Introduction to Computer Algebra

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– Computer Algebra and Particle Physics 2023, Hamburg, July 17, 2023 –

Motivation

Large Hadron Collider

Challenges

The Big Questions

- What is the nature of dark matter?
- What are the properties of the Higgs boson?
- What is the quantum structure of the vacuum?
- ...

The challenge

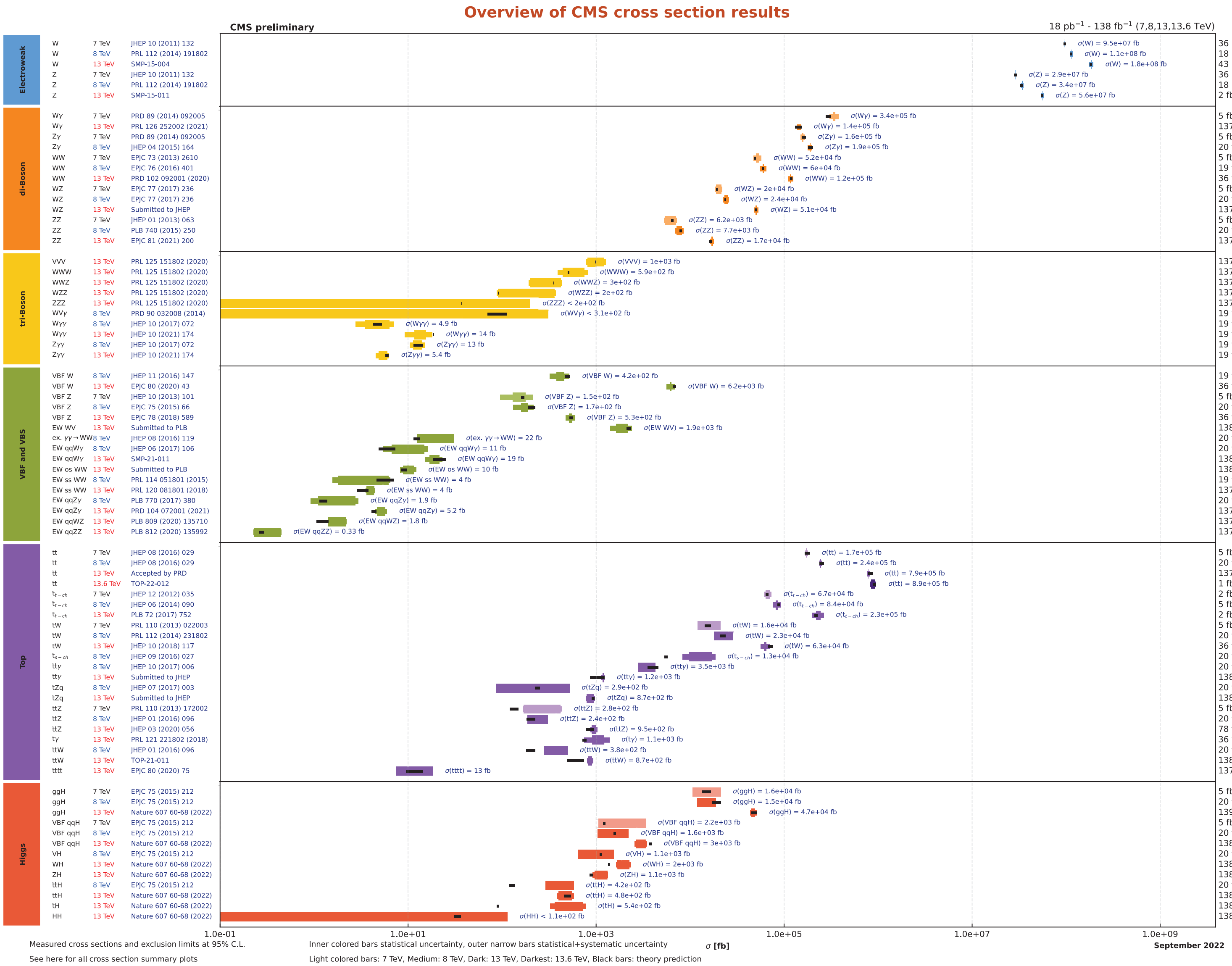
- Solve master equation

$$\text{new physics} = \text{data} - \text{Standard Model}$$

- LHC experiments deliver high precision measurements
  - searches require understanding of SM background
  - theory has to match or exceed accuracy of LHC data

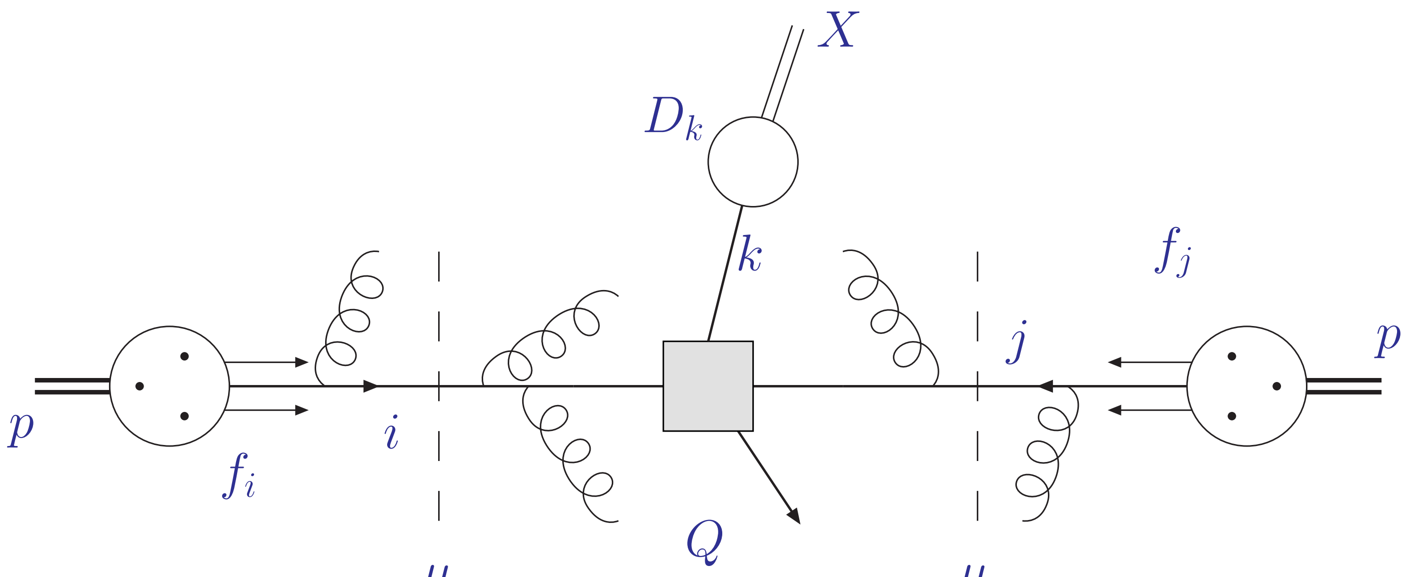
Standard Model cross sections

- Standard Model cross sections and predictions at the LHC CMS coll. '22



QCD factorization

QCD factorization



$$\sigma_{pp\to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \hat{\sigma}_{ij\to X}\left(\alpha_s(\mu^2), Q^2, \mu^2, m_X^2\right)$$

- Factorization at scale μ
  - separation of sensitivity to dynamics from long and short distances
- Hard parton cross section $\hat{\sigma}_{ij\to X}$ calculable in perturbation theory
  - cross section $\hat{\sigma}_{ij\to k}$ for parton types i, j and hadronic final state X
- Non-perturbative parameters: parton distribution functions f_i, strong coupling α_s, particle masses m_X
  - known from global fits to exp. data, lattice computations, ...

