Algorithmic proving of special function identities in Mathematica

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Motivation

$$\sum_{k=0}^{n} \binom{n}{k}^2 \binom{k+n}{k}^2 = \sum_{k=0}^{n} \binom{n}{k} \binom{k+n}{k} \sum_{j=0}^{k} \binom{k}{j}^3 \tag{1}$$

$$\int_0^\infty \frac{1}{(x^4+2ax^2+1)^{m+1}}\,\mathrm{d}x = \frac{\pi P_m^{\left(m+\frac{1}{2},-m-\frac{1}{2}\right)}(a)}{2^{m+\frac{3}{2}}(a+1)^{m+\frac{1}{2}}} \tag{2}$$

$$e^{-x}x^{a/2}n!L_n^a(x) = \int_0^\infty e^{-t}t^{\frac{a}{2}+n}J_a\left(2\sqrt{tx}\right)\,\mathrm{d}t \tag{3}$$

$$\int_{-\infty}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{H_m(x)H_n(x)r^m s^n e^{-x^2}}{m!n!}\,\mathrm{d}x = \sqrt{\pi}e^{2rs} \tag{4}$$

$$\int_{-1}^{1} \left(1-x^2\right)^{\nu-\frac{1}{2}} e^{iax} C_n^{(\nu)}(x)\,\mathrm{d}x = \frac{\pi 2^{1-\nu} i^n \Gamma(n+2\nu) a^{-\nu} J_{n+\nu}(a)}{n!\Gamma(\nu)} \tag{5}$$

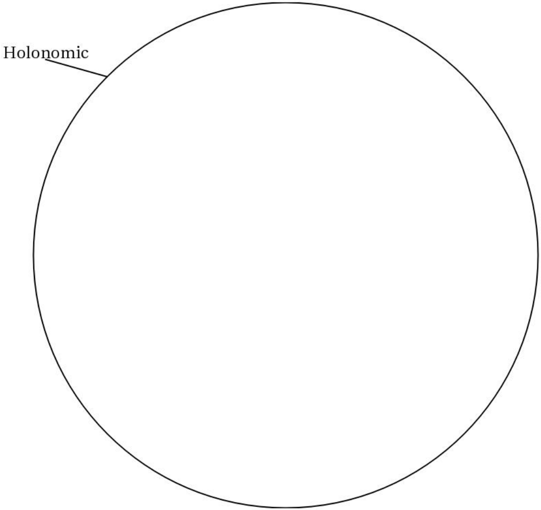
$$\frac{\sin\left(\sqrt{z^2+2tz}\right)}{z} = \sum_{n=0}^{\infty} \frac{(-t)^n y_{n-1}(z)}{n!} \tag{6}$$

HolonomicFunctions…

…is the name of our new Mathematica package (to be released in a few weeks).

- addresses exactly such identities
- provides algorithmic proofs
- applicable to functions that are both holonomic and ∂-finite
- functions are described via recurrences and differential equations (multivariate, also of mixed type)
- these are represented in operator notation

holonomic and ∂-finite functions



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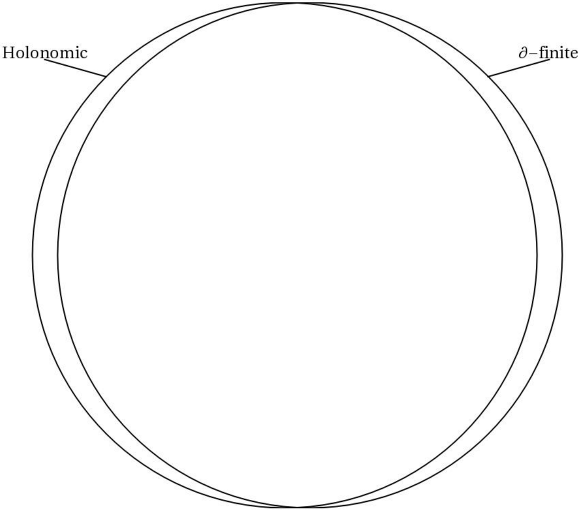

