

Computer Algebra for Combinatorics

Alin Bostan

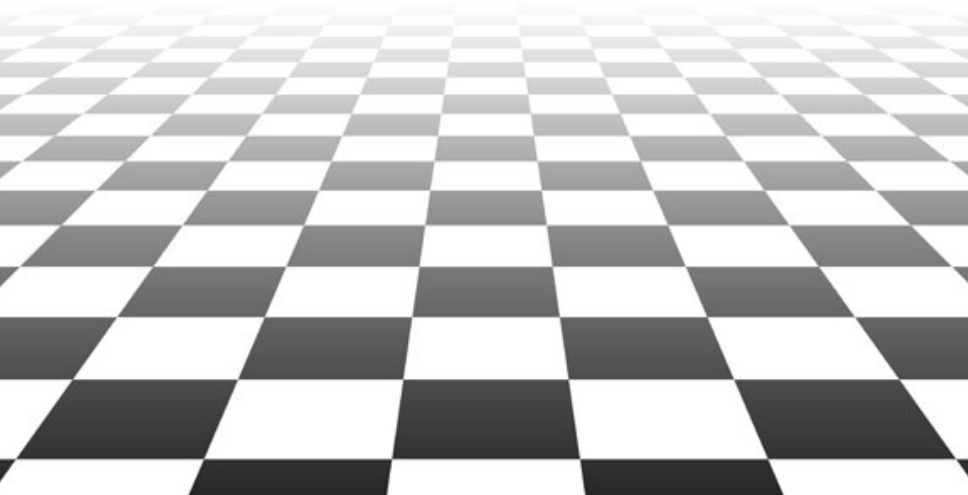


MPRI, C-2-22, January 31, 2019

- Part 1: General presentation
- Part 2: Guess'n'Prove
- Part 3: Creative telescoping



Part 2: Guess'n'Prove



Guess'n'Prove

–The easiest example–

$\{\rightarrow, \uparrow\}$ -walks with prescribed endpoint

Question: Find $B_{i,j}$, the number of $\{\rightarrow, \uparrow\}$ -walks in \mathbb{Z}^2 from $(0,0)$ to (i,j)

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- ▷ There are two ways to get to (i,j) , either from $(i-1,j)$, or from $(i,j-1)$:

$$B_{i,j} = B_{i-1,j} + B_{i,j-1}.$$

- ▷ There is only one way to get to a point on an axis:

$$B_{i,0} = B_{0,j} = 1$$

- ▷ These two rules completely determine all the numbers $B_{i,j}$

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The answer can be guessed from the triangle:

$$B_{i,j} = \frac{(i+j)!}{i!j!}$$

$$\begin{aligned} &\longrightarrow \dots \\ &\longrightarrow \frac{(i+1)(i+2)}{2} \\ &\longrightarrow i+1 \\ &\longrightarrow 1 \end{aligned}$$

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Answer: binomials

$$B_{i,j} = \frac{(i+j)!}{i!j!} =: \binom{i+j}{i}$$

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$$B_{i,j} = \frac{(i+j)!}{i!j!} =: \binom{i+j}{i}$$

Proof: If $C_{i,j} \stackrel{\text{def}}{=} \frac{(i+j)!}{i!j!}$,

$$\frac{C_{i-1,j}}{C_{i,j}} + \frac{C_{i,j-1}}{C_{i,j}} = \frac{i}{i+j} + \frac{j}{i+j} = 1$$

$$C_{i,0} = C_{0,j} = 1$$

Thus $B_{i,j} = C_{i,j}$

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This is a typical
guess-and-prove
proof!

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Exercise 3

$$B_{n,0} + B_{n-1,1} + \cdots + B_{0,n} = 2^n$$

$$B_{n,0}^2 + B_{n-1,1}^2 + \cdots + B_{0,n}^2 = B_{n,n}$$

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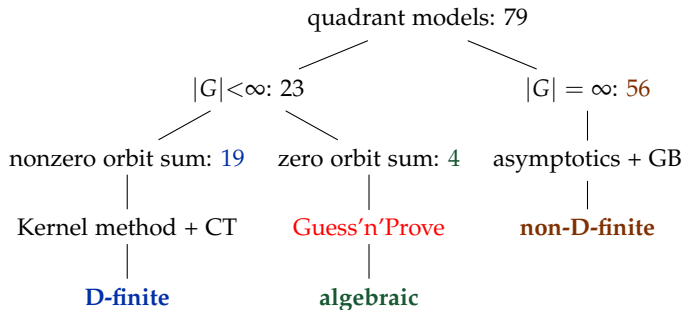
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Summary of Part 1: Walks with unit steps in \mathbb{N}^2