Parton luminosity

- Long distance dynamics due to proton structure

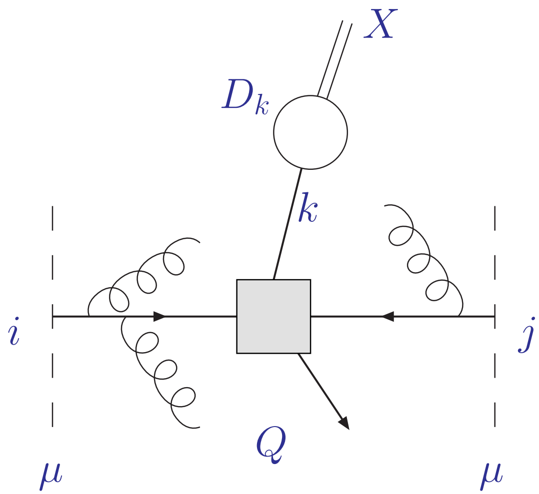
- Cross section depends on parton distributions f_i

$$\sigma_{pp \to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \left[\ldots \right]$$

- Parton distributions known from global fits to exp. data
  - available fits accurate to NNLO
  - information on proton structure depends on kinematic coverage

Hard scattering cross section

- Parton cross section $\hat{\sigma}_{ij \to k}$ calculable pertubatively in powers of α_s
  - known to NLO, NNLO, ... ($\mathcal{O}(\text{few}\%)$ theory uncertainty)



- Accuracy of perturbative predictions
  - LO (leading order) ($\mathcal{O}(50 - 100\%)$ unc.)
  - NLO (next-to-leading order) ($\mathcal{O}(10 - 30\%)$ unc.)
  - NNLO (next-to-next-to-leading order) ($\lesssim$ $\mathcal{O}(10\%)$ unc.)
  - N^3LO (next-to-next-to-next-to-leading order)
  - ...

Perturbation theory at work

QCD Lagrangian

- Classical part of QCD Lagrangian

$$\mathcal{L}_{\rm cl} \quad = \quad -\frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + \sum_{\rm flavors} \bar{\psi}_i \left({\rm i} \not{D} - m_q \right)_{ij} \psi_j$$

- Matter fields $\psi_i, \bar{\psi}_j$ with $i, j = 1, \dots, 3$ (fundamental rep.)
  - covariant derivative $D_{\mu,ij} = \partial_\mu \delta_{ij} + {\rm i} g_s \left(t_a \right)_{ij} A^a_\mu$
- Field strength tensor $F^a_{\mu\nu}$ with $a = 1, \dots, 8$ (adjoint rep.)
  - covariant derivative $D_{\mu,ab} = \partial_\mu \delta_{ab} - g_s f_{abc} A^c_\mu$
  - $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$
- Formal parameters of the theory (no observables)
  - strong coupling $\alpha_s = g_s^2/(4\pi)$
  - quark masses m_q

Quantization

- Gauge fixing (Feynman gauge $\lambda = 1$) $\mathcal{L}_{\rm gauge-fix} \; = \; -\frac{1}{2\lambda} \left(\partial^\mu A^a_\mu \right)^2$
- Ghosts (Grassmann fields η) $\mathcal{L}_{\rm ghost} \; = \; \partial_\mu \eta^{a\,\dagger} \left(D^\mu_{ab} \eta^b \right)$
  (removal of unphysical degrees of freedom for gauge fields) Fadeev, Popov

From Lagrangian to Feynman rules

- Consider action S

$$S = \mathrm{i} \int d^4x \, (\mathcal{L}_{\rm cl} + \mathcal{L}_{\rm gauge-fix} + \mathcal{L}_{\rm ghost}) = S_{\rm free} + S_{\rm int}$$

- Decompose action into free $S_{\rm free}$ and interacting part $S_{\rm int}$
  - $S_{\rm free}$ contains bi-linear terms in fields
  - $S_{\rm int}$ contains interactions
- Derivation of Feynman rules
  - inverse propagators from $S_{\rm free}$
  - interacting parts from $S_{\rm int}$ (in perturbative expansion)

From Lagrangian to Feynman rules

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- Decompose action into free S_{free} and interacting part S_{int}
  - S_{free} contains bi-linear terms in fields
  - S_{int} contains interactions
- Derivation of Feynman rules
  - inverse propagators from S_{free}
  - interacting parts from S_{int} (in perturbative expansion)

Examples (I)

- Fermion propagator in QCD from $\bar{\psi}_i \delta_{ij} \, (\mathrm{i}\not{\partial} - m_q) \, \psi_j$
  - substitution $\partial_\mu = -\mathrm{i} p_\mu$ (Fourier transformation)
- Inverse propagator (momentum space) $\Gamma_{ij}^{\bar{\psi}\psi}(p) = -\mathrm{i} \, \delta_{ij} \, (\not{p} - m_q)$
- Check: quark propagator $\Delta_{ij}(p) = +\mathrm{i} \, \delta_{ij} \, \dfrac{1}{\not{p} - m_q + \mathrm{i}0}$
  - causality in Minkowski space: prescription $+\mathrm{i}0$

Examples (II)

- Gluon propagator in QCD from bi-linear terms in $F^a_{\mu\nu} F_a^{\mu\nu}$ and $\mathcal{L}_{\rm gauge-fix}$
  - recall $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$
  - recall $\mathcal{L}_{\rm gauge-fix} \;=\; -\frac{1}{2\lambda} \left(\partial^\mu A^a_\mu\right)^2$
- Inverse propagator (momentum space)

$$\Gamma^{AA}_{ab;\mu\nu}(p) \;=\; +{\rm i}\,\delta_{ab} \left[p^2 g_{\mu\nu} - \left(1 - \frac{1}{\lambda}\right) p_\mu p_\nu\right]$$

- Gluon propagator $\Delta^{ab;\mu\nu}(p) \;=\; +{\rm i}\,\delta_{ab} \left[\frac{-g_{\mu\nu}}{p^2} + (1-\lambda)\frac{p_\mu p_\nu}{p^4}\right]$
  - Check: $\Gamma^{AA}_{ac;\mu\rho}(p)\,\Delta^{cb;\rho\nu}(p) \;=\; \delta_a^{\;b}\, g_\mu^{\;\nu}$

Examples (II)

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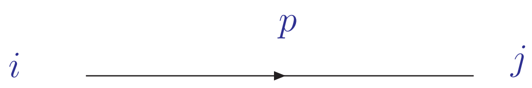
  - Check: $\Gamma^{AA}_{ac;\mu\rho}(p)\, \Delta^{cb;\rho\nu}(p) = \delta_a^{\ b}\, g_\mu^{\ \nu}$

Examples (III)

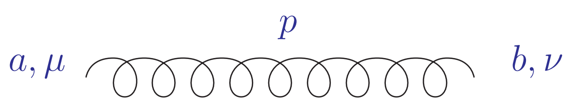
- Interactions derived from S_{int}
  - fermion-gluon interaction from $\bar{\psi}_i \mathrm{i} \not{A}_{ij} \psi_j \longrightarrow -\mathrm{i} t^a_{ij} \gamma_\mu$
- General rule
  - replacement of all ∂_μ by momenta p_μ
    (tedious for 3- and 4-gluon interactions)

