The Power of Holonomic Computation

Christoph Koutschan

Johann Radon Institute for Computational and Applied Mathematics (RICAM)
Austrian Academy of Sciences

March 15, 2023
Zu Chongzhi Mathematics Research Seminar

ÖAW RICAM

Special Functions

- arise in mathematical analysis and in real-world phenomena

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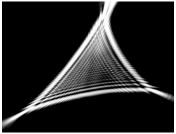

Airy function

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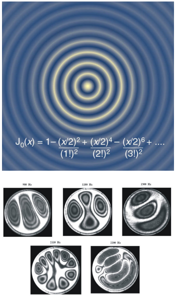

Bessel function

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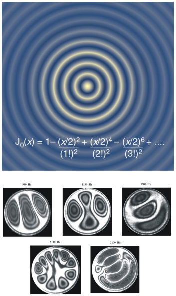

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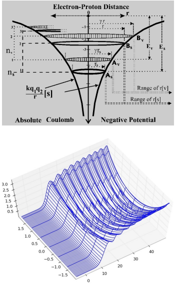

Coulomb function

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- are solutions to certain differential equations

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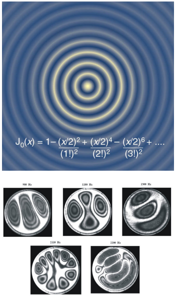

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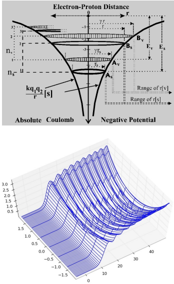

Coulomb function

Special Functions

- arise in mathematical analysis and in real-world phenomena
- are solutions to certain differential equations
- cannot be expressed in terms of the usual elementary functions ($\sqrt{\ }$, exp, log, sin, cos, ...)

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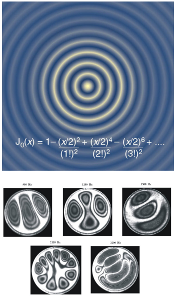

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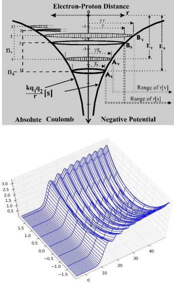

Coulomb function

Holonomic Functions

Definition: A function $f(x)$ is called **holonomic** if it satisfies a linear ordinary differential equation with polynomial coefficients:

$$p_r(x)f^{(r)}(x) + \cdots + p_1(x)f'(x) + p_0(x)f(x) = 0,$$

$p_0, \ldots, p_r \in \mathbb{K}[x]$ (not all zero).

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$$p_r(n)f(n+r) + \cdots + p_1(n)f(n+1) + p_0(n)f(n) = 0,$$

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$\longrightarrow$ In both cases, one needs only **finitely many** initial conditions.

Differential Equations and Recurrences

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Many special functions can be characterized as solutions to systems of linear differential equations and recurrences, and in fact are holonomic.

Finiteness Property

Example: The **Legendre polynomials** are orthogonal polynomials w.r.t. the L^2 inner product $\int_{-1}^{1} f(x)g(x)\,\mathrm{d}x$, and satisfy the ODE

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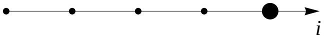
Consider the set $\left\{P_n^{(i)}(x) : i \geqslant 0\right\}$.

$$P_n^{(4)}(x) =$$



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$$(x^2-1)P_n^{(4)}(x) + 6xP_n^{(3)}(x) - (n-2)(n+3)P_n''(x) = 0$$

Consider the set $\left\{P_n^{(i)}(x) : i \geqslant 0\right\}$.

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$$P_n^{(4)}(x) = \frac{n^2x^2-n^2+nx^2-n+18x^2+6}{(x^2-1)^2}P_n''(x) - \frac{6(n-1)(n+2)x}{(x^2-1)^2}P_n'(x)$$

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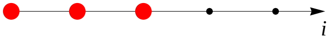

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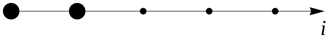
$\longrightarrow P_n(x)$ is **holonomic** w.r.t. x.