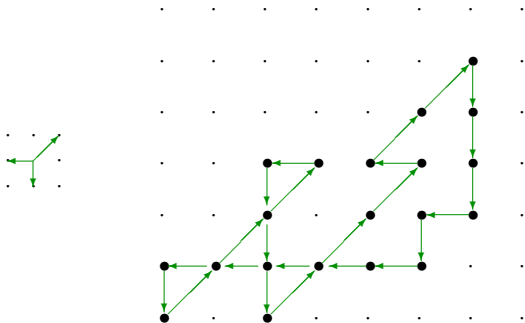


Two important models: **Kreweras** and **Gessel** walks

$$\mathcal{S} = \{\downarrow, \leftarrow, \nearrow\} \quad F_{\mathcal{S}}(t; x, y) \equiv K(t; x, y)$$



$$\mathcal{S} = \{\nearrow, \swarrow, \leftarrow, \rightarrow\} \quad F_{\mathcal{S}}(t; x, y) \equiv G(t; x, y)$$

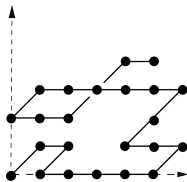


Example: A Kreweras excursion.

- **Gessel walks:** walks in \mathbb{N}^2 using only steps in $\mathcal{S} = \{\nearrow, \swarrow, \leftarrow, \rightarrow\}$
- $g(n; i, j)$ = number of **walks** from $(0,0)$ to (i, j) with n steps in \mathcal{S}

Question: Find the nature of the generating function

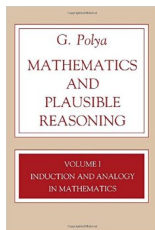
$$G(t; x, y) = \sum_{i, j, n=0}^{\infty} g(n; i, j) x^i y^j t^n \in \mathbb{Q}[[x, y, t]]$$



Theorem (B.-Kauers, 2010) $G(t; x, y)$ is an algebraic function[†].

→ Effective, computer-driven discovery and proof

[†] Minimal polynomial $P(x, y, t, G(t; x, y)) = 0$ has $> 10^{11}$ terms; ≈ 30 Gb (!)



Guessing and Proving

George Pólya

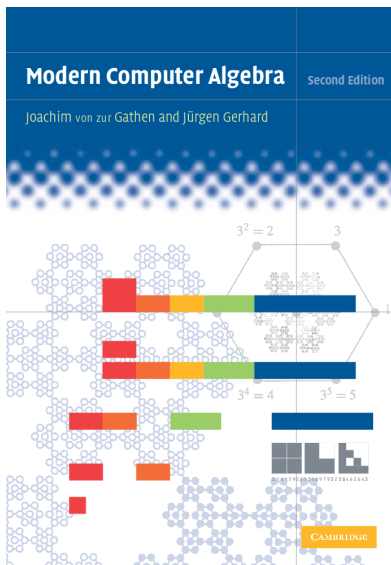
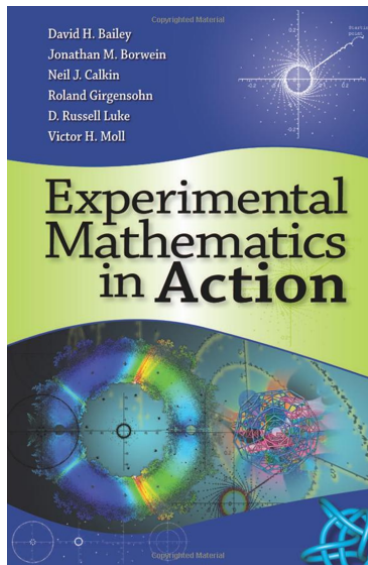


What is “scientific method”? Philosophers and non-philosophers have discussed this question and have not yet finished discussing it. Yet as a first introduction it can be described in three syllables:

Guess and test.

Mathematicians too follow this advice in their research although they sometimes refuse to confess it. They have, however, something which the other scientists cannot really have. For mathematicians the advice is

First guess, then prove.