Feynman rules (I)

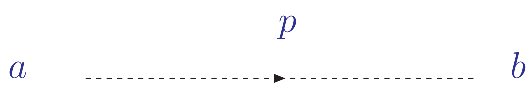
- Propagators
  - fermions, gluons, ghosts
  - covariant gauge



$$\delta^{ij}\,\frac{\mathrm{i}}{\not{p}-m}$$



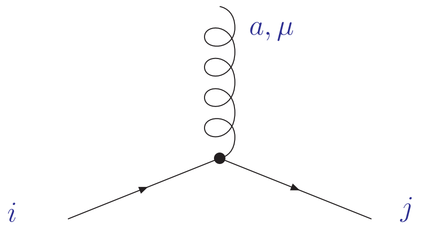
$$\delta^{ab}\,\mathrm{i}\left(\frac{-g^{\mu\nu}}{p^2}+(1-\lambda)\frac{p^\mu p^\nu}{(p^2)^2}\right)$$



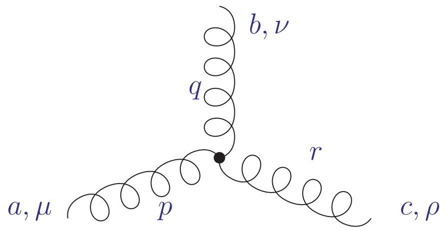
$$\delta^{ab}\,\frac{\mathrm{i}}{p^2}$$

Feynman rules (II)

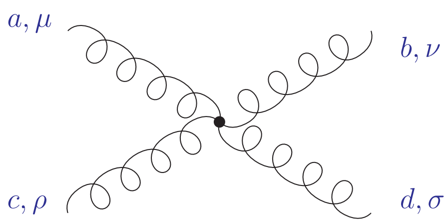
- Vertices



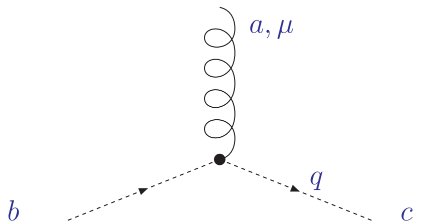
$$-\mathrm{i}\, g\; (t^a)_{ji}\; \gamma^\mu$$



$$-g\, f^{abc}\; \left((p-q)^\rho g^{\mu\nu} + (q-r)^\mu g^{\nu\rho} + (r-p)^\nu g^{\mu\rho}\right)$$



$$-\mathrm{i}\, g^2\, f^{xac} f^{xbd}\; (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\sigma} g^{\nu\rho})$$
$$-\mathrm{i}\, g^2\, f^{xad} f^{xbc}\; (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma})$$
$$-\mathrm{i}\, g^2\, f^{xab} f^{xcd}\; (g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho})$$



$$g\, f^{abc}\, q^\mu$$

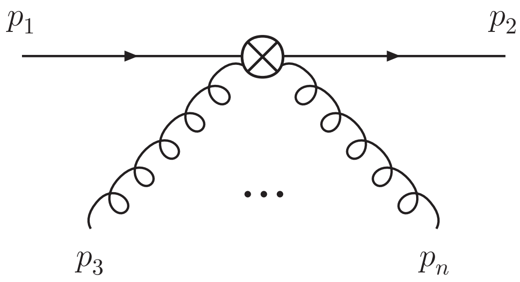
Perturbation theory at work

- Perturbative approach straightforward in principle
  - draw all Feynman diagrams
  - apply Feynman rules and evaluate expressions for matrix elements
  - use standard reduction techniques for loops and phase space integrals
- (Extremely) hard in practice
  - intermediate expressions more complicated than final results
- Known bottlenecks
  - **many diagrams** — many diagrams are related by gauge invariance
  - **many terms in each diagram** — nonabelian gauge boson self-interactions are complicated
  - **many kinematic variables** — allowing the construction of very complicated expressions
- Computer algebra programs are a standard tool

Text book example (I)

Operator matrix elements

- Quark operator of spin-N and twist two
  $O^{\psi}_{\{\mu_1,\dots,\mu_N\}} = \overline{\psi}\,\gamma_{\{\mu_1} D_{\mu_2} \dots D_{\mu_N\}}\,\psi$



- N covariant derivatives $D_{\mu,ij} = \partial_\mu \delta_{ij} + \mathrm{i} g_s \, (t_a)_{ij}$ between quark fields ψ, $\overline{\psi}$
- Feynman rules with new vertices for additional gluons coupling to operator
- Evaluation of operators in matrix elements $A^{\psi\psi}$ with external quark states

$$A^{\psi\psi}_{\{\mu_1,\dots,\mu_N\}} = \langle \psi(p_1) | O^{\psi}_{\{\mu_1,\dots,\mu_N\}}(-p_1 - p_2) | \overline{\psi}(p_2) \rangle$$

- Zero-momentum transfer through operator reduces problem to computation of propagator-type diagrams

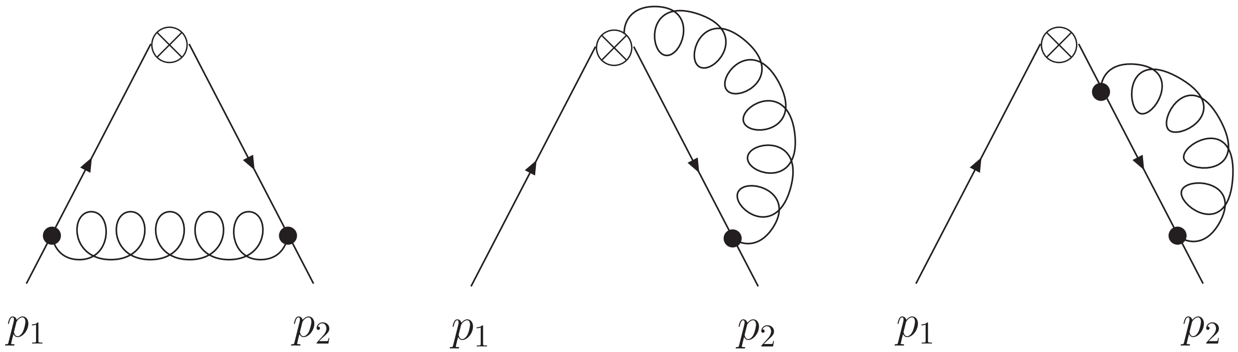
Real life

- Computation of quantum corrections to $A^{\psi\psi}$ up to four loops

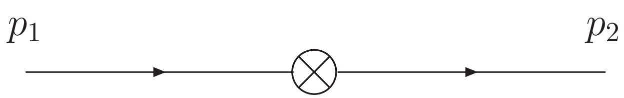
Text book example (II)