Consider the set $\left\{P_n^{(i)}(x) : i \geqslant 0\right\}$.

$$P_n^{(4)}(x) = -\frac{8x(n^2x^2-n^2+nx^2-n+3x^2+3)}{(x^2-1)^3}P_n'(x) + \frac{n(n+1)(n^2x^2-n^2+nx^2-n+18x^2+6)}{(x^2-1)^3}P_n(x)$$



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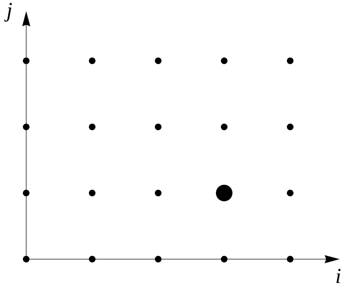

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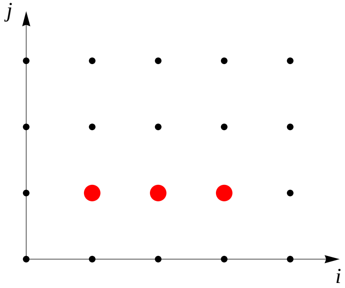

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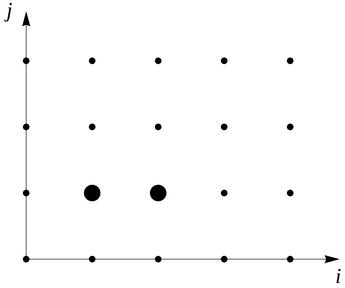

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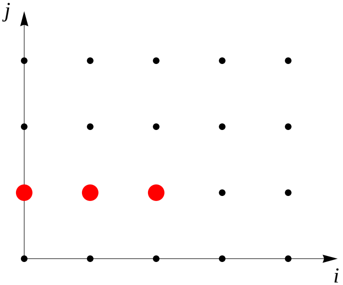

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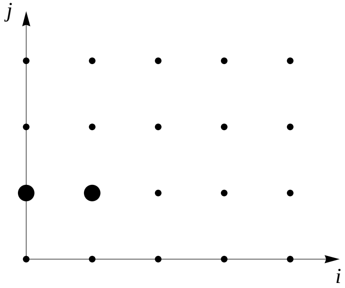

$$P_{n+1}^{(3)}(x) = \frac{(n^2x^2-n^2+3nx^2-3n+8x^2)}{(x^2-1)^2}P_{n+1}'(x) - \frac{4(n^2x+3nx+2x)}{(x^2-1)^2}P_{n+1}(x)$$

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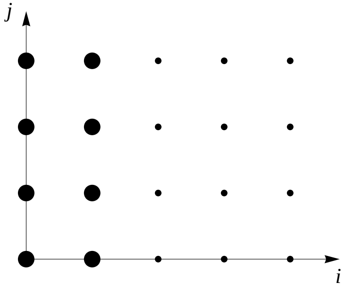

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Example: The **Legendre polynomials** can be defined recursively:

$$P_0(x) = 1, \quad P_1(x) = x$$
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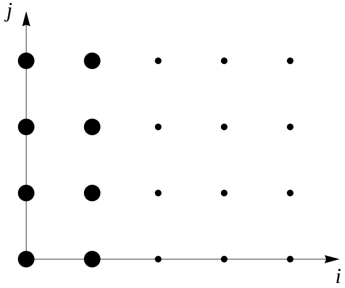

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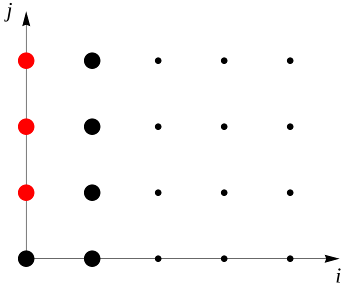

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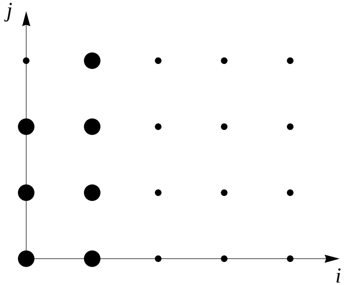

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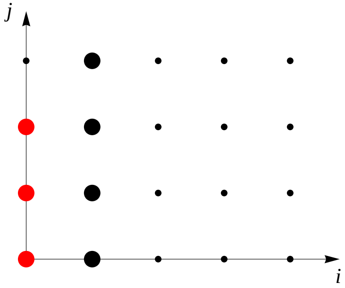