**Guess'n'Prove for
-PROVING ALGEBRAICITY-**

Experimental mathematics –**Guess'n'Prove**– approach:

(S1) **Generate data**

(S2) **Conjecture**

(S3) **Prove**

Experimental mathematics –**Guess'n'Prove**– approach:

- (S1) **Generate data**
compute a **high order expansion** of the series $F_{\mathcal{F}}(t; x, y)$;
- (S2) **Conjecture**
guess a candidate for the minimal polynomial of $F_{\mathcal{F}}(t; x, y)$, using Hermite-Padé approximation;
- (S3) **Prove**
rigorously certify the minimal polynomials, using (exact) polynomial computations.

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+ **Efficient Computer Algebra**

Step (S1): high order series expansions

$f_{\mathcal{S}}(n; i, j)$ satisfies the recurrence with constant coefficients

$$f_{\mathcal{S}}(n+1; i, j) = \sum_{(u,v) \in \mathcal{S}} f_{\mathcal{S}}(n; i-u, j-v) \quad \text{for } n, i, j \geq 0$$

+ initial conditions $f_{\mathcal{S}}(0; i, j) = \delta_{0,i,j}$ and $f_{\mathcal{S}}(n; -1, j) = f_{\mathcal{S}}(n; i, -1) = 0$.

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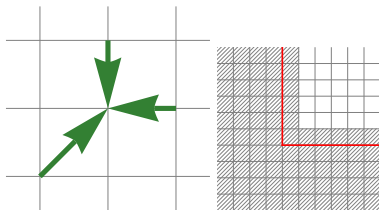
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Example: for the Kreweras walks,

$$\begin{aligned} k(n+1; i, j) = & k(n; i+1, j) \\ & + k(n; i, j+1) \\ & + k(n; i-1, j-1) \end{aligned}$$



Step (S1): high order series expansions

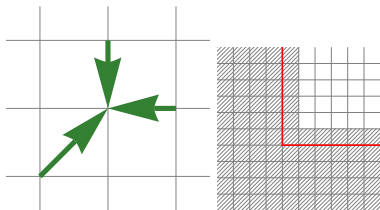
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▷ Recurrence is used to compute $F_{\mathcal{S}}(t; x, y) \bmod t^N$ for large N .

$$\begin{aligned} K(t; x, y) = & 1 + xyt + (x^2y^2 + y + x)t^2 + (x^3y^3 + 2xy^2 + 2x^2y + 2)t^3 \\ & + (x^4y^4 + 3x^2y^3 + 3x^3y^2 + 2y^2 + 6xy + 2x^2)t^4 \\ & + (x^5y^5 + 4x^3y^4 + 4x^4y^3 + 5xy^3 + 12x^2y^2 + 5x^3y + 8y + 8x)t^5 + \dots \end{aligned}$$

Step (S2): guessing equations for $F_{\mathcal{S}}(t; x, y)$, a first idea

In terms of generating functions, the recurrence on $k(n; i, j)$ reads

$$\begin{aligned} & (xy - (x + y + x^2y^2)t)K(t; x, y) \\ & = xy - xt K(t; x, 0) - yt K(t; 0, y) \end{aligned} \quad (\text{KerEq})$$

▷ A similar kernel equation holds for $F_{\mathcal{S}}(t; x, y)$, for any \mathcal{S} -walk.

Corollary. $F_{\mathcal{S}}(t; x, y)$ is algebraic (resp. D-finite) if and only if $F_{\mathcal{S}}(t; x, 0)$ and $F_{\mathcal{S}}(t; 0, y)$ are both algebraic (resp. D-finite).

▷ **Crucial** simplification: equations for $G(t; x, y)$ are **huge** (≈ 30 Gb)

Step (S2): guessing equations for $F_{\mathcal{F}}(t; x, 0)$ and $F_{\mathcal{F}}(t; 0, y)$

Task 1: Given the first N terms of $S = F_{\mathcal{F}}(t; x, 0) \in \mathbb{Q}[x][[t]]$, search for a **differential equation** satisfied by S at precision N :

$$c_r(x, t) \cdot \frac{\partial^r S}{\partial t^r} + \cdots + c_1(x, t) \cdot \frac{\partial S}{\partial t} + c_0(x, t) \cdot S = 0 \bmod t^N.$$

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Task 2: Search for an **algebraic equation** $\mathcal{P}_{x,0}(S) = 0 \bmod t^N$.