One-loop computation

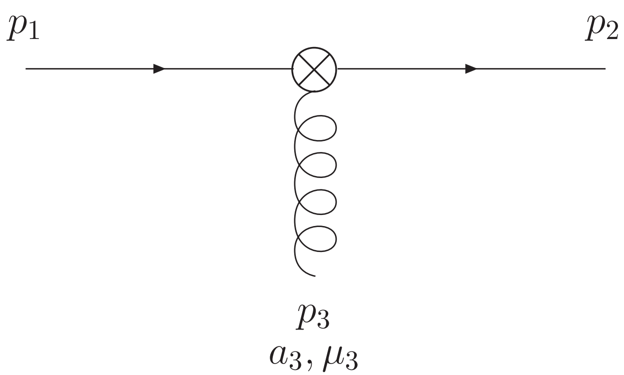
- Feynman diagrams



- New Feynman rules for vertices with light-like vector Δ, $\Delta^2 = 0$



$$\not\Delta \, (\Delta \cdot p_2)^{N-1}$$



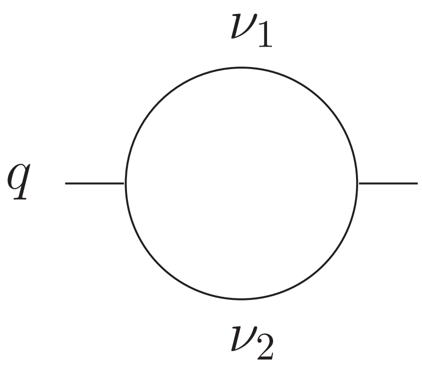
$$-g t^{a_3} \not\Delta \Delta^{\mu_3} \sum_{j_1=0}^{N-2} (p_2 \cdot \Delta)^{N-2-j_1} (-p_1 \cdot \Delta)^{j_1}$$

Text book example (III)

Two-point integrals

- Massless one-loop scalar two-point function $\mathrm{L1}$
  - dimensional regularization with $D = 4 - 2\epsilon$

$$\mathrm{L1} = \int d^D p_1 \, \frac{1}{(p_1^2)^{\nu_1} \, ((p_1 - q)^2)^{\nu_2}}$$



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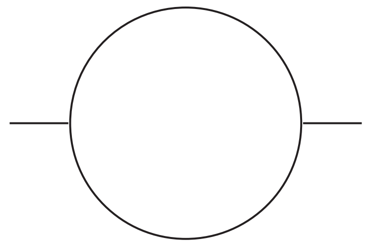

- Results for $\mathrm{L1}$

$$\mathrm{L1} \;=\; \mathrm{i}\,(-1)^{\nu_1+\nu_2}\,\pi^{-D/2}\,(-p^2)^{D/2-\nu_1-\nu_2} \;\times$$
$$\times\; \frac{\Gamma(\nu_1+\nu_2-D/2)\Gamma(D/2-\nu_1)\Gamma(D/2-\nu_2)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(D-\nu_1-\nu_2)}$$

- Laurent-expansion of Gamma-function in $\epsilon = 2 - \frac{D}{2}$ around positive integers values ($\nu_i \geq 0$)
  - Riemann zeta values $\Gamma(1+\epsilon) = 1 - \epsilon\gamma_E + \frac{\epsilon^2}{2}(\zeta_2 + \gamma_E^2) + \ldots$

Text book example (IV)

One-loop result

- Computation of loop integral in $D = 4 - 2\epsilon$ dimensions and expansion in ϵ

$$\Delta^{\mu_1} \dots \Delta^{\mu_N} \langle \psi(p_1) | O^{\psi}_{\{\mu_1, \dots, \mu_N\}}(0) | \overline{\psi}(-p_1) \rangle =$$

$$= \quad 1 + \frac{\alpha_s}{4\pi} C_F \frac{1}{\epsilon} \left\{ 4 S_1(N) + \frac{2}{N+1} - \frac{2}{N} - 3 \right\} + \mathcal{O}(\alpha_s \epsilon^0) + \mathcal{O}(\alpha_s^2)$$

- Details in chapt. 4.6 of
  The Theory of Quark and Gluon Interactions
  F.J. Yndurain

- One-loop result contains harmonic sum $S_1(N)$ (harmonic numbers)

$$S_1(N) \quad = \quad \sum_{i=1}^{N} \frac{1}{i} \quad = \quad 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{N}$$

$$S_1(N+1) - S_1(N) \quad = \quad \frac{1}{N+1}$$

Symbolic Summation

Symbolic Summation

Polynomial summation

- Examples

$$\sum_{i=0}^{n-1} i = \frac{1}{2}n(n-1)$$

$$\sum_{i=0}^{n-1} i^2 = \frac{1}{6}n(n-1)(2n-1)$$

$$\sum_{i=0}^{n-1} i^3 = \frac{1}{4}n^2(n-1)^2$$

$$\sum_{i=0}^{n-1} i^4 = \frac{1}{30}n(n-1)(2n-1)(3n^2-3n-1)$$

Difference operator

- Introduce operator Δ with $(\Delta f)(n) = f(n+1) - f(n)$
- If $g = (\Delta f)$, then (for $a, b \in \mathbf{N}, a \leq b$)

$$\sum_{i=a}^{b-1} g(i) \qquad = \sum_{i=a}^{b-1} \big(f(i+1) - f(i)\big)$$

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$$= \sum_{i=a+1}^{b} f(i) - \sum_{i=a}^{b-1} f(i)$$

Difference operator

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$$\begin{aligned}\sum_{i=a}^{b-1} g(i) &= \sum_{i=a}^{b-1} \big(f(i+1) - f(i)\big) = \sum_{i=a}^{b-1} f(i+1) - \sum_{i=a}^{b-1} f(i) \\ &= \sum_{i=a+1}^{b} f(i) - \sum_{i=a}^{b-1} f(i) = f(b) - f(a)\end{aligned}$$

Difference operator

- Introduce operator Δ with $(\Delta f)(n) = f(n+1) - f(n)$
- If $g = (\Delta f)$, then (for $a, b \in \mathbf{N}, a \leq b$)

$$\sum_{i=a}^{b-1} g(i) = \sum_{i=a}^{b-1} \big(f(i+1) - f(i)\big) = \sum_{i=a}^{b-1} f(i+1) - \sum_{i=a}^{b-1} f(i)$$

$$= \sum_{i=a+1}^{b} f(i) - \sum_{i=a}^{b-1} f(i) = f(b) - f(a)$$

- Consecutive cancellation of summands: telescoping
- Symbolic summation problem
  $g = (\Delta f)$ with $f = (\sum g)$, operator Δ is left inverse $\Delta(\sum f) = f$
- Cf. symbolic integration (differential operator D)

$$g = Df = \frac{d}{dx} f \quad \longrightarrow \quad \int_a^b dx g(x) = f(b) - f(a)$$

Difference operator (cont'd)

- Differential operator D acts in continuum as $D(x^m) = mx^{m-1}$

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Rising and falling factorials

- Define rising factorials as $f^{\overline{m}} = f(x)f(x+1)\ldots f(x+m-1)$ (also known as Pochhammer symbols $(x)_m$)

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Rising and falling factorials

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Difference operator (cont'd)

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Rising and falling factorials

- Define falling factorials as $f^{\underline{m}} = f(x)f(x-1)\dots f(x-m+1)$
- Then, with falling factorials

$$\Delta(x^{\underline{m}}) \;=\; mx^{\underline{m-1}} \qquad\qquad \sum_{i=0}^{n-1} i^{\underline{m}} \;=\; \frac{1}{m+1} n^{\underline{m+1}}$$

- Conversion of polynomial powers x^m
  (decomposition with Stirling numbers of second kind $\left\{ \begin{matrix} m \\ i \end{matrix} \right\}$)

$$x^m = \sum_{i=0}^{m} \left\{ \begin{matrix} m \\ i \end{matrix} \right\} x^{\underline{i}}$$

  - Stirling numbers of second kind denote # of ways to partition n things in k non-empty sets

