Zeilberger’s Holonomic Ansatz for Pfaffians

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Introduction

The HOLONOMIC ANSATZ II.
Automatic DISCOVERY(!) and PROOF(!!)
of Holonomic Determinant Evaluations
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det A_n = \det_{1 \leq i, j \leq n} a_{i,j} = b_n \quad (n \geq 1)
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- \( a_{i,j} \) is a bivariate **holonomic** sequence, not depending on \( n \),
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where

- \( a_{i,j} \) is a bivariate **holonomic** sequence, not depending on \( n \),

  - linear recurrences
  - polynomial coefficients
  - finitely many initial values
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\]

where

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

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

\[
\det_{0 \leq i,j \leq n-1} \begin{pmatrix} 2i + 2a \\ j + b \end{pmatrix} = 2^{n(n-1)/2} \prod_{k=0}^{n-1} \frac{(2k + 2a)!k!}{(k + b)!(2k + 2a - b)!}
\]

\[
\det_{0 \leq i,j \leq n-1} \sum_{k} \binom{i}{k} \binom{j}{k} 2^k = 2^{n(n-1)/2}
\]
A Prominent Example

C. K., M. Kauers, D. Zeilberger:

Proof of George Andrews’s and David Robbins’s
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By evaluating the $q$-holonomic determinant

$$\det_{1 \leq i,j \leq n} \left( q^{i+j-1} \left[ \begin{array}{c} i+j-2 \\ i-1 \end{array} \right]_q + q^{i+j} \left[ \begin{array}{c} i+j-1 \\ i \end{array} \right]_q + (1 + q^i) \delta_{i,j} - \delta_{i,j+1} \right)$$

$$= \prod_{1 \leq i \leq j \leq k \leq n} \left( \frac{1 - q^{i+j+k-1}}{1 - q^{i+j+k-2}} \right)^2$$

a long-standing combinatorial problem (first stated in 1983) was solved, the $q$-enumeration of totally symmetric plane partitions.
Determinant Evaluation: Proof by Induction

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

Base case: verify that $a_{1,1} = b_1$.

Induction hypothesis: assume that $\det A_{n-1} = b_{n-1} \neq 0$.

Induction step: the assumption implies that the linear system:

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

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

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

$\det A_n = \sum_{i=1}^n M_{n,n} c_{n,i} a_{n,i}$.

Showing that the sum evaluates to $b_n$ completes the induction step.
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\det A_n = \sum_{i=1}^{n} M_{n,n} c_{n,i} a_{n,i}.
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Explanation for $c_{n,i}$

It’s easy to see that $c_{n,i} = (-1)^{n+i} M_{n,i} / M_{n,n}$ is the solution of the system

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\end{pmatrix}.$$

Let $A(j)_n$ denote the matrix that is obtained from $A_n$ by replacing the last row by the $j$-th row ($1 \leq j < n$).

Laplace expansion of $A(j)_n$ w.r.t. the last row:

$$\det A(j)_n = 0 = n \sum_{i=1} M_{n,n} c_{n,i} a_{j,i}.$$
Explanation for \( c_{n,i} \)

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Let \( A_{n}^{(j)} \) denote the matrix that is obtained from \( A_n \) by replacing the last row by the \( j \)-th row \((1 \leq j < n)\).
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Let $A_{n}^{(j)}$ denote the matrix that is obtained from $A_n$ by replacing the last row by the $j$-th row ($1 \leq j < n$).