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- Both tasks amount to **linear algebra** in size N over $\mathbb{Q}(x)$.
- In practice, we use **modular** Hermite-Padé approximation (**Beckermann-Labahn** algorithm) combined with (rational) **evaluation-interpolation** and **rational number reconstruction**.
- Fast (FFT-based) arithmetic in $\mathbb{F}_p[t]$ and $\mathbb{F}_p[t]\langle \frac{t}{\partial t} \rangle$.

Step (S2): guessing equations for $K(t; x, 0)$

Using $N = 80$ terms of $K(t; x, 0)$, one can guess

▷ a linear differential equation of order 4, degrees (14, 11) in (t, x) , such that

$$\begin{aligned} & t^3 \cdot (3t - 1) \cdot (9t^2 + 3t + 1) \cdot (3t^2 + 24t^2x^3 - 3xt - 2x^2) \cdot \\ & \cdot (16t^2x^5 + 4x^4 - 72t^4x^3 - 18x^3t + 5t^2x^2 + 18xt^3 - 9t^4) \cdot \\ & \cdot (4t^2x^3 - t^2 + 2xt - x^2) \cdot \frac{\partial^4 K(t; x, 0)}{\partial t^4} + \dots \\ & = 0 \pmod{t^{80}} \end{aligned}$$

▷ a polynomial of tridegree (6, 10, 6) in (T, t, x)

$$\begin{aligned} \mathcal{P}_{x,0} = & x^6 t^{10} T^6 - 3x^4 t^8 (x - 2t) T^5 + \\ & + x^2 t^6 \left(12t^2 + 3t^2 x^3 - 12xt + \frac{7}{2} x^2 \right) T^4 + \dots \end{aligned}$$

such that $\mathcal{P}_{x,0}(K(t; x, 0), t, x) = 0 \pmod{t^{80}}$.

Step (S2): guessing equations for $G(t; x, 0)$ and $G(t; 0, y)$

Using $N = 1200$ terms of $G(t; x, y)$, our guesser found candidates

- $\mathcal{P}_{x,0}$ in $\mathbb{Z}[T, t, x]$ of degree $(24, 43, 32)$, coefficients of 21 digits
- $\mathcal{P}_{0,y}$ in $\mathbb{Z}[T, t, y]$ of degree $(24, 44, 40)$, coefficients of 23 digits

such that

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▷ Guessing $\mathcal{P}_{x,0}$ by **undetermined coefficients** would have required to solve a dense linear system of size $\approx 100\,000$, and ≈ 1000 digits entries!

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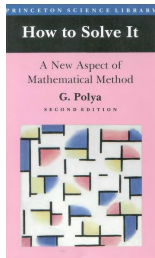
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- ▷ Guessing $\mathcal{P}_{x,0}$ by **undetermined coefficients** would have required to solve a dense linear system of size $\approx 100\,000$, and ≈ 1000 digits entries!
- ▷ [B., Kauers '09] actually first guessed **differential equations**[†], then computed their **p -curvatures** to empirically certify them. This led them suspect the algebraicity of $G(t; x, 0)$ and $G(t; 0, y)$, using a conjecture of Grothendieck's (on differential equations modulo p) as an oracle.

† of order 11, and bidegree $(96, 78)$ for $G(t; x, 0)$, and $(68, 28)$ for $G(t; 0, y)$



Guessing and Proving

George Pólya



Guessing is good, proving is better.

Step (S3): warm-up – Gessel excursions are algebraic

Theorem

$$g(t) := G(\sqrt{t}; 0, 0) = \sum_{n=0}^{\infty} \frac{(5/6)_n (1/2)_n}{(5/3)_n (2)_n} (16t)^n \text{ is algebraic.}$$

Theorem

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- ① Find P such that $P(t, g(t)) = 0 \pmod{t^{100}}$ by **(structured) linear algebra**.
- ② **Implicit function theorem:** $\exists!$ root $r(t) \in \mathbb{Q}[[t]]$ of P .
- ③ $r(t) = \sum_{n=0}^{\infty} r_n t^n$ **being algebraic, it is D-finite**, and so is (r_n) :

$$(n+2)(3n+5)r_{n+1} - 4(6n+5)(2n+1)r_n = 0, \quad r_0 = 1$$

$$\Rightarrow \text{solution } r_n = \frac{(5/6)_n (1/2)_n}{(5/3)_n (2)_n} 16^n = g_n, \text{ thus } g(t) = r(t) \text{ is algebraic.}$$