Examples

- Polynomials

$$\sum_{i=0}^{n-1} i = \sum_{i=0}^{n-1} i^{\underline{1}} = \frac{1}{2}n^{\underline{2}} = \frac{1}{2}n(n-1)$$

$$\sum_{i=0}^{n-1} i^2 = \sum_{i=0}^{n-1} (i^{\underline{2}} + i^{\underline{1}}) = \frac{1}{3}n^{\underline{3}} + \frac{1}{2}n^{\underline{2}} = \frac{1}{6}n(n+1)(2n+1)$$

$$\sum_{i=0}^{n-1} i^3 = \sum_{i=0}^{n-1} (i^{\underline{3}} + 3i^{\underline{2}} + i^{\underline{1}}) = \frac{1}{4}n^{\underline{4}} + n^{\underline{3}} + \frac{1}{2}n^{\underline{2}} = \frac{1}{4}n^2(n+1)^2$$

Harmonic summation

- Harmonic numbers $S_1(N)$
  Euler 1775

$$S_1(N) \quad = \quad \sum_{i=1}^{N} \frac{1}{i} \; = \; 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{N}$$

- Harmonic sums $S_{m_1,\ldots,m_k}(n)$
  Gonzalez-Arroyo, Lopez, Ynduráin ‘79; Vermaseren ‘98; S.M., Uwer, Weinzierl ‘01
  - recursive definition $S_{\pm m_1,\ldots,m_k}(n) = \sum_{i=1}^{n} \frac{(\pm 1)^i}{i^{m_1}} S_{m_2,\ldots,m_k}(i)$

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  Gonzalez-Arroyo, Lopez, Ynduráin ‘79; Vermaseren ‘98; S.M., Uwer, Weinzierl ‘01
  - recursive definition $S_{\pm m_1,\ldots,m_k}(n) = \sum_{i=1}^{n} \frac{(\pm 1)^i}{i^{m_1}} S_{m_2,\ldots,m_k}(i)$
- Expansion of Gamma-function in $\epsilon = 2 - \frac{D}{2}$ around positive integers values ($n \geq 0$)

$$\frac{\Gamma(n+1+\epsilon)}{\Gamma(1+\epsilon)} \quad = \quad \Gamma(n+1) \, \exp\left(- \sum_{k=1}^{\infty} \epsilon^k \, \frac{(-1)^k}{k} \, S_k(n) \right)$$

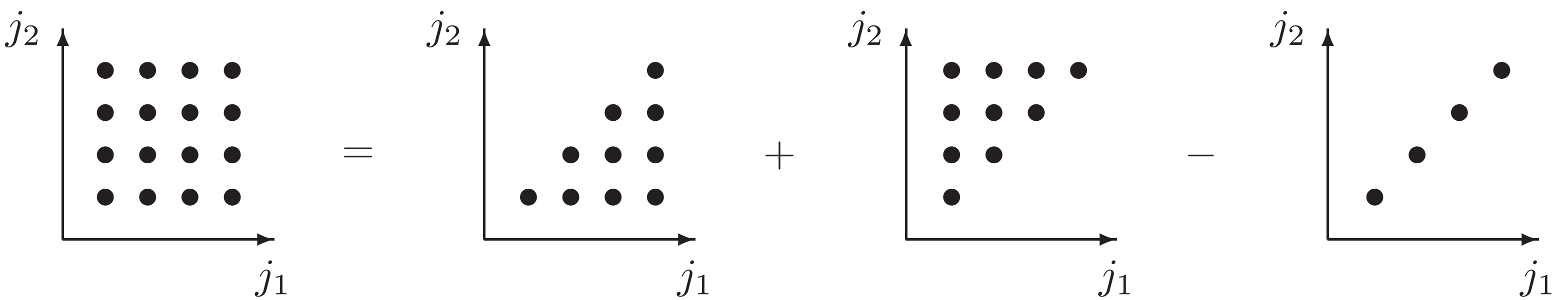
Algorithms for harmonic sums

- Multiplication (Hopf algebra)
  - basic formula (recursion)

$$
\begin{aligned}
S_{m_1,\ldots,m_k}(n) \times S_{m'_1,\ldots,m'_l}(n) \quad = \quad & \sum_{j_1=1}^{n} \frac{1}{j_1^{m_1}} S_{m_2,\ldots,m_k}(j_1) S_{m'_1,\ldots,m'_l}(j_1) \\
& + \sum_{j_2=1}^{n} \frac{1}{j_2^{m'_1}} S_{m_1,\ldots,m_k}(j_2) S_{m'_2,\ldots,m'_l}(j_2) \\
& - \sum_{j=1}^{n} \frac{1}{j^{m_1+m'_1}} S_{m_2,\ldots,m_k}(j) S_{m'_2,\ldots,m'_l}(j)
\end{aligned}
$$

- Proof uses decomposition

$$
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \quad = \quad \sum_{i=1}^{n} \sum_{j=1}^{i} a_{ij} + \sum_{j=1}^{n} \sum_{i=1}^{j} a_{ij} - \sum_{i=1}^{n} a_{ii}
$$



Algorithms for harmonic sums (cont'd)

- Convolution (sum over $n-j$ and j)

$$\sum_{j=1}^{n-1} \frac{1}{j^{m_1}} S_{m_2,\ldots,m_k}(j) \frac{1}{(n-j)^{n_1}} S_{n_2,\ldots,n_l}(n-j)$$

- Conjugation

$$-\sum_{j=1}^{n} \binom{n}{j} (-1)^j \frac{1}{j^{m_1}} S_{m_2,\ldots,m_k}(j)$$

- Binomial convolution (sum over binomial, $n-j$ and j)

$$-\sum_{j=1}^{n-1} \binom{n}{j} (-1)^j \frac{1}{j^{m_1}} S_{m_2,\ldots,m_k}(j) \frac{1}{(n-j)^{n_1}} S_{n_2,\ldots,n_l}(n-j)$$

Hypergeometric summation

Definition

- Hypergeometric function ${}_mF_n$

$$ {}_mF_n\left(\begin{array}{c} a_1, \ldots, a_m \\ b_1, \ldots, b_n \end{array} \middle| z \right) = \sum_{i \geq 0} \frac{a_1^{\overline{i}} \ldots a_m^{\overline{i}}}{b_1^{\overline{i}} \ldots b_n^{\overline{i}}} \frac{z^i}{i!} $$

Hypergeometric summation

Definition

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$${}_mF_n\left(\begin{array}{c} a_1,\ldots,a_m \\ b_1,\ldots,b_n \end{array}\middle| z\right) = \sum_{i\geq 0} \frac{a_1^{\overline{i}}\ldots a_m^{\overline{i}}}{b_1^{\overline{i}}\ldots b_n^{\overline{i}}}\,\frac{z^i}{i!}$$

Examples

$${}_0F_0\left(\middle| z\right) = \sum_{i\geq 0} \frac{z^i}{i!} = \exp(z)$$

$${}_2F_1\left(\begin{array}{c} a, 1 \\ 1 \end{array}\middle| z\right) = \sum_{i\geq 0} a^{\overline{i}}\,\frac{z^i}{i!} = \frac{1}{(1-z)^a}$$

$${}_2F_1\left(\begin{array}{c} 1, 1 \\ 2 \end{array}\middle| z\right) = z\sum_{i\geq 0} \frac{1^{\overline{i}}1^{\overline{i}}}{2^{\overline{i}}}\,\frac{z^i}{i!} = -\ln(1-z)$$

Higher transcendental functions

- Hypergeometric function

$$ {}_2F_1(a,b;c,x_0) = \sum_{i=0}^{\infty} \frac{a^{\overline{i}} b^{\overline{i}}}{c^{\overline{i}}} \frac{x_0^i}{i!} $$