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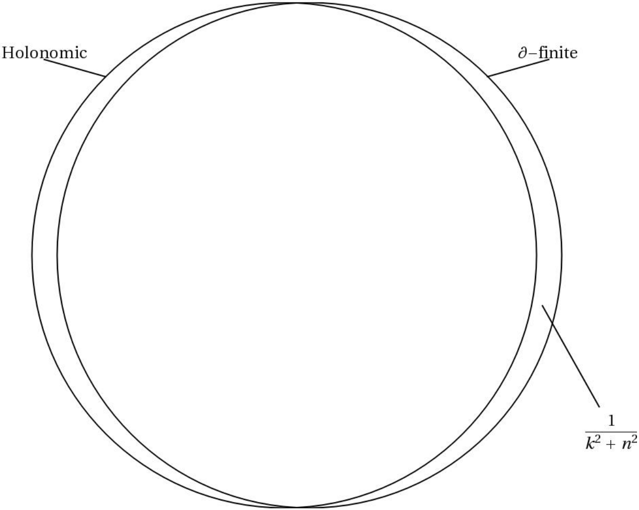

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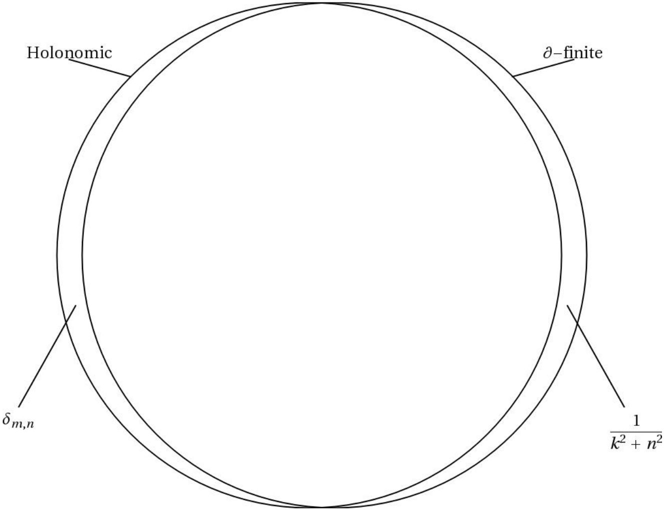

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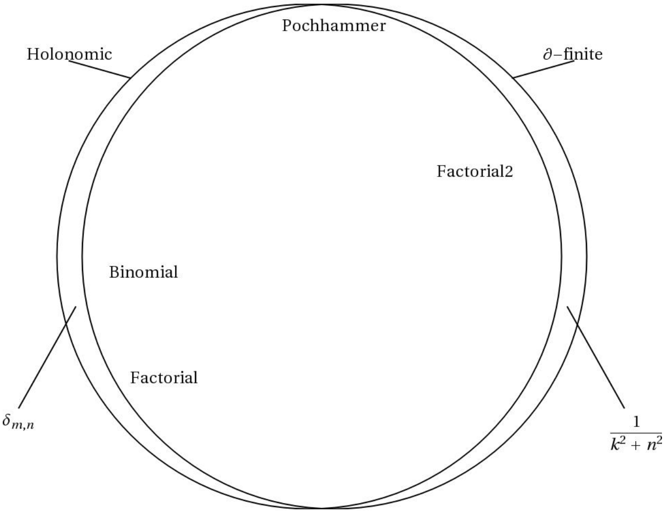

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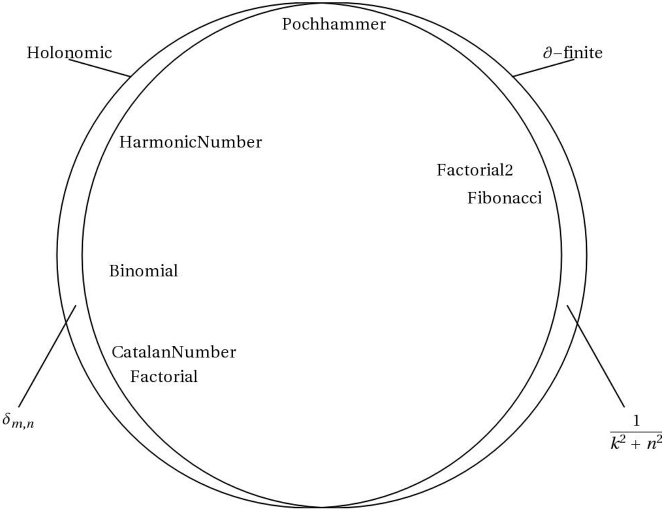