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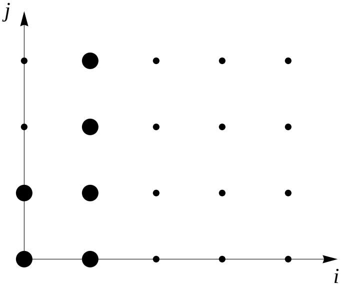

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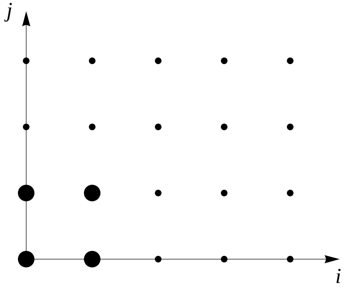

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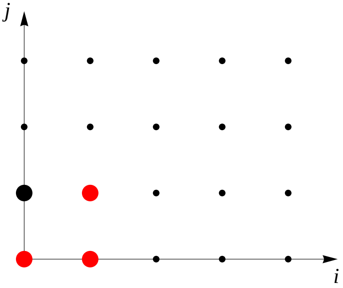

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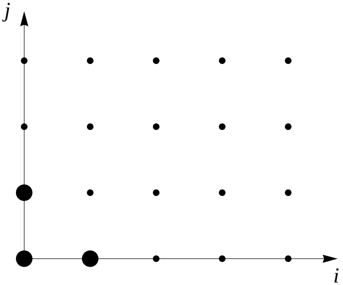

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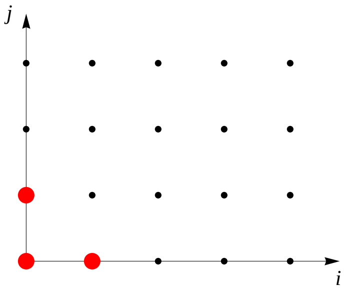

Finiteness Property

Example: The **Legendre polynomials** can be defined recursively:

$$P_0(x) = 1, \quad P_1(x) = x$$
$$nP_n(x) = (2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x).$$

$\longrightarrow$ $P_n(x)$ is **holonomic** w.r.t. n and x (of rank 2).

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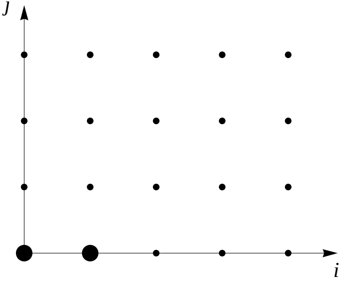

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- $f_n(h(x))$, where $h(x)$ is an algebraic function.

Many Functions are Holonomic

ArcCsc, KelvinBei, HypergeometricPFQ, ExpIntegralE, ArcTanh, HankelH2, AngerJ, JacobiP, ChebyshevT, AiryBi, AiryAi, Sinc, Multinomial, CatalanNumber, QBinomial, CosIntegral, ArcSech, SphericalHankelH2, HermiteH, ExpIntegralEi, Beta, AiryBiPrime, SphericalBesselJ, Binomial, ParabolicCylinderD, Erfc, EllipticK, Fibonacci, QFactorial, Cos, Hypergeometric2F1, Erf, KelvinKer, HypergeometricPFQRegularized, Log, Factorial, BesselY, Cosh, CoshIntegral, ArcTan, ArcCoth, LegendreP, LaguerreL, EllipticE, SinhIntegral, Sinh, BetaRegularized, SphericalHankelH1, ArcSin, EllipticThetaPrime, Root, LucasL, AppellF1, FresnelC, LegendreQ, ChebyshevU, GammaRegularized, Erfi, HarmonicNumber, BesselI, KelvinKei, ArithmeticGeometricMean, Exp, ArcCot, EllipticTheta, Hypergeometric0F1, EllipticPi, GegenbauerC, ArcCos, WeberE, FresnelS, EllipticF, ArcCosh, Subfactorial, QPochhammer, Gamma, StruveH, WhittakerM, ArcCsch, Hypergeometric1F1, SinIntegral, BesselJ, StruveL, ArcSec, Factorial2, KelvinBer, BesselK, ArcSinh, HankelH1, Sqrt, PolyGamma, HypergeometricU, AiryAiPrime, Sin,