- First Appell function

$$ F_1(a,b_1,b_2;c;x_1,x_2) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{a^{\overline{m_1+m_2}} b_1^{\overline{m_1}} b_2^{\overline{m_2}}}{c^{\overline{m_1+m_2}}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

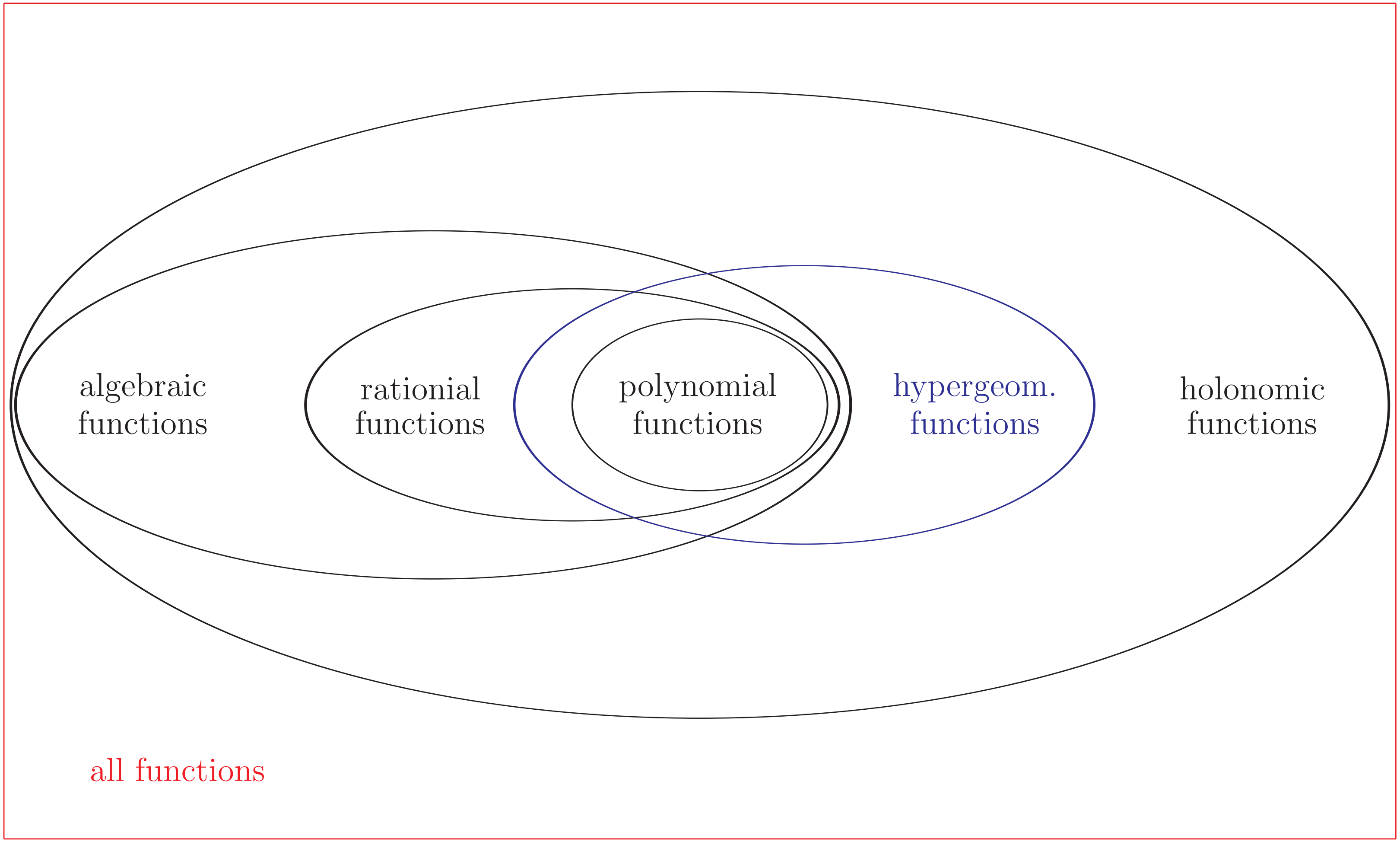
- Second Appell function

$$ F_2(a,b_1,b_2;c_1,c_2;x_1,x_2) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{a^{\overline{m_1+m_2}} b_1^{\overline{m_1}} b_2^{\overline{m_2}}}{c_1^{\overline{m_1}} c_2^{\overline{m_2}}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

Holonomic functions

Classes of functions

- Some common classes of functions



Holonomic functions

- Definition (continuous case of one variable): A function f is called holonomic if there exist polynomials $p_0, \dots, p_r$ not all zero, such that

$$p_0(x)f(x) + p_1(x)f'(x) + p_2(x)f''(x) + \cdots + p_r(x)f^{(r)}(x) = 0$$

- Examples:
  - $\exp(x)$: $f'(x) - f(x) = 0$
  - $\ln(1-x)$: $(x-1)f''(x) - f'(x) = 0$
  - $\frac{1}{1+\sqrt{1-x^2}}$: $(x^3 - x)f''(x) + (4x^2 - 3)f'(x) + 2xf(x) = 0$
  - Bessel functions, Hankel functions, Struve functions, Airy functions, Polylogarithms, Elliptic integrals, the Error function, Kelvin functions, Mathieu functions, . . .
  - many functions which have no name and no closed form

Holonomic functions

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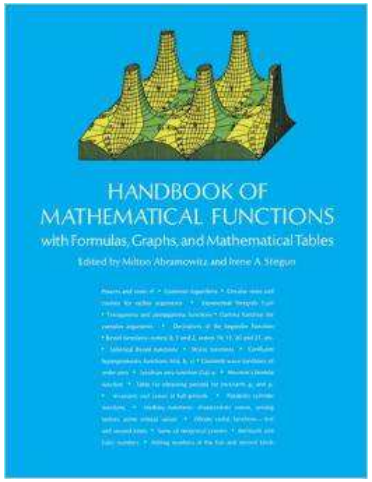
$$p_0(x) f(x) + p_1(x) f'(x) + p_2(x) f''(x) + \cdots + p_r(x) f^{(r)}(x) = 0$$

- Not holonomic:
  - $\exp(\exp(x) - 1)$
  - Riemann Zeta function
  - many functions which have no name and no closed form
- This means that these functions can (provably) not be viewed as solutions of a linear differential equation with polynomial coefficients.

Holonomic functions

- Approximately 60% of the functions in Abramowitz and Stegun's handbook fall into the category of holonomic functions in one variable.

  - *Handbook of Mathematical Functions*
    M. Abramowitz, I. Stegun



Differential equations

Theorem

- The solution set of a linear differential equation of order r is a vector space of dimension r.

Consequences

- A holonomic function f is uniquely determined by
  - the differential equation
  - a finite number of initial values $f(0)$, $f'(0)$, $f''(0)$, . . . , $f^{(k)}(0)$ (usually, $k = r$ suffices.)
- A holonomic function can be represented exactly by a finite amount of data (assuming that the constants appearing in equation and initial values belong to a suitable subfield of $\mathbb{C}$, e.g., to $\mathbb{Q}$.)

