

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

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

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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- ▶ Work with an implicit (recursive) definition of $c_{n,j}$.
- ▶ 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 $c_{n,j}$:

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

$$c_{n,j} = \frac{(n-1)(j+n-2)}{2(2n-3)(j-n)} c_{n-1,j},$$

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Show that the definition implies $c_{n,n} = 1$ for all n :

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$$c_{n,j} = \frac{(j-n-1)(j+n-2)}{(j-1)^2} \frac{(n-1)(j-1+n-2)}{2(2n-3)(j-1-n)} c_{n-1,j-1}$$

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

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Show that the definition implies $c_{n,n} = 1$ for all n :

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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: $S(n) = \frac{1}{2n-1} \binom{2n-2}{n-1}^{-2}$.

Zeilberger's Holonomic Ansatz

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

$$c_{n,n} = 1 \quad (n \geq 1), \tag{1}$$

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

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

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

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

Back to Inverse Inequalities

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

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

Back to Inverse Inequalities

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Back to Inverse Inequalities

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

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

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

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

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

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

$$\det A_5^{(0)} = -\frac{1073741824\lambda^5}{177624332221127738821875} + \frac{1073741824\lambda^4}{119612344930052349375} -$$

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

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

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

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

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

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

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

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

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

- ▶ ℓ_n is the leading coefficient of $\det A_n^{(0)}$.
- ▶ Define $c_{n,j}^{(0)} := (-1)^{n+j} \frac{M_{n,j}}{\ell_n}$.
- ▶ Thanks to the parameter λ this normalization is easy to achieve.

We conjecture

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

We conjecture

$$c_{n,j}^{(0)} = \frac{2^{2n+2j-3} \left(\frac{3}{2}\right)_{2n-1} \left(n + \frac{1}{2}\right)_{j-1}}{(n-1)! (2j-1)!}$$
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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

$$c_n = \det \left(\lim_{\lambda \rightarrow \infty} \frac{1}{\lambda} A_n^{(0)} \right) = \left(-\frac{1}{2} \right)^n \prod_{i=1}^n \frac{(i-1)!}{\left(i + \frac{1}{2} \right)_n}$$

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And hence we obtain:

Theorem.

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

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

Recall that we had

$$\det(B_n - \lambda A_n) = 2^n \det\left(A_{\lceil n/2 \rceil}^{(1)}\right) \cdot \det\left(A_{\lfloor n/2 \rfloor}^{(0)}\right).$$

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To be continued with:

Part III: Using the closed form, derive bounds $b_1(n)$ and $b_2(n)$ s.t.

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