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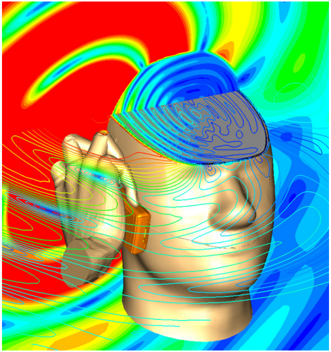
- evaluate symbolic determinants (e.g., in combinatorics)

Finite Elements



(joint work with Joachim Schöberl and Peter Paule)

Problem Setting

Simulate the propagation of electromagnetic waves according to

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \operatorname{curl} E, \quad \frac{\mathrm{d}E}{\mathrm{d}t} = -\operatorname{curl} H \qquad \text{(Maxwell)}$$

where H and E are the magnetic and the electric field respectively.

Define basis functions (2D case):

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

using Legendre and Jacobi polynomials.

Problem: Represent the partial derivatives of $\varphi_{i,j}(x,y)$ in the basis (i.e., as linear combinations of shifts of the $\varphi_{i,j}(x,y)$ itself).

Solution

Ansatz: One needs a relation of the form

$$\sum_{(k,l)\in A} a_{k,l}(i,j)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+k,j+l}(x,y) \;=\; \sum_{(m,n)\in B} b_{m,n}(i,j)\varphi_{i+m,j+n}(x,y),$$

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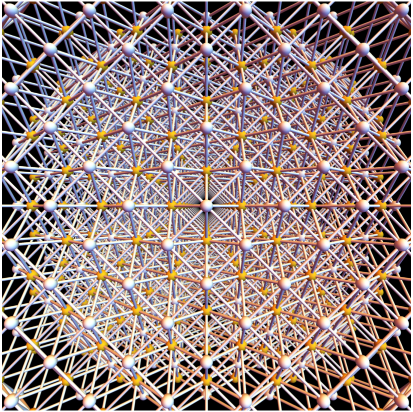
Result: With our holonomic methods, we find the relation

$$\begin{aligned}
&(2i+j+3)(2i+2j+7)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+1}(x,y)+\\
&2(2i+1)(i+j+3)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+2}(x,y)-\\
&(j+3)(2i+2j+5)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i,j+3}(x,y)+\\
&(j+1)(2i+2j+7)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j}(x,y)-\\
&2(2i+3)(i+j+3)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j+1}(x,y)-\\
&(2i+j+5)(2i+2j+5)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j+2}(x,y)+\\
&2(i+j+3)(2i+2j+5)(2i+2j+7)\varphi_{i,j+2}(x,y)+\\
&2(i+j+3)(2i+2j+5)(2i+2j+7)\varphi_{i+1,j+1}(x,y)=0.
\end{aligned}$$

Creative Telescoping



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$$\underbrace{\sum_{k=1}^{\infty} \frac{1}{k(k+n)}}_{=:\, f_n} \rightsquigarrow (n+2)^2 f_{n+2} = (n+1)(2n+3) f_{n+1} - n(n+1) f_n$$

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Method for doing integrals and sums
(aka Feynman's differentiating under the integral sign)

Consider the following summation problem: $F(n) := \sum_{k=a}^{b} f(n,k)$

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Summing from a to b yields a recurrence for $F(n)$:

$$c_r(n)F(n+r) + \cdots + c_0(n)F(n) = g(n,b+1) - g(n,a).$$

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Method for doing integrals and sums
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Consider the following integration problem: $F(x) := \int_a^b f(x,y)\,\mathrm{d}y$

Telescoping: write $f(x,y) = \frac{\mathrm{d}}{\mathrm{d}y} g(x,y)$.

Then $F(n) = \int_a^b \left(\frac{\mathrm{d}}{\mathrm{d}y} g(x,y)\right) \mathrm{d}y \qquad = g(x,b) - g(x,a)$.