Laplace expansion of $A_{n}^{(j)}$ w.r.t. the last row:

$$
\det A_{n}^{(j)} = 0 = \sum_{i=1}^{n} M_{n,n} c_{n,i} a_{j,i}.
$$

This is just the $j$-th row in the above system.
How to get $c_{n,i}$

We cannot expect to be able to compute $c_{n,i}$ explicitly!
(at least not for symbolic $n$)
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Instead:

- Hope that $c_{n,i}$ is holonomic.
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Instead:

- Hope that $c_{n,i}$ is holonomic.
- Try to work with an implicit (recursive) definition of $c_{n,i}$.
- The values of $c_{n,i}$ can be computed for concrete $n, i \in \mathbb{N}$.
- If recurrences exist they can be guessed automatically (e.g. with M. Kauers’s Mathematica package Guess)
Zeilberger’s Holonomic Ansatz

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

$$c_{n,n} = 1 \quad (n \geq 1),$$  \hspace{1cm} (D1)

$$\sum_{i=1}^{n} c_{n,i} a_{j,i} = 0 \quad (1 \leq j < n),$$  \hspace{1cm} (D2)

$$\sum_{i=1}^{n} c_{n,i} a_{n,i} = \frac{b_n}{b_{n-1}} \quad (n \geq 1).$$  \hspace{1cm} (D3)

Note: all these steps can be executed automatically!
Pfaffians

Consider a skew-symmetric matrix $A$, i.e., $A = -A^T$:

\[
A = \begin{pmatrix}
  0 & a_{1,2} & a_{1,3} & \cdots \\
-a_{1,2} & 0 & a_{2,3} & \cdots \\
-a_{1,3} & -a_{2,3} & 0 & \cdots \\
  \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]

(it is easy to see that $\det A = 0$ if $A$ has odd dimensions).
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\end{pmatrix}$$

(it is easy to see that $\det A = 0$ if $A$ has odd dimensions).

Now let $A$ be a skew-symmetric matrix of size $2n \times 2n$. Then the Pfaffian of $A$ is defined as

$$\text{Pf } A := \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \text{sgn}(\sigma) \prod_{i=1}^{n} a_{\sigma(2i-1), \sigma(2i)}.$$

Note that $(\text{Pf } A)^2 = \det A$. 
Try to Apply Determinant Techniques
Zeilberger’s holonomic ansatz doesn’t work, since it requires
\[ \det A_n \neq 0 \text{ for all } n. \]
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In the paper

Advanced Computer Algebra for Determinants


C.K. and T. Thanatipanonda presented a variant of Zeilberger’s holonomic ansatz that considers the quotient

\[ \frac{\det A_n}{\det A_{n-2}}. \]
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$$\frac{\det A_n}{\det A_{n-2}}.$$ 

- This double step method works in theory,
- but is complicated in practice and
- leads to very large computations.
Laplace Expansion for Pfaffians

- Let $A = (a_{i,j})_{1 \leq i, j \leq 2n}$ be a skew-symmetric matrix.
- Denote by $A(i, j)$ the $(2n - 2) \times (2n - 2)$ matrix which is obtained by deleting the rows and columns $i$ and $j$ from $A$.
- Define the cofactors $\Gamma_{i,j} := \begin{cases} (-1)^{j-i-1} \text{Pf } A(i, j) & \text{if } i < j, \\ (-1)^{i-j} \text{Pf } A(j, i) & \text{if } j < i, \\ 0 & \text{if } i = j. \end{cases}$
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• Let $A = (a_{i,j})_{1 \leq i,j \leq 2n}$ be a skew-symmetric matrix.

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Then there exists a Laplace-type expansion for the Pfaffian of $A$:

$$\delta_{j,k} \text{Pf} A = \sum_{i=1}^{2n} a_{j,i} \Gamma_{k,i} = \sum_{i=1}^{2n} a_{i,j} \Gamma_{i,k}.$$
Laplace Expansion for Pfaffians

• Let \( A = (a_{i,j})_{1 \leq i,j \leq 2n} \) be a skew-symmetric matrix.

• Denote by \( A(i, j) \) the \((2n - 2) \times (2n - 2)\) matrix which is obtained by deleting the rows and columns \( i \) and \( j \) from \( A \).