Examples

- $f(x) = \exp(x)$
  $\longleftrightarrow f'(x) - f(x) = 0$ with $f(0) = 1$

- $f(x) = \ln(1-x)$
  $\longleftrightarrow (x-1)f''(x) - f'(x) = 0$ with $f(0) = 0, f'(0) = -1$

- $f(x) = \frac{1}{1+\sqrt{1-x^2}}$
  $\longleftrightarrow (x^3 - x)f''(x) + (4x^2 - 3)f'(x) + 2xf(x) = 0$ with
  $f(0) = \frac{1}{2}, f'(0) = 0$

- $f(x) = I_5(x)$ (fifth modified Bessel function of the first kind)
  $\longleftrightarrow x^2 f''(x) + xf'(x) - (x^2 + 25)f(x) = 0$
  with $f(0) = f'(0) = \cdots = f^{(4)}(0) = 0, f^{(5)}(0) = \frac{1}{32}$

- ...

Holonomic sequences

- Definition (discrete case of one variable): A sequence $(a_n)_{n=0}^{\infty}$ is called holonomic if there exist polynomials $p_0, \ldots, p_r$ not all zero, such that

$$p_0(n)a_n + p_1(n)a_{n+1} + p_2(n)a_{n+2} + \cdots + p_r(n)a_{n+r} = 0$$

- Examples:
  - 2^n : $\quad a_{n+1} - 2a_n = 0$
  - $n!$: $\quad a_{n+1} - (n+1)a_n = 0$
  - $\sum_{i=0}^{n} \frac{(-1)^i}{i!}$: $\quad (n+2)a_{n+2} - (n+1)a_{n+1} - a_n = 0$
  - Fibonacci numbers, Harmonic numbers, Perrin numbers, diagonal Delannoy numbers, Motzkin numbers, Catalan numbers, Apery numbers, Schröder numbers, . . .
  - many sequences which have no name and no closed form

Holonomic sequences

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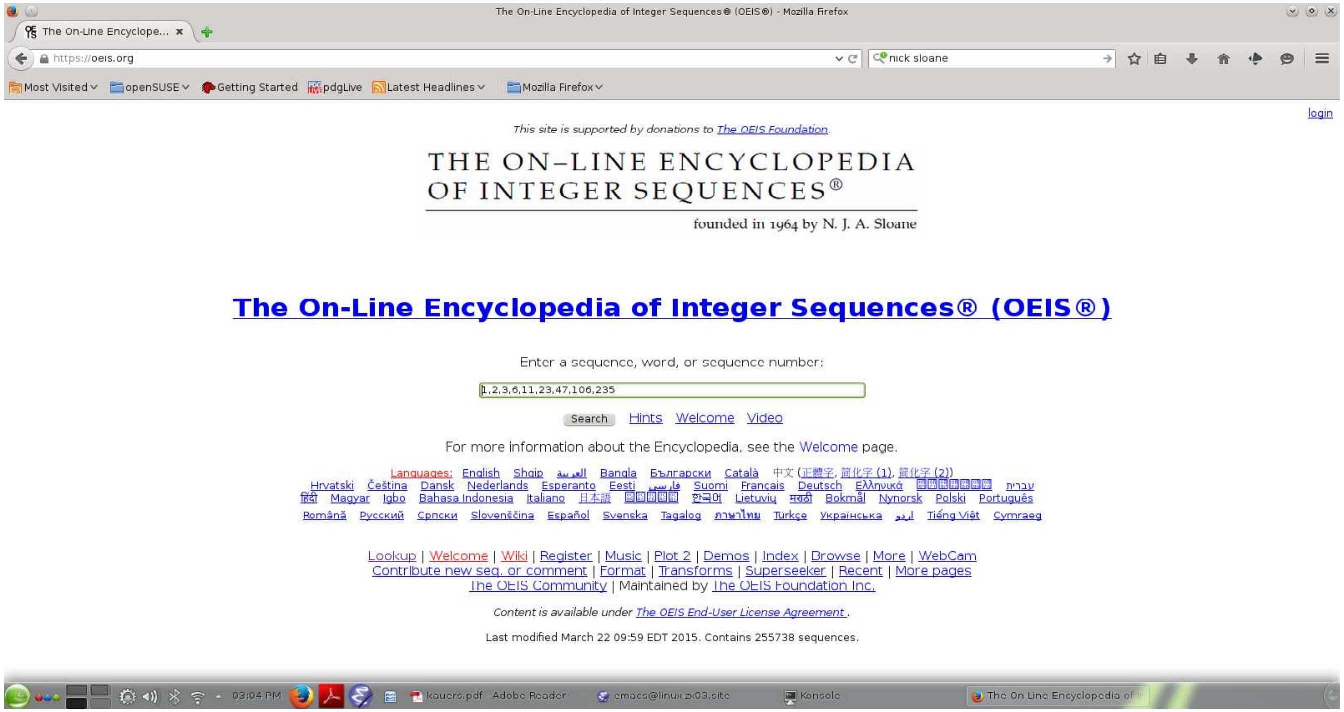
$$p_0(n)a_n + p_1(n)a_{n+1} + p_2(n)a_{n+2} + \cdots + p_r(n)a_{n+r} = 0$$

- Not holonomic:
  - 2^{2^n}
  - sequence of prime numbers
  - many sequences which have no name and no closed form
- This means that these sequences can (provably) not be viewed as solutions of a linear recurrence equation with polynomial coefficients.

Holonomic sequences

- Approximately 25% of the sequences in Sloane's Online Encyclopedia of Integer Sequences fall into the category of holonomic sequences in one variable.
  - Online Encyclopedia of Integer Sequences `https://oeis.org/`



Difference equations

Theorem

- The solution set of a linear recurrence equation of order r whose leading coefficient has s integer roots greater than r is a vector space of dimension $s + r$.

Consequences

- A holonomic sequence $(a_n)_{n=0}^{\infty}$ is uniquely determined by a holonomic function f is uniquely determined by
  - the recurrence equation
  - a finite number of initial values a_0, a_1, a_2, ..., a_k (usually, $k = r$ suffices.)
- A holonomic sequence can be represented exactly by a finite amount of data. (assuming that the constants appearing in equation and initial values belong to a suitable subfield of $\mathbb{C}$, e.g., to $\mathbb{Q}$.)

Examples

- $a_n = 2^n$
  $\longleftrightarrow a_{n+1} - 2a_n = 0$ with $a_0 = 1$

- $a_n = n!$
  $\longleftrightarrow a_{n+1} - (n+1)a_n = 0$ with $a_0 = 1$

- $a_n = \sum_{i=0}^{n} \frac{(-1)^i}{i!}$
  $\longleftrightarrow (n+2)a_{n+2} - (n+1)a_{n+1} - a_n = 0$ with $a_0 = 1, a_1 = 0$

- $a_n = I(n)$ (number of involutions of n letters)
  $\longleftrightarrow a_{n+3} + na_{n+2} - (3n+6)a_{n+1} - (n+1)(n+2)a_n = 0$ with
  $a_0 = 1, a_1 = 1, a_2 = 2$

- ...