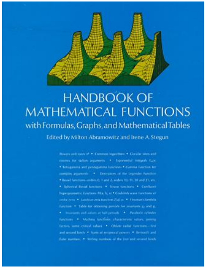
Creative Telescoping: write

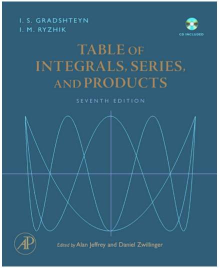
$$c_r(x)\frac{\mathrm{d}^r}{\mathrm{d}x^r} f(x,y) + \cdots + c_0(x) f(x,y) \; = \frac{\mathrm{d}}{\mathrm{d}y} g(x,y).$$

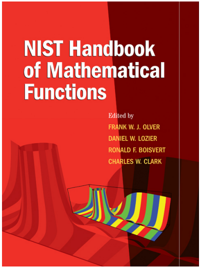
Integrating from a to b yields a differential equation for $F(x)$:

$$c_r(x)\frac{\mathrm{d}^r}{\mathrm{d}x^r} F(x) + \cdots + c_0(x) F(x) \; = g(x,b) - g(x,a)$$

Special Function Identities







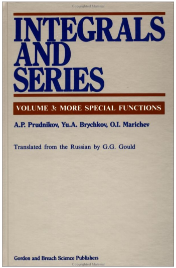
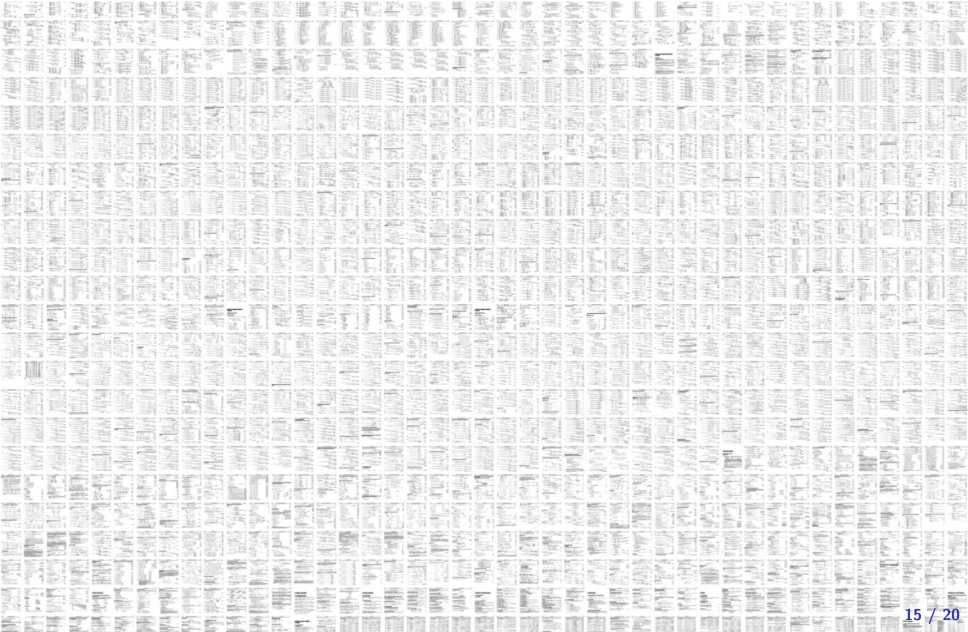


Table of Integrals by Gradshteyn and Ryzhik



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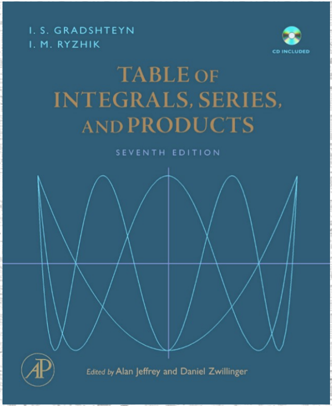