• Define the cofactors \( \Gamma_{i,j} := \begin{cases} (-1)^{j-i+1} \text{Pf } A(i, j) & \text{if } i < j, \\ (-1)^{i-j} \text{Pf } A(j, i) & \text{if } j < i, \\ 0 & \text{if } i = j. \end{cases} \)

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\delta_{j,k} \text{Pf } A = \sum_{i=1}^{2n} a_{j,i} \Gamma_{k,i} = \sum_{i=1}^{2n} a_{i,j} \Gamma_{i,k}.
\]

Setting \( j = k = 2n \) leads to

\[
\text{Pf } A = \sum_{i=1}^{2n} a_{2n,i} \Gamma_{2n,i} = \sum_{i=1}^{2n} a_{i,2n} \Gamma_{i,2n}.
\]
Pfaffian Evaluation: Proof by Induction

**Problem:** Prove that $Pf A_{2n} = Pf(a_{i,j})_{1 \leq i,j \leq 2n} = b_n$ for all $n \in \mathbb{N}$.
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Base case: verify that $a_{1,2} = b_1$. 

Induction hypothesis: assume that $\text{Pf } A_{2n-2} = b_{n-1} \neq 0$.

Induction step: the assumption implies that the linear system
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\begin{pmatrix}
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    \vdots & \ddots & \vdots \\
    a_{1,2n-2} & \cdots & a_{2n-2,2n-2} \\
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has a unique solution, namely $c_{2n,i} = \frac{\Gamma_i}{\Gamma_{2n-1}}$. Now use $c_{2n,i}$ in the expansion formula for the Pfaffian of $A_{2n}$:

\[
\text{Pf } A_{2n} = (-1)^{n(n-1)/2} \sum_{i=1}^{2n} b_{n-1} c_{2n,i} a_{i,2n}.
\]

Showing that the sum evaluates to $b_n$ completes the induction step.
Problem: Prove that \( \text{Pf} A_{2n} = \text{Pf}(a_{i,j})_{1 \leq i,j \leq 2n} = b_n \) for all \( n \in \mathbb{N} \).

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\]

Now use \( c_{2n,i} \) in the expansion formula for the Pfaffian of \( A_{2n} \):

\[
\text{Pf} \ A_{2n} = 2^{n-1} \sum_{i=1}^{b_n-1} c_{2n,i} a_{i,2n} = b_n
\]

Showing that the sum evaluates to \( b_n \) completes the induction step.
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\end{pmatrix}
\]

has a unique solution, namely \( c_{2n,i} = \Gamma_{i,2n}/\Gamma_{2n-1,2n} = \Gamma_{i,2n}/b_{n-1} \).

Now use \( c_{2n,i} \) in the expansion formula for the Pfaffian of \( A_{2n} \):

\[
\text{Pf} A_{2n} = \sum_{i=1}^{2n-1} b_{n-1} c_{2n,i} a_{i,2n}.
\]

Showing that the sum evaluates to \( b_n \) completes the induction step.
Now the holonomic ansatz can be formulated for Pfaffians:

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

\[
c_{2n,2n-1} = 1 \quad (n \geq 1), \\
\sum_{i=1}^{2n-1} c_{2n,i}a_{i,j} = 0 \quad (1 \leq j < 2n), \\
\sum_{i=1}^{2n-1} c_{2n,i}a_{i,2n} = \frac{b_n}{b_{n-1}} \quad (n \geq 1).
\]

*implementations are available in F. Chyzak's Maple package Mgfun and C.K.'s Mathematica package HolonomicFunctions; here we will use the latter one.
A Worked Example

Consider the Pfaffian $\text{Pf} \left( (j - i)M_{i+j-3} \right)_{1 \leq i,j \leq 2n}$ where

$$M_n = \sum_{k=0}^{[n/2]} \frac{1}{k+1} \binom{n}{2k} \binom{2k}{k}$$

denotes the $n$-th Motzkin number: 1, 2, 4, 9, 21, 51, 127, 323, . . .