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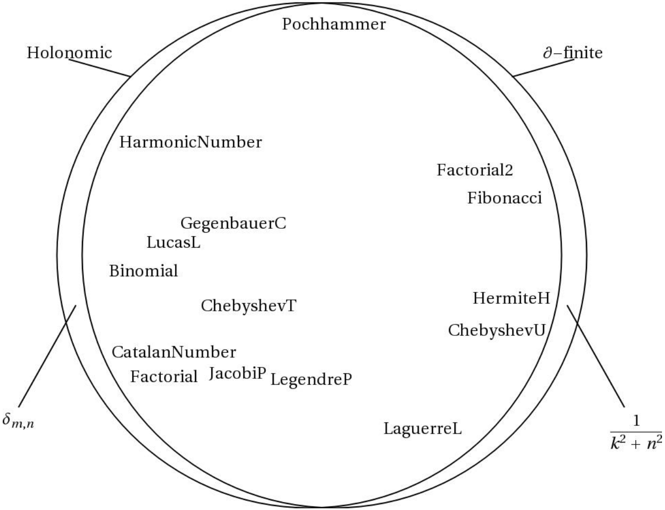

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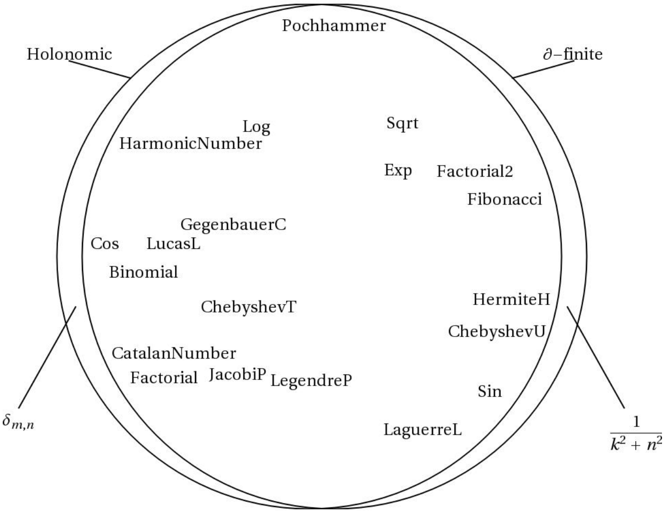

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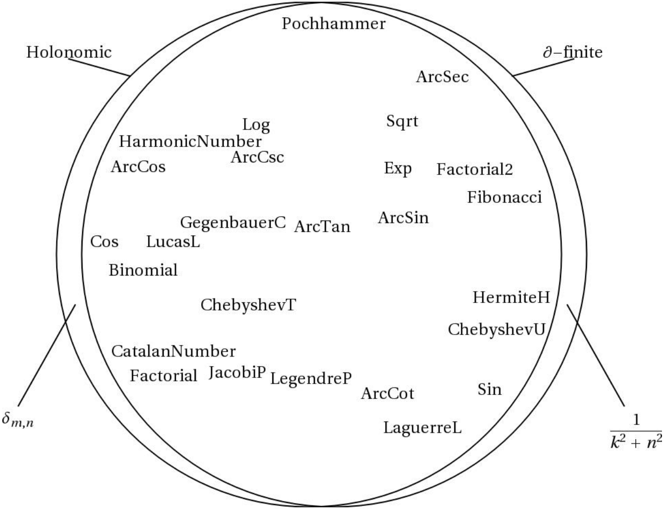


Holonomic

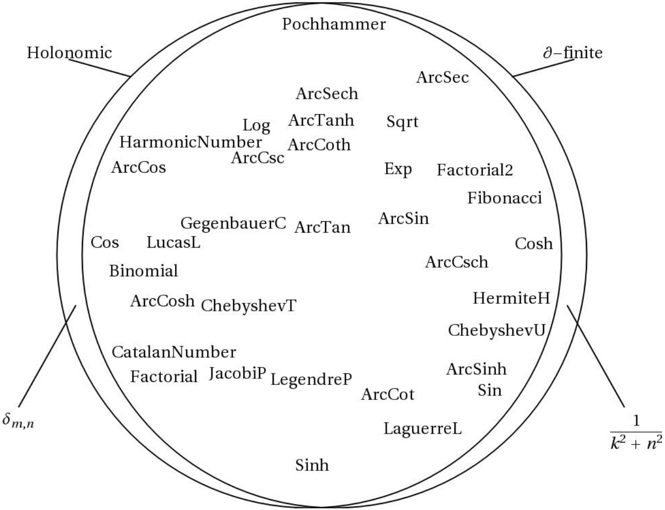
∂–finite

$\delta_{m,n}$

$\frac{1}{k^2+n^2}$

Pochhammer
ArcSec
Log
Sqrt
HarmonicNumber
ArcCsc
ArcCos
Exp
Factorial2
Fibonacci
GegenbauerC
ArcTan
ArcSin
Cos
LucasL
Binomial
HermiteH
ChebyshevT
ChebyshevU
CatalanNumber
Factorial
JacobiP
LegendreP
ArcCot
Sin
LaguerreL