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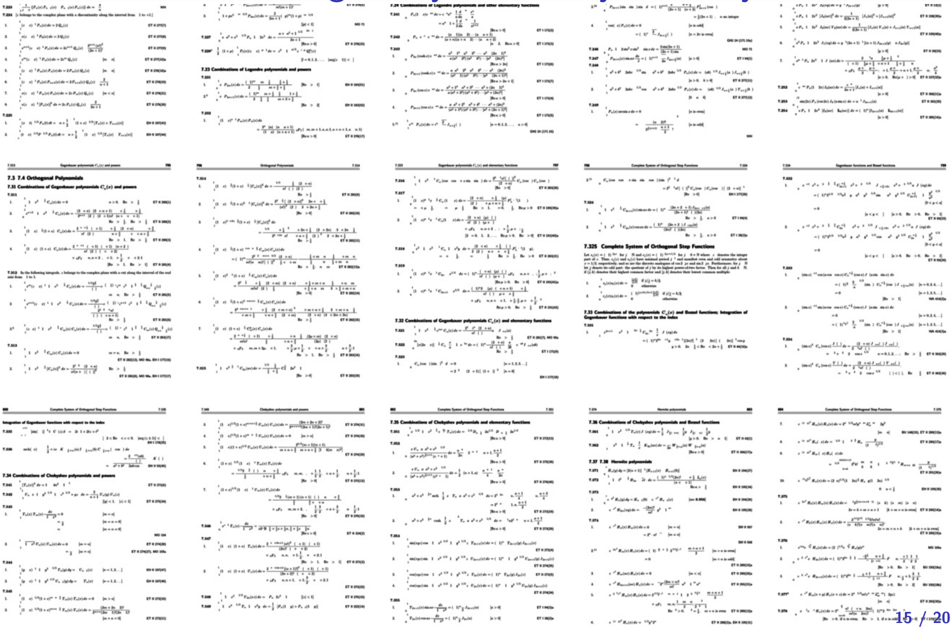

7.319

1. $$\int_0^1 (1-x)^{\mu-1} x^{\nu-1}\, C_{2n}^{\lambda}\left(\gamma x^{1/2}\right) dx = (-1)^n \frac{\Gamma(\lambda+n)\,\Gamma(\mu)\,\Gamma(\nu)}{n!\,\Gamma(\lambda)\,\Gamma(\mu+\nu)}\ {}_3F_2\left(-n, n+\lambda, \nu; \frac{1}{2}, \mu+\nu; \gamma^2\right)$$

$[\operatorname{Re}\mu > 0, \quad \operatorname{Re}\nu > 0]$ ET II 191(41)a

2. $$\int_0^1 (1-x)^{\mu-1} x^{\nu-1}\, C_{2n+1}^{\lambda}\left(\gamma x^{1/2}\right) dx = \frac{(-1)^n 2\gamma\,\Gamma(\mu)\,\Gamma(\lambda+n+1)\,\Gamma\left(\nu+\frac{1}{2}\right)}{n!\,\Gamma(\lambda)\,\Gamma\left(\mu+\nu+\frac{1}{2}\right)} \times {}_3F_2\left(-n, n+\lambda+1, \nu+\tfrac{1}{2}; \tfrac{3}{2}, \mu+\nu+\frac{1}{2}; \gamma^2\right)$$

$[\operatorname{Re}\mu > 0, \quad \operatorname{Re}\nu > -\frac{1}{2}]$ ET II 191(42)

7.32 Combinations of Gegenbauer polynomials $C_n^{\nu}(x)$ and elementary functions

7.321 $$\int_{-1}^1 \left(1-x^2\right)^{\nu-\frac{1}{2}} e^{iax}\, C_n^{\nu}(x)\, dx = \frac{\pi 2^{1-\nu} i^n\, \Gamma(2\nu+n)}{n!\,\Gamma(\nu)} a^{-\nu} J_{\nu+n}(a)$$

$[\operatorname{Re}\nu > -\frac{1}{2}]$ ET II 281(7), MO 99a

7.322 $$\int_0^{2a} [x(2a-x)]^{\nu-\frac{1}{2}}\, C_n^{\nu}\left(\frac{x}{a}-1\right) e^{-bx}\, dx = (-1)^n \frac{\pi\,\Gamma(2\nu+n)}{n!\,\Gamma(\nu)} \left(\frac{a}{2b}\right)^{\nu} e^{-ab}\, I_{\nu+n}(ab)$$

$[\operatorname{Re}\nu > -\frac{1}{2}]$ ET I 171(9)

7.323

1. $$\int_0^{\pi} C_n^{\nu}(\cos\varphi)\,(\sin\varphi)^{2\nu}\, d\varphi = 0$$ $[n = 1, 2, 3, \ldots]$

Table of Integrals by Gradshteyn and Ryzhik

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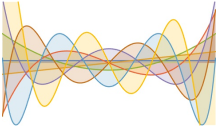

Gegenbauer polynomials $C_n^{(\alpha)}(x)$

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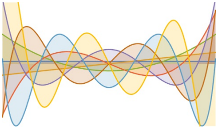