Step (S3): rigorous proof for Kreweras walks



- ① Setting $y_0 = \frac{x-t-\sqrt{x^2-2tx+t^2(1-4x^3)}}{2tx^2} = t + \frac{1}{x}t^2 + \frac{x^3+1}{x^2}t^3 + \dots$ in the kernel equation

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- ③ The guessed candidate $\mathcal{P}_{x,0}(T, t, x)$ **has a root** $H(t, x)$ in $\mathbb{Q}[[x, t]]$.
- ④ $U = H(t, x)$ also satisfies (RKerEq) **Resultant computations!**
- ⑤ **Uniqueness** $\implies H(t, x) = K(t; x, 0) \implies K(t; x, 0)$ is algebraic!

Algebraicity of *Kreweras walks*: a computer proof in a nutshell

```
# HIGH ORDER EXPANSION (S1)
> st,bu:=time(),kernelopts(bytesused):
> f:=proc(n,i,j) option remember;
    if i<0 or j<0 or n<0 then 0
    elif n=0 then if i=0 and j=0 then 1 else 0 fi
    else f(n-1,i-1,j-1)+f(n-1,i,j+1)+f(n-1,i+1,j) fi
end:
> S:=series(add(add(f(k,i,0)*x^i,i=0..k)*t^k,k=0..80),t,80):

# GUESSING (S2)
> libname:=".",libname:gfun:-version();
    3.76
> P:=subs(Fx0(t)=T,gfun:-seriestoalgeq(S,Fx0(t))[1]):

# RIGOROUS PROOF (S3)
> ker := (T,t,x) -> (x+T+x^2*T^2)*t-x*T:
> pol := unapply(P,T,t,x):
> p1 := resultant(pol(z-T,t,x),ker(t*z,t,x),z):
> p2 := subs(T=x*T,resultant(numer(pol(T/z,t,x)),ker(z,t,x),z)):
> normal(primpart(p1,T)/primpart(p2,T));
    1

# time (in sec) and memory consumption (in Mb)
> trunc(time()-st),trunc((kernelopts(bytesused)-bu)/1000^2);
    8, 785
```

Step (S3): rigorous proof for Gessel walks

Same strategy, but several complications:

- stepset diagonal symmetry is lost: $G(t; x, y) \neq G(t; y, x)$;
- $G(t; 0, 0)$ occurs in (KerEq) (because of the step \swarrow);
- equations are $\approx 5\,000$ times bigger.

→ replace equation (RKerEq) by a **system** of 2 reduced kernel equations.

→ fast algorithms needed (e.g., [B., Flajolet, Salvy, Schost, 2006] for computations with algebraic series).



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Journal of Symbolic Computation 41 (2006) 1–29

Journal of
Symbolic
Computation

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Fast computation of special resultants

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Received 3 September 2003; accepted 9 July 2005

Available online 25 October 2005

BACK TO THE EXERCISE

-A hint-

The exercise

Let $\mathfrak{S} = \{\uparrow, \leftarrow, \searrow\}$. A \mathfrak{S} -walk is a path in \mathbb{Z}^2 using only steps from \mathfrak{S} . Show that, for any integer n , the following quantities are equal:

- (i) the number a_n of \mathfrak{S} -walks of length n confined to the upper half plane $\mathbb{Z} \times \mathbb{N}$ that start and end at the origin $(0,0)$;
- (ii) the number b_n of \mathfrak{S} -walks of length n confined to the quarter plane \mathbb{N}^2 that start at the origin $(0,0)$ and finish on the diagonal $x = y$.