holonomic and ∂-finite functions



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ChebyshevU

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ArcSinh

Factorial

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ArcCot

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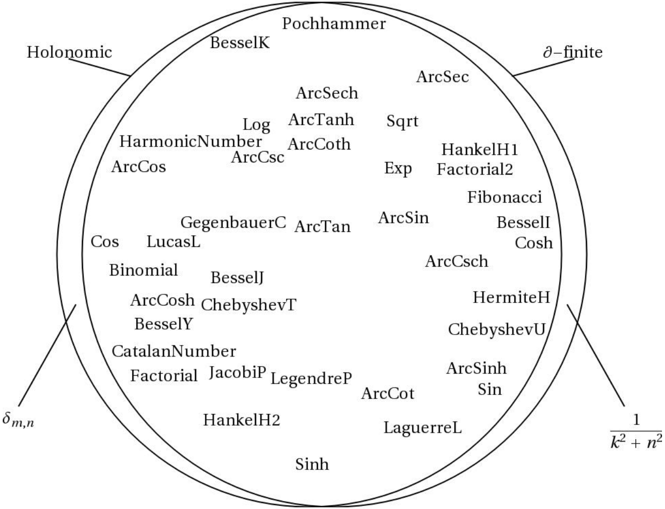
$\frac{1}{k^2 + n^2}$

LaguerreL

Sinh

holonomic and ∂-finite functions



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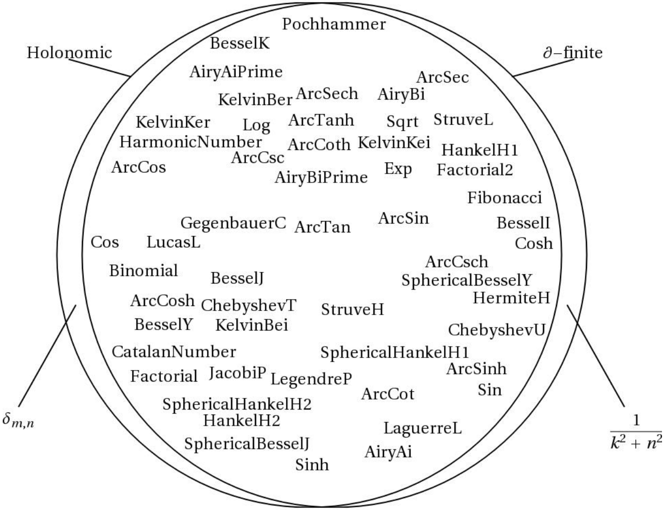

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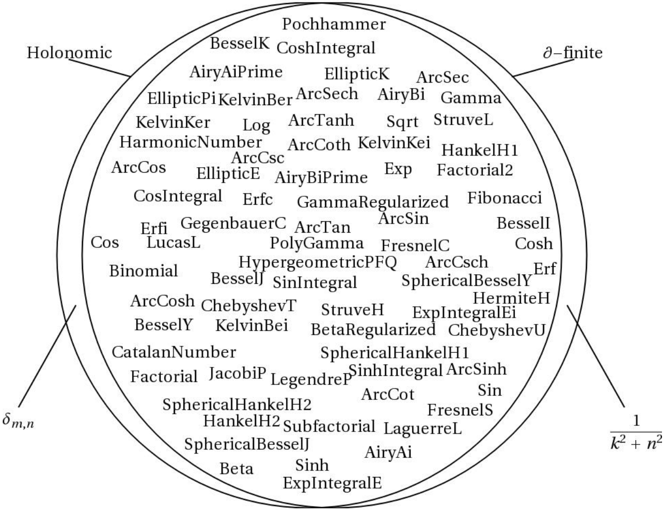