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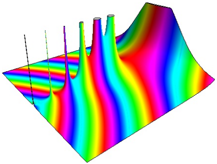

Gamma function $\Gamma(x)$

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

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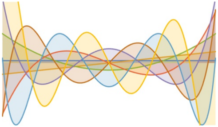
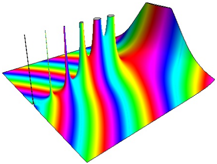
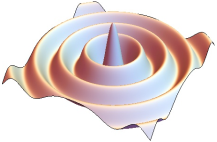


Gegenbauer polynomials $C_n^{(\alpha)}(x)$



Gamma function $\Gamma(x)$



Bessel function $J_\nu(x)$

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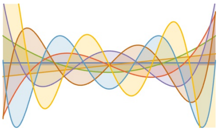

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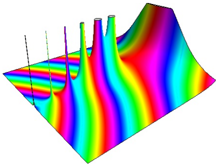

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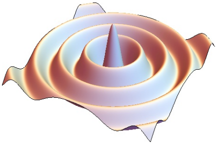

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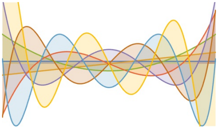
- A large portion of such identities can be proven via the holonomic systems approach.

Table of Integrals by Gradshteyn and Ryzhik



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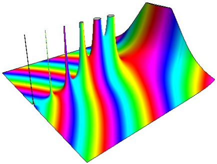

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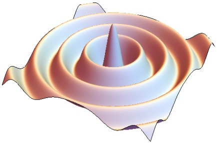

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- A large portion of such identities can be proven via the holonomic systems approach.
- Algorithms are implemented in the HolonomicFunctions package.

Example: Holonomic system, satisfied by both sides of the identity:

$$ia(n+2\nu)f_n'(a) + a(n+1)f_{n+1}(a) - in(n+2\nu)f_n(a) = 0,$$

$$a(n+1)(n+2)f_{n+2}(a) - 2i(n+1)(n+\nu+1)(n+2\nu+1)f_{n+1}(a) \\ \quad - a(n+2\nu)(n+2\nu+1)f_n(a) = 0.$$

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```
In[42]:= Annihilator[Pi * 2 ^ (1 - ν) * I ^ n * Gamma[2 ν + n] / n ! / Gamma[ν] * a ^ (-ν) *
           BesselJ[ν + n, a], {Der[a], S[n]}] // Factor
Out[42]=
         {i a (n + 2 ν) D_a + a (1 + n) S_n - i n (n + 2 ν),
          a (1 + n) (2 + n) S_n^2 - 2 i (1 + n) (1 + n + ν) (1 + n + 2 ν) S_n - a (n + 2 ν) (1 + n + 2 ν)}