Conversion

Theorem

- Conversion of difference to differential equations:
  Let $a(x) = \sum_{n=0}^{\infty} a_n\, x^n$, then $a(x)$ is holonomic as function $\longleftrightarrow$ $(a_n)_{n=0}^{\infty}$ is holonomic as sequence

Consequences

- Given a differential equation for $a(x)$, one can compute a recurrence for $(a_n)_{n=0}^{\infty}$
- Given a recurrence for $(a_n)_{n=0}^{\infty}$, we can compute a differential equation for $a(x)$

Polynomials

Polynomials as sequences

- Examples

$$\frac{1}{1-x} = \sum_{i=0}^{\infty} 1\, x^i$$

$$D_x \frac{1}{1-x} = \frac{1}{(1-x)^2} = \sum_{i=0}^{\infty} i\, x^{i-1} = \sum_{i=0}^{\infty} (i+1)\, x^i$$

$$D_x^2 \frac{1}{1-x} = \frac{2}{(1-x)^3} = \sum_{i=0}^{\infty} i\,(i-1)\, x^{i-2} = \sum_{i=0}^{\infty} (i+1)\,(i+2)\, x^i$$

$$D_x^3 \frac{1}{1-x} = \frac{6}{(1-x)^4} = \sum_{i=0}^{\infty} i\,(i-1)\,(i-2)\, x^{i-3} = \sum_{i=0}^{\infty} (i+1)\,(i+2)\,(i+3)\, x^i$$

Harmonic polylogarithms

- Harmonic polylogarithms $H_{m_1,\ldots,m_k}(x)$
  Remiddi, Vermaseren '99
  - physical quantities in momentum (x)-space

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  - physical quantities in momentum (x)-space
    - basic functions of lowest weight
      $H_0(x) = \ln x\,, \quad H_1(x) = -\ln(1-x)\,, \quad H_{-1}(x) = \ln(1+x)$
    - higher functions defined by recursion
      $$H_{m_1,\ldots,m_w}(x) = \int_0^x dz\; f_{m_1}(z)\; H_{m_2,\ldots,m_w}(z)$$
      $$f_0(x) = \frac{1}{x}\,, \qquad f_1(x) = \frac{1}{1-x}\,, \qquad f_{-1}(x) = \frac{1}{1+x}$$

Harmonic polylogarithms

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      $$H_{m_1,\ldots,m_w}(x) = \int_0^x dz\; f_{m_1}(z)\; H_{m_2,\ldots,m_w}(z)$$
      $$f_0(x) = \frac{1}{x}\,, \qquad f_1(x) = \frac{1}{1-x}\,, \qquad f_{-1}(x) = \frac{1}{1+x}$$
- Algebra under multiplication
  $H_{m_1,\ldots,m_r}(x) H_{n_1,\ldots,n_s}(x) \longrightarrow H_{m_1,\ldots,m_{r+s}}(x)$
- Integral transformation (Mellin transform to discrete N)
  $$\tilde{f}(N) \;=\; \int_0^1 dx\;\, x^{\,N}\, f(x)$$
  - unique mapping $\dfrac{H_{m_1,\ldots,m_w}(x)}{(1 \pm x)} \longleftrightarrow S_{n_1,\ldots,n_{w+1}}(N)$

Algebra of words

- Consider alphabet alphabet of length $l = 3$
  - harmonic polylogarithms arise from iterated integrals over letters $x, 1 \pm x$

Iterated integrals

- Generalization:
  - hyperlogarithms (mathematics definition Poincaré)
  - generalized polylogarithms $\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1)$ Goncharov '98; Borwein, Bradley, Broadhurst, Lisonek '99
- Words $w = m_{\sigma_1} \ldots m_{\sigma_n}$ from letters $w = m_{\sigma_i}$ associated to generalized polylogarithms

$$\mathrm{Li}_{m_k,\ldots,m_1}(x_k,\ldots,x_1) =$$

$$= \int_0^{x_1 x_2 \ldots x_k} \underbrace{\left(\frac{dt'}{t'}\circ\right)^{m_1-1}}_{\underbrace{\frac{dt'_{m_1-1}}{t'_{m_1-1}} \cdots \frac{dt'_1}{t'_1}}_{(m_1-1)\text{ times}}} \frac{dt_k}{x_2 x_3 \ldots x_k - t_k} \cdots \int_0^{t_2} \left(\frac{dt'}{t'}\circ\right)^{m_k-1} \frac{dt_1}{1-t_1}$$

Summary

Perturbation theory at work

- Computer algebra is indispensable tool for computation of perturbative corrections

Symbolic sums

- Algorithms for symbolic summation and recurrence relations

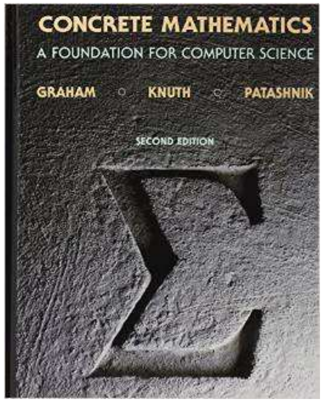
Polylogarithms

- Holonomic functions as solutions to set of a linear differential equations

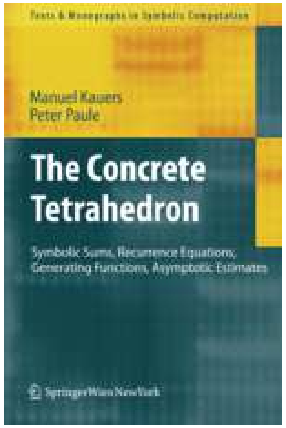
Literature (I)

- Text books
  - *Modern Computer Algebra*
    J. von zur Gathen, J. Gerhard

  - *Concrete Mathematics*
    R. L Graham, D. E. Knuth, O. Pataschnik

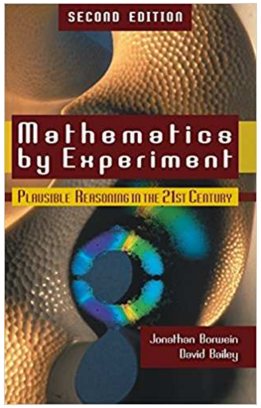


  - *Concrete Tetrahydron*
    M. Kauers, P. Paule



  - *A=B*
    M. Petkovsek, H. S. Wilf, D. Zeilberger `www.math.upenn.edu/~wilf/AeqB.html`

  - *Mathematics by Experiment*
    J.M. Borwein, D. Bailey



Literature (II)

- Selected research articles
  - *Harmonic sums, Mellin transforms and integrals*, J. Vermaseren; hep-ph/9806280
  - *Nested sums, expansion of transcendental functions and multi-scale multi-loop integrals*, S.M., P. Uwer, S. Weinzierl; hep-ph/0110083
  - *Gauss hypergeometric function: Reduction, epsilon-expansion for integer/half-integer parameters and Feynman diagrams*, M. Yu. Kalmykov; hep-th/0602028
  - *HypExp 2, Expanding Hypergeometric Functions about Half-Integer Parameters*, T. Huber, D. Maitre; 0708.2443
  - *On the analytic computation of massless propagators in dimensional regularization*, E. Panzer; 1305.2161
  - . . .

Software (I)

Requirements in particle physics

- Symbolic calculations characterized by need for basic operations
  - sorting, gcd, factorization, multiplication
  - symbolic integration/summation
  - solution of systems of equations
  - ...
- Specialized code usually written by the user
  - largely dependent on the physics problem
  - add-on libraries

Software (II)

- Commercial programs: *Mathematica*, *Maple*, . . .
- Freeware/Add-on packages
  - *Mathematica*, *Maple*
    - several packages for hypergeometric summation
      [see for instance `www.math.upenn.edu/~wilf/AeqB.html`]
    - RISC software for symbolic summation and integration
      `www.risc.jku.at/research/combinat/software`
    - expansion of hypergeometric functions *HypExp*, T. Huber, D. Maitre
    - reduction of hypergeometric functions *HyperDire*, V. Bytev
    - hyperlogarithmic integration *HyperInt*, E. Panzer
  - GiNaC `www.ginac.de`
    - *nestedsums*, S. Weinzierl
  - Form `www.nikhef.nl/~form`
    - *Summer6*, J. Vermaseren
    - *XSummer*, S.M., P. Uwer