Holonomic

∂−finite

Pochhammer

BesselK CoshIntegral

AiryAiPrime EllipticK ArcSec

EllipticPi KelvinBer ArcSech AiryBi Gamma

KelvinKer Log ArcTanh Sqrt StruveL

HarmonicNumber ArcCoth KelvinKei HankelH1

ArcCsc

ArcCos EllipticE AiryBiPrime Exp Factorial2

CosIntegral Erfc GammaRegularized Fibonacci

Erfi GegenbauerC ArcTan ArcSin BesselI

Cos LucasL PolyGamma FresnelC Cosh

Binomial HypergeometricPFQ ArcCsch Erf

BesselJ SinIntegral SphericalBesselY

ArcCosh ChebyshevT StruveH ExpIntegralEi HermiteH

BesselY KelvinBei BetaRegularized ChebyshevU

CatalanNumber SphericalHankelH1

Factorial JacobiP LegendreP SinhIntegral ArcSinh

ArcCot Sin

SphericalHankelH2 FresnelS

HankelH2 Subfactorial LaguerreL

SphericalBesselJ AiryAi

Beta Sinh

ExpIntegralE

$\delta_{m,n}$

$\frac{1}{k^2 + n^2}$

Functionality of the package

What can we do with holonomic/∂-finite functions?

- compute the defining equations (recurrences, differential equations)
- execute closure properties
- doing summation / integration (Takayama's algorithm, Chyzak's algorithm)
- find annihilating relations of certain type

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All that is implemented in `HolonomicFunctions`. Additionally:

- arithmetic with noncommutative Ore polynomials
- Gröbner bases in Ore algebras
- finding rational solutions of systems of difference or differential equations

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In Maple, there is `Mgfun` (by F. Chyzak).

Ore algebras

Notation:

- S_n denotes the shift operator $S_n \bullet f(n) = f(n+1)$,
- D_x denotes the derivative w.r.t. x.

In Mathematica they can be input as `S[n]` and `Der[x]`.

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Define some Ore algebras:

```
OreAlgebra[S[n],Der[x]]
```

$$K(n,x)[S_n; S_n, 0][D_x; 1, D_x]$$

```
OreAlgebra[x,S[n],Der[x]]
```

$$K(n)[x][S_n; S_n, 0][D_x; 1, D_x]$$

Ore polynomials

```
p = ToOrePolynomial[Der[x]^3]
```

$$D_x^3$$

```
p = p ** (x^2+x)
```

$$(x^2+x)D_x^3+(6x+3)D_x^2+6D_x$$

```
ChangeOreAlgebra[p, OreAlgebra[Der[x],x]]
```

$$D_x^3x^2+D_x^3x$$

Gröbner bases

There are no zero-dimensional ideals in the Weyl algebra:

```
OreGroebnerBasis[{Der[x]^5, x^7}, OreAlgebra[x,Der[x]]]
```

$$\{1\}$$

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```

$$\{1\}$$

Recurrence and differential equation of Hermite polynomials:

```
OreGroebnerBasis[{S[n]^2-2*x*S[n]+2*n+2,
                  Der[x]^2-2*x*Der[x]+2*n},
                 OreAlgebra[S[n],Der[x]]]
```

$$\left\{-D_x - S_n + 2x, D_x^2 - 2xD_x + 2n\right\}$$

Olver's problems (1)

From a letter by Frank Olver to my advisor Peter Paule:

"The writing of DLMF Chapter BS by Leonard Maximon and myself is now largely complete; ... However, a problem has arisen in connection with about a dozen formulas from Chapter 10 of Abramowitz and Stegun for which we have not yet tracked down proofs, and the author of this chapter, Henry Antosiewiecz, died about a year ago. Since it is the editorial policy for the DLMF not to state formulas without indications of proofs, I am hoping that you will be willing to step into the breach and supply verifications by computer algebra methods ... I will fax you the formulas later today ..."