Clearly, $a_{i,j} = (j - i)M_{i+j-3}$ is a holonomic sequence:

$$(i - j - 2)a_{i,j} = (i - j)a_{i-1,j+1}$$

$$(i - j + 1)(i - j + 2)(i + j - 1)a_{i,j} =$$

$$(i - j)(i - j + 2)(2i + 2j - 5)a_{i,j-1} +$$

$$3(i - j)(i - j + 1)(i + j - 4)a_{i,j-2}$$
Guessed Recurrences for \(c_{2n,i}\)

\[
(i - 1)(2n - 3)(4n - 7)c_{2n,i} = \\
-(2n + i - 4)(8in - 8i - 8n^2 + 6n + 3)c_{2(n-1),i-1} + \\
(i - 1)(16in - 16i + 8n^2 - 34n + 27)c_{2(n-1),i} + \\
24i(i - 1)(n - 1)c_{2(n-1),i+1} - (2n - 3)(4n - 7)(2n - i)c_{2n,i-1}
\]

\[
(n - 2)(2n - 5)(4n - 11)(4n - 7)(2n - i - 2)(2n - i - 1)c_{2n,i} = \\
(2n - 5)(4n - 11)(8i^2n^2 - 24i^2n + 17i^2 - 16in^2 + 48in - \\
33i - 16n^4 + 108n^3 - 258n^2 + 258n - 92)c_{2(n-1),i} - \\
(n - 1)(4n - 7)(2n + i - 5)(32in^2 - 122in + \\
117i - 32n^3 + 168n^2 - 280n + 144)c_{2(n-2),i} + \\
6i(4i + 1)(n - 2)(n - 1)(2n - 3)(4n - 7)c_{2(n-2),i+1} + \\
36i(i + 1)(n - 2)(n - 1)(2n - 3)(4n - 7)c_{2(n-2),i+2}
\]

\[
18n(i - 3)(i - 2)(i - 1)c_{2n,i} = \\
(2n + i - 4)(10i^2n - 24in^2 - 63in + i + 16n^3 + 76n^2 + 97n - 3)c_{2n,i-3} + \\
2(i - 3)n(7i^2 - 12in - 46i + 33n + 73)c_{2n,i-2} - \\
3(i - 3)(i - 2)n(14i - 12n - 39)c_{2n,i-1} - \\
(2n - 1)(4n - 3)(2n - i + 4)(2n - i + 3)c_{2(n+1),i-3}
\]
Guessed Recurrences for $c_{2n,i}$

The support of these recurrences looks as follows:

The annihilating ideal they generate has rank 4.
Identity (P1)

\[ c_{2n,2n-1} = 1 \quad (n \geq 1), \]  

(P1)

Apply the holonomic closure property “integer-linear substitution”:

\[
DFiniteSubstitute[c2ni, \{i \rightarrow 2 \ n - 1\}] 
\]
Identity (P1)

\[ c_{2n,2n-1} = 1 \quad (n \geq 1), \quad (P1) \]

Apply the holonomic closure property “integer-linear substitution”:

\[ \text{DFiniteSubstitute}[c_{2ni}, \{i -> 2n - 1\}] \]

The result is a recurrence of order 4 for \( c_{2n,2n-1} \):

\[
648(n + 2)(n + 3)(2n + 3)(2n + 5)(4n + 9) \\
(1003520n^7 + 6117888n^6 + 12424768n^5 + 9388056n^4 \\
+ 318598n^3 - 2766651n^2 - 1249360n - 163269)c_{2(n+4),2(n+4)-1} \\
- 9(n + 2)(2n + 3)(2247884800n^{10} + \ldots)c_{2(n+3),2(n+3)-1} \\
+ 2(4n + 7)(6470696960n^{11} + \ldots)c_{2(n+2),2(n+2)-1} \\
-(4n + 3)(4n + 7)(1485209600n^{10} + \ldots)c_{2(n+1),2(n+1)-1} \\
+ 2(4n + 1)(4n + 3)(4n + 7)(4n - 1)^2(1003520n^7 + \ldots)c_{2n,2n-1} = 0
\]

which has \( S_n - 1 \) as a right factor and initial values 1, 1, 1, 1, 1.
Identity (P2)

\[ \sum_{i=1}^{2n-1} c_{2n,i} a_{i,j} = 0 \quad (1 \leq j < 2n), \quad (P2) \]