In[43]:= CreativeTelescoping[(1 - x ^ 2) ^ (ν - 1 / 2) * Exp[I * a * x] * GegenbauerC[n, ν, x],
           Der[x], {Der[a], S[n]}] // Factor
Out[43]=
         {{a (n + 2 ν) D_a - i a (1 + n) S_n - n (n + 2 ν),
           a (1 + n) (2 + n) S_n^2 - 2 i (1 + n) (1 + n + ν) (1 + n + 2 ν) S_n - a (n + 2 ν) (1 + n + 2 ν)},
          {(1 + n) S_n - x (n + 2 ν), 2 i (1 + n) x (1 + n + ν) S_n - 2 i (1 + n + ν) (n + 2 ν)}}
```

Holonomic Special Function Identities

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

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

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

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Symbolic Determinants via Holonomic Ansatz

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

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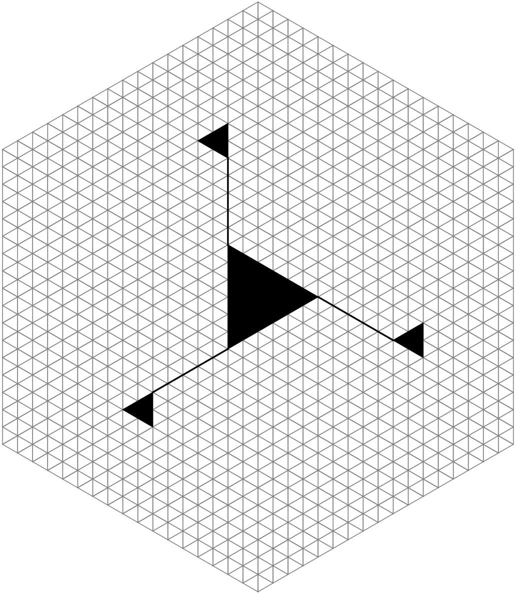
$$\det_{1\leqslant i,j\leqslant 2m+1}\left[\binom{\mu+i+j+2r}{j+2r-2}-\delta_{i,j+2r}\right]$$

$$= \frac{(-1)^{m-r+1}\,(\mu+3)\,(m+r+1)_{m-r}}{2^{2m-2r+1}\left(\frac{\mu}{2}+r+\frac{3}{2}\right)_{m-r+1}}\cdot\prod_{i=1}^{2m}\frac{(\mu+i+3)_{2r}}{(i)_{2r}}$$

$$\times\prod_{i=1}^{m-r}\frac{\left(\mu+2i+6r+3\right)_i^2\left(\frac{\mu}{2}+2i+3r+2\right)_{i-1}^2}{(i)_i^2\left(\frac{\mu}{2}+i+3r+2\right)_{i-1}^2}.$$

Combinatorial Interpretation



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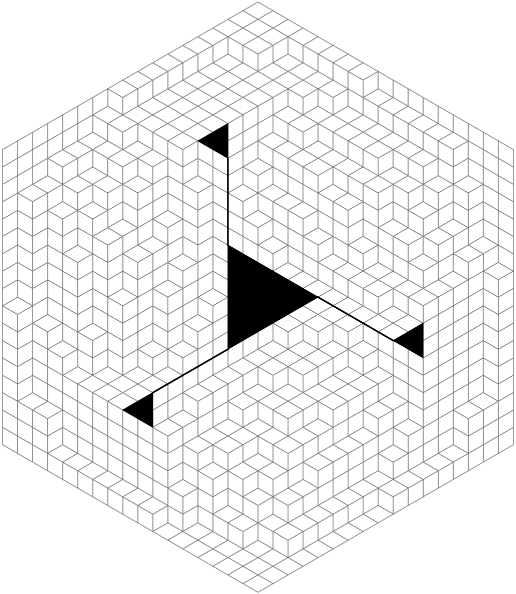

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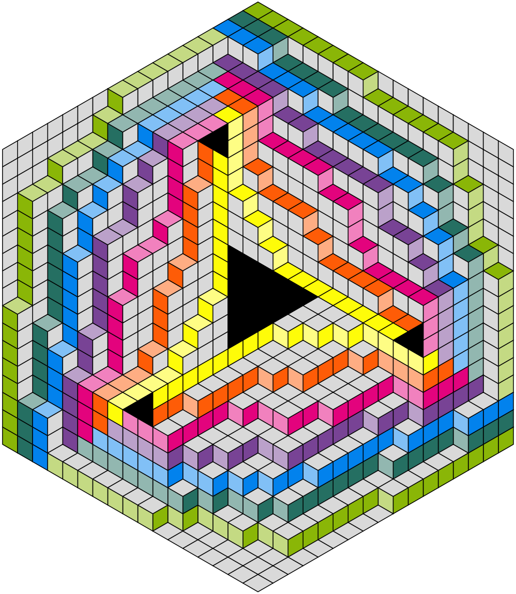

Further Reading

- **Survey article:** *Creative telescoping for holonomic functions.* DOI: 10.1007/978-3-7091-1616-6_7, arXiv:1307.4554.
- **PhD thesis:** *Advanced applications of the holonomic systems approach* (RISC, Johannes Kepler University, Linz, Austria, 2009).
- **Software package:** *HolonomicFunctions (user's guide)*. https://risc.jku.at/sw/holonomicfunctions/
- **Electromagnetic waves application:** *Method, device and computer program product for determining an electromagnetic near field of a field excitation source for an electrical system* (with J. Schöberl and P. Paule), Patents EP2378444 and US8868382.
- **Combinatorial determinants:** *Binomial determinants for tiling problems yield to the holonomic ansatz* (with H. Du, T. Thanatipanonda, E. Wong). DOI: 10.1016/j.ejc.2021.103437, arXiv:2105.08539.