Olver's problems (2)

Prove the following identity:

$$\frac{1}{z}\sinh\sqrt{z^2-2izt}=\sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\sqrt{\frac{\pi}{2z}}I_{\frac{1}{2}-n}(z)$$

Olver's problems (2)

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$$\frac{1}{z}\sinh\sqrt{z^2-2izt}=\sum_{n=0}^{\infty}\frac{(-it)^n}{n!}\sqrt{\frac{\pi}{2z}}I_{\frac{1}{2}-n}(z)$$

For the left hand side, we can immediately compute annihilating operators (using closure properties + database):

```
F[t_,z_] := Sinh[Sqrt[z^2 - 2*I*z*t]]/z
lhs = Annihilator[F[t,z], {Der[t], Der[z]}]
```

$$\begin{aligned}\{&(-t-iz)D_t+zD_z+1,\\ &(-z^4+3itz^3+2t^2z^2)D_z^2+(-2z^3+6itz^2+5t^2z)D_z\\ &+(z^4-3itz^3-3t^2z^2+it^3z+t^2)\}\end{aligned}$$

Olver's problems (3)

On the right hand side $\sum_{n=0}^{\infty} \frac{(-it)^n}{n!} \sqrt{\frac{\pi}{2z}} I_{\frac{1}{2}-n}(z)$, we perform creative telescoping:

```
f[n_,t_,z_]:= (-I*t)^n/n!*Sqrt[Pi/2/z]*BesselI[-n+1/2,z];
{opQ, opR} =
  CreativeTelescoping[f[n,t,z], S[n]-1, {Der[t],Der[z]}]
```

We obtain two operators $Q_i + (S_n - 1) \cdot R_i \in \operatorname{Ann} f$ where

$$\begin{aligned}
Q_1 &= -t(t+iz)D_t + tzD_z + t, \\
Q_2 &= (t+iz)(2t+iz)z^2 D_z^2 - z(-5t^2 - 6izt + 2z^2)D_z \\
&\quad +i(-iz^4 - 3tz^3 + 3it^2z^2 + t^3z - it^2), \\
R_1 &= -inz, \\
R_2 &= i(n^2+n)(t+iz)zS_n + 2t^2n^2 - z^2n^2 + 3itzn^2 - t^2n \\
&\quad +z^2n - 3itzn
\end{aligned}$$

Olver's problems (4)

Next verify that $[R_1 \bullet f]_{n=0} = 0$ and that $R_1 \bullet f$ tends to 0 when n goes to infinity (the same for R_2):

```
ApplyOreOperator[opR, f[n,t,z]] /. n->0
```

$$\{0, 0\}$$

(do the same thing for $n \to \infty$)
$\longrightarrow$ The delta part vanishes.
Hence Q_1 and Q_2 are annihilating operators for the sum. In fact, we find that they agree with the annihilating operators that we computed for the left hand side.

Olver's problems (5)

In order to establish equality, we have to compare initial values. Look at the vector space under the stairs of the Gröbner basis:

```
u = UnderTheStaircase[lhs]
```

$$\{1, D_z\}$$

This means we have to compute two initial values:

```
ApplyOreOperator[u, F[t,z]] /. {t->0,z->1} //FullSimplify
```

$$\{\sinh(1), \tfrac{1}{e}\}$$

```
ApplyOreOperator[u, f[n,t,z]] /. {t->0,z->1}
```

$$\left\{\frac{0^n\sqrt{\frac{\pi}{2}}I_{\frac{1}{2}-n}(1)}{n!}, \frac{0^n\sqrt{\frac{\pi}{2}}\left(I_{-n-\frac{1}{2}}(1)+I_{\frac{3}{2}-n}(1)\right)}{2n!} - \frac{0^n\sqrt{\frac{\pi}{2}}I_{\frac{1}{2}-n}(1)}{2n!}\right\}$$

```
% /. (0^n)->1 /. n->0 // FullSimplify
```

$$\{\sinh(1), \tfrac{1}{e}\}$$

Olver's problems (6)

All this can be done in one step, completely automatically!

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Another problem was to prove

$$\left.\frac{\partial}{\partial\nu} j_\nu(x)\right|_{\nu=0} = \frac{\mathrm{Ci}(2x)\sin(x) - \mathrm{Si}(2x)\cos(x)}{x}$$

Olver's problems (6)

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Another problem was to prove

$$\frac{\partial}{\partial \nu} j_\nu(x)\bigg|_{\nu=0} = \frac{\mathrm{Ci}(2x)\sin(x) - \mathrm{Si}(2x)\cos(x)}{x}$$

Rewrite left hand side to

$$\sqrt{\frac{\pi}{2x}}\left(\sqrt{\frac{2}{\pi x}}\log\left(\frac{x}{2}\right)\sin(x) - \sqrt{\frac{x}{2}}\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{x^2}{4}\right)^k\psi\left(\frac{1}{2}+k+1\right)}{k!\Gamma\left(\frac{1}{2}+k+1\right)}\right)$$