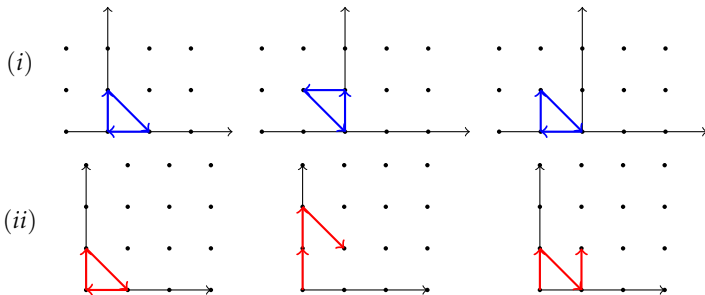
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For instance, for $n = 3$, this common value is $a_3 = b_3 = 3$:



A recurrence relation for $\{\uparrow, \leftarrow, \searrow\}$ -walks in $\mathbb{Z} \times \mathbb{N}$

$h(n; i, j)$ = nb. of $\{\uparrow, \leftarrow, \searrow\}$ -walks in $\mathbb{Z} \times \mathbb{N}$ of length n from $(0, 0)$ to (i, j)

The numbers $h(n; i, j)$ satisfy

$$h(n; i, j) = \begin{cases} 0 & \text{if } j < 0 \text{ or } n < 0, \\ \mathbb{1}_{i=j=0} & \text{if } n = 0, \\ \sum_{(i', j') \in \mathcal{S}} h(n-1; i-i', j-j') & \text{otherwise.} \end{cases}$$

```
> h:=proc(n,i,j)
  option remember;
  if j<0 or n<0 then 0
  elif n=0 then if i=0 and j=0 then 1 else 0 fi
  else h(n-1,i,j-1) + h(n-1,i+1,j) + h(n-1,i-1,j+1) fi
end:

> A:=series(add(h(n,0,0)*t^n, n=0..12), t, 12);
```

$$A = 1 + 3t^3 + 30t^6 + 420t^9 + O(t^{12})$$

A recurrence relation for $\{\uparrow, \leftarrow, \searrow\}$ -walks in \mathbb{N}^2

$q(n; i, j)$ = nb. of $\{\uparrow, \leftarrow, \searrow\}$ -walks in \mathbb{N}^2 of length n from $(0, 0)$ to (i, j)
The numbers $q(n; i, j)$ satisfy

$$q(n; i, j) = \begin{cases} 0 & \text{if } i < 0 \text{ or } j < 0 \text{ or } n < 0, \\ \mathbb{1}_{i=j=0} & \text{if } n = 0, \\ \sum_{(i', j') \in \mathcal{S}} q(n-1; i-i', j-j') & \text{otherwise.} \end{cases}$$

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end:

> B:=series(add(add(q(n,k,k), k=0..n)*t^n, n=0..12), t,12);
```

$$B = 1 + 3t^3 + 30t^6 + 420t^9 + O(t^{12})$$

```

> seriestorec(A, u(n))[1];
      2          2
{(-27 n  - 81 n - 54) u(n) + (n  + 9 n + 18) u(n + 3),
      u(0) = 1, u(1) = 0, u(2) = 0}

> rsolve(%, u(n)):

> A:=sum(subs(n=3*n, op(2,%))*t^(3*n), n=0..infinity);
      3
      A := hypergeom([1/3, 2/3], [2], 27 t )
    
```

▷ Thus, **differential guessing** predicts

$$A(t) = B(t) = {}_2F_1\left(\begin{matrix} 1/3 & 2/3 \\ 2 \end{matrix} \middle| 27t^3\right) = \sum_{n=0}^{\infty} \frac{(3n)!}{n!^3} \frac{t^{3n}}{n+1}.$$


```
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      A := hypergeom([1/3, 2/3], [2], 27 t )
```

- ▷ This can be algorithmically **proved** using **creative telescoping**

- Automatic classification of restricted lattice walks, with M. Kauers. *Proceedings FPSAC*, 2009.
- The complete generating function for Gessel walks is algebraic, with M. Kauers. *Proceedings of the American Mathematical Society*, 2010.
- Explicit formula for the generating series of diagonal 3D Rook paths, with F. Chyzak, M. van Hoeij and L. Pech. *Séminaire Lotharingien de Combinatoire*, 2011.
- Non-D-finite excursions in the quarter plane, with K. Raschel and B. Salvy. *Journal of Combinatorial Theory A*, 2013.
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- A human proof of Gessel's lattice path conjecture, with I. Kurkova, K. Raschel, *Transactions of the American Mathematical Society*, 2017.
- Hypergeometric expressions for generating functions of walks with small steps in the quarter plane, with F. Chyzak, M. van Hoeij, M. Kauers and L. Pech, *European Journal of Combinatorics*, 2017.
- *Computer Algebra for Lattice Path Combinatorics*, preprint, 2017.

Thanks for your attention!