Apply closure property “times” and use creative telescoping:

\[
\text{smnd} = \text{DFiniteTimes}[c_{2n,i}, a_{i,j}]
\]

\[
\text{FindCreativeTelescoping}[\text{smnd}, S[i] - 1]
\]
Identity (P2)

\[ \sum_{i=1}^{2n-1} c_{2n,i} a_{i,j} = 0 \quad (1 \leq j < 2n), \quad \text{(P2)} \]

Apply closure property “times” and use creative telescoping:

\[
\text{smnd} = \text{DFiniteTimes}[c_{2ni}, a_{ij}]
\]
\[
\text{FindCreativeTelescoping}[	ext{smnd}, S[i] - 1]
\]

The result is a system of recurrences which is satisfied by the sum

\[
j(4n - 3)(j + 2n)s_{n+1,j} - n(4n + 1)(-j + 2n - 1)s_{n,j+1} - j(4n + 1)(j - n)s_{n,j} = 0,
\]
\[
(j - 2n + 2)(j + 2n)s_{n,j+2} - (j+1)(2j+1)s_{n,j+1} - 3j(j+1)s_{n,j} = 0,
\]

and whose initial values are all equal to 0.
Identity (P3)

\[ \sum_{i=1}^{2n-1} c_{2n,i} a_{i,2n} = \frac{b_n}{b_{n-1}} \quad (n \geq 1). \] (P3)

This is done by closure property “times” and creative telescoping.
Identity (P3)

\[
\sum_{i=1}^{2n-1} c_{2n,i}a_{i,2n} = \frac{b_n}{b_{n-1}} \quad (n \geq 1). \tag{P3}
\]

This is done by closure property “times” and creative telescoping.

The result is a recurrence for the ratio \( r_n := \det A_n / \det A_{n-1} \):

\[
2(4n - 11)(4n - 7)(4n - 5)(7n - 13)r_n
- (4n - 11)(350n^3 - 1413n^2 + 1798n - 714)r_{n-1}
+ 9(n - 2)(2n - 3)(4n - 7)(7n - 6)r_{n-2} = 0
\]

with initial values \( r_1 = 1 \) and \( r_2 = 5 \).
Identity (P3)

\[
\sum_{i=1}^{2n-1} c_{2n,i}a_{i,2n} = \frac{b_n}{b_{n-1}} \quad (n \geq 1).
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\]

with initial values \( r_1 = 1 \) and \( r_2 = 5 \).

Its closed-form solution is \( r_n = 4n - 3 \) and therefore

\[
Pf \left( (j - i)M_{i+j-3} \right)_{1 \leq i,j \leq 2n} = \prod_{k=1}^{n} (4k - 3).
\]
Theorem 2. Let $M_n = \sum_{k=0}^{n} \frac{1}{k+1} \binom{n}{2k} \binom{2k}{k}$ denote the $n$-th Motzkin number. Then for $n \in \mathbb{N}$ we have

$$\text{Pf} \left( (j - i) M_{i+j-3} \right)_{1 \leq i, j \leq 2n} = \prod_{k=0}^{n-1} (4k + 1).$$

Theorem 3. Let $D_n = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k}$ denote the $n$-th central Delannoy number. Then for $n \in \mathbb{N}$ we have

$$\text{Pf} \left( (j - i) D_{i+j-3} \right)_{1 \leq i, j \leq 2n} = 2^{n+1}(n+1)! (2n - 1) \prod_{k=1}^{n-1} (4k - 1).$$

Theorem 4. Let $N_n(x)$ denote the $n$-th Narayana polynomial defined by $N_0(x) = 1$ and $N_n(x) = \sum_{k=0}^{n} \frac{1}{n} \binom{n}{k} \binom{n}{k-1} x^k$, $n \geq 1$. Then for $n \in \mathbb{N}$ we have

$$\text{Pf} \left( (j - i) N_{i+j-2}(x) \right)_{1 \leq i, j \leq 2n} = x^{n^2} \prod_{k=0}^{n-1} (4k + 1).$$