Olver's problems (7)

$$\sqrt{\frac{\pi}{2x}}\left(\sqrt{\frac{2}{\pi x}}\log\left(\frac{x}{2}\right)\sin(x)-\sqrt{\frac{x}{2}}\sum_{k=0}^{\infty}\frac{(-1)^k\left(\frac{x^2}{4}\right)^k\psi\left(\frac{1}{2}+k+1\right)}{k!\Gamma\left(\frac{1}{2}+k+1\right)}\right)$$

```
Annihilator[Sqrt[Pi/(2*x)]*(
  Sqrt[2/(Pi*x)]*Log[x/2]*Sin[x]-
  Sqrt[x/2]*Sum[(-1)^k*(x^2/4)^k*PolyGamma[0,3/2+k]/
                 (k!*Gamma[3/2+k]), {k,0,Infinity}]),
  Der[x]]
```

$$\{x^3D_x^6+14x^2D_x^5+(3x^3+52x)D_x^4+(28x^2+48)D_x^3$$
$$+(3x^3+64x)D_x^2+(14x^2+32)D_x+(x^3+12x)\}$$

Non-holonomic identities

In their ISSAC 2009 paper, Chyzak/Kauers/Salvy propose to extend the algorithms for holonomic/∂-finite functions to non-holonomic functions. These ideas have already been included into the package, e.g.

$$\sum_{k=0}^{n} \binom{k}{m} \mathcal{S}_n^{(k)} (-(k-m)+x+1)_{k-m} = \sum_{k=0}^{n} \binom{n}{k} \mathcal{S}_k^{(m)} x^{n-k}$$

```
Annihilator[Sum[Binomial[k,m]*Pochhammer[x-(k-m)+1,k-m]*
  StirlingS2[n,k], {k,0,n}], {S[m],S[n]},
  Assumptions -> Element[n, Integers] && n >= 0]
```

$$\{S_m S_n + (-m-x-1)S_m - 1\}$$

(similarly for the right hand side)

Proof of Gessel's conjecture

`HolonomicFunctions` was used in proving an open problem in enumerative combinatorics: Ira Gessel's conjecture on the number lattice paths with a certain step set.

Reference:
Manuel Kauers, Christoph Koutschan, Doron Zeilberger: *Proof of Ira Gessel's lattice path conjecture.* Proceedings of the National Academy of Sciences, 2009, to appear.

Simulation of electromagnetic waves

- joint work with Joachim Schöberl (RWTH Aachen) and Peter Paule (RISC)
- wide range of applications in constructing antennas, mobile phones, etc.
- merchandised by the company CST (Computer Simulation Technology)

- simulation with finite element methods
- significant contributions from Computer Algebra using the package `HolonomicFunctions`
- symbolically derived formulae allow a considerable speed-up
- they are planned to be part of a patent

Mathematical and physical background

Simulate the propagation of electromagnetic waves using the Maxwell equations

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \operatorname{curl} E, \quad \frac{\mathrm{d}E}{\mathrm{d}t} = -\operatorname{curl} H$$

where H and E are the magnetic and the electric field respectively. Define basis functions (in 2D) in order to approximate the solution:

$$\varphi_{i,j}(x,y) := (1-x)^i P_j^{(2i+1,0)}(2x-1) P_i\left(\tfrac{2y}{1-x} - 1\right)$$

(basis functions in 3D are more involved)

Task: Rewrite derivatives of these basis functions.

Result

In order to speed up the numerical computations, certain relations for the basis functions $\varphi_{i,j}(x,y)$ are needed.

Using `HolonomicFunctions` relations like the following can easily be derived:

$$\begin{aligned}
&2(i+2j+5)(2i+2j+7)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+1}(x,y)\\
&+(2i+1)(i+2j+1)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+2}(x,y)\\
&-(j+3)(i+2j+5)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+3}(x,y)\\
&+(j+1)(2i+2j+7)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j}(x,y)\\
&-2(2i+3)(i+j+3)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j+1}(x,y)\\
&+(i+2j+5)(2i+2j+5)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j+2}(x,y)=\\
&2(i+j+4)(2i+2j+5)(2i+2j+7)\varphi_{i,j+2}(x,y)\\
&+2(i+j+2)(i+2j+5)(2i+2j+7)\varphi_{i+1,j+1}(x,y)
\end{aligned}$$

How to (1)

```
ann = Annihilator[
  (1-x)^i*JacobiP[j,2i+1,0,2x-1]*LegendreP[i,2y/(1-x)-1],
  {S[i],S[j],Der[x]}]
```

$$\{(4i^2x^5 + 4i^2x^4y - 16i^2x^4 - 12i^2x^3y + 20i^2x^3 + 8i^2x^2y - 8i^2x^2 + 8ijx^5 + 8ijx^4y - 28ijx^4 -$$

$$20ijx^3y + 32ijx^3 + 12ijx^2y - 12ijx^2 + 12ix^5 + 12ix^4y - 46ix^4 - 34ix^3y + 56ix^3 + 22ix^2y - 22ix^2 +$$

$$4j^2x^5 + 4j^2x^4y - 12j^2x^4 - 8j^2x^3y + 12j^2x^3 + 4j^2x^2y - 4j^2x^2 + 12jx^5 + 12jx^4y - 40jx^4 - 28jx^3y +$$

$$44jx^3 + 16jx^2y - 16jx^2 + 9x^5 + 9x^4y - 33x^4 - 24x^3y + 39x^3 + 15x^2y - 15x^2)D_x^2 + (8i^4x^2 - 8i^4x +$$

$$16i^3jx^2 - 16i^3jx + 40i^3x^2 - 40i^3x + 10i^2j^2x^2 - 10i^2j^2x + 58i^2jx^2 - 58i^2jx + 74i^2x^2 - 74i^2x +$$

$$2ij^3x^2 - 2ij^3x + 23ij^2x^2 - 23ij^2x + 69ijx^2 - 69ijx + 60ix^2 - 60ix + 2j^3x^2 - 2j^3x + 13j^2x^2 -$$

$$13j^2x + 27jx^2 - 27jx + 18x^2 - 18x)S_i + (-12i^3jx^2 - 16i^3jxy + 24i^3jx + 16i^3jy - 16i^3j - 12i^3x^2 -$$

$$16i^3xy + 24i^3x + 16i^3y - 16i^3 - 26i^2j^2x^2 - 32i^2j^2xy + 48i^2j^2x + 24i^2j^2y - 24i^2j^2 - 68i^2jx^2 -$$

$$84i^2jxy + 130i^2jx + 72i^2jy - 72i^2j - 42i^2x^2 - 52i^2xy + 82i^2x + 48i^2y - 48i^2 - 18ij^3x^2 - 20ij^3xy +$$

$$30ij^3x + 12ij^3y - 12ij^3 - 77ij^2x^2 - 86ij^2xy + 135ij^2x + 60ij^2y - 60ij^2 - 107ijx^2 - 120ijxy +$$

$$195ijx + 94ijy - 94ij - 48ix^2 - 54ixy + 90ix + 46iy - 46i - 4j^4x^2 - 4j^4xy + 6j^4x + 2j^4y - 2j^4 -$$

$$24j^3x^2 - 24j^3xy + 38j^3x + 14j^3y - 14j^3 - 53j^2x^2 - 53j^2xy + 88j^2x + 35j^2y - 35j^2 - 51jx^2 -$$

$$51jxy + 88jx + 37jy - 37j - 18x^2 - 18xy + 32x + 14y - 14)S_j + (8i^3x^4 + 8i^3x^3y - 24i^3x^3 - 16i^3x^2y +$$

$$32i^3x^2 + 16i^3xy - 16i^3x + 24i^2jx^4 + 24i^2jx^3y - 72i^2jx^3 - 48i^2jx^2y + 80i^2jx^2 + 32i^2jxy -$$

How to (2)

```
FindRelation[ann, Eliminate -> {x,y},
                  Pattern -> {_,_,0|1}]
```

$$(-4i^2-6ij-20i-2j^2-15j-25)S_iS_j^2D_x+(-2ij-6i-2j^2-11j-15)S_j^3D_x+(-4i^2-4ij-18i-6j-18)S_iS_jD_x+(4i^2+4ij+14i+2j+6)S_j^2D_x+(8i^3+24i^2j+72i^2+24ij^2+144ij+214i+8j^3+72j^2+214j+210)S_iS_j+(2ij+2i+2j^2+9j+7)S_iD_x+(8i^3+24i^2j+72i^2+24ij^2+144ij+214i+8j^3+72j^2+214j+210)S_j^2+(4i^2+6ij+20i+2j^2+13j+21)S_jD_x$$