Summation Techniques for Feynman Diagrams via Special Functions

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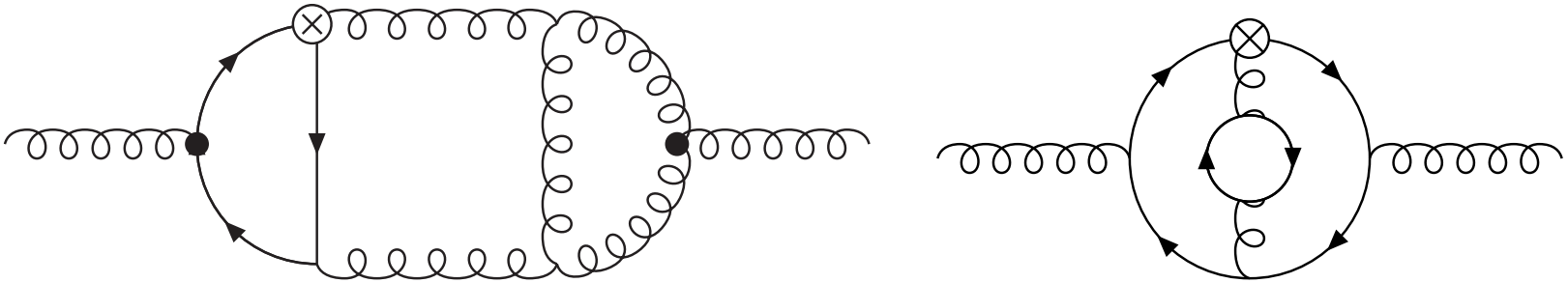
Talk Outline

This talk is aimed at 3 audiences; physicists, mathematicians and computer algebraists. There is something for everyone but no-one will be completely satisfied...

1. A summation phrasing of Feynman integrals
2. Existing summation tools
3. A refined holonomic approach (implemented in ρSum)
4. Illustrative results and examples

High Precision QFT Calculations
QCD

- Consider perturbative QFT. Such as corrections to the high energy proton sub-structure from heavy quarks at 3-loops (and for $p^2 >> m^2_{\mathrm{HQ}}$). Bierenbaum, Blümlein, Klein '09



- Such diagrams yield nasty integrals which are extremely hard to work with. A simpler form is needed. Our goal is to simplify the object.
- Physically speaking, the only restriction on the Feynman diagrams is that they contain atmost one mass.

High Precision QFT Calculations

First Algorithmic Steps

- Momentum integrals are straightforward but the Feynman parameters integrals are not. Notice the operator insertion (the $\otimes$ in the diagram) will give us a Mellin parameter, n. Diagrams obey homogeneous difference equations in n. Blümlein, Kauers, Klein, Schneider '09
- A first step in trying to understand the remaining integrals is to convert them into definite nested hypergeometric and harmonic multi-sums. Blümlein & Kurth '98 and Vermaseren '98
- There is an algorithm to do this! Blümlein, Klein, Schneider & Stan '12

Mathematical Results

To arrive at special functions we will need just a few classical results,

1. The B-function,

$$B(x,y) = \int_0^1 (1-t)^{y-1} t^{x-1} dt$$

2. The Γ-function,

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$$

which is related to the B-function by,

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$$

Mathematical Results

1. The hypergeometric function, or ${}_2F_1$,

$$ {}_2F_1(a,b,c;z) = \frac{1}{B(b,c-b)} \int_0^1 x^{b-1}(1-x)^{c-b-1}(1-zx)^{-a}dx $$

2. The Pfaff transformations which allow one to change the ${}_2F_1$ argument,

$$ {}_2F_1(a,b,c;z) = (1-z)^{-b}{}_2F_1\left(b, c-a, c; \frac{z}{z-1}\right) $$

3. Euler's transformation,

$$ {}_{p+1}F_{q+1}\left[\begin{array}{c} a_1,\ldots,a_p,c \\ b_1,\ldots,b_q,d \end{array};z\right] = $$
$$ \frac{\Gamma(d)}{\Gamma(c)\Gamma(d-c)} \int_0^1 t^{c-1}(1-t)^{d-c-1}{}_pF_q\left[\begin{array}{c} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{array};tz\right]dt $$

which defines the generalised hypergeometric functions. Such as the ${}_3F_2$.

Mathematical Results

1. The generalised hypergeometric functions admit a sum representation,

$$ {}_pF_q\left[\begin{array}{c} a_1,\ldots,a_p \\ b_1,\ldots,b_q \end{array};z\right] = \sum_{i=0}^{\infty} \frac{(a_1)_i\cdots(a_p)_i}{(b_1)_i\cdots(b_q)_i}\frac{z^i}{i!} $$

   which makes use of the Pochhammer symbol,

$$ x_n = \frac{\Gamma(x+n)}{\Gamma(x)}. $$

2. Later harmonic sums will also be encountered,

$$ S_1(n) = \sum_{r=0}^{n}\frac{1}{r}, \quad S_{b,\vec{a}}(n) = \sum_{r=0}^{n}[\mathrm{sign}(b)]^r\frac{S_{\vec{a}}(r)}{r^{|b|}}, \quad S_{\emptyset}(n) = 1. $$

Producing Sums

General Approach

Returning to the problem: A parameter integral takes the form,

$$\int_0^1 dx_i \frac{\sum_j \prod_k P_{j,k}(x_i)^{\alpha_{j,k}(\epsilon)}}{[Q(x_i)]^{\beta(\epsilon)}} \quad \epsilon > 0 \; \alpha_{j,k}(\epsilon), \beta(\epsilon) \in \mathbb{Q}(\epsilon), P_{j,k}, Q \in \mathbb{Q}[x_i]$$

One uses a Mellin-Barnes representation to convert sums to products in the $P_{j,k}$ and Q,

$$(1-z)^{-a} = {}_2F_1(a,1,1;z) = \frac{1}{2\pi i}\int_C ds \frac{\Gamma(a+s)\Gamma(-s)}{\Gamma(a)}(-z)^s$$

then recognises the integrals as special functions. Closing the Mellin-Barnes contour C and using the residue theorem leads to a sum representation. Blümlein, Klein, Schneider & Stan '12

Producing Sums

General Approach

An illustrative example is,

$$\int_0^1 dx_1 dx_2 \frac{x_1(1-x_1)x_2^\epsilon(1-x_2)^2}{(x_1-x_2)^N} = \int_0^1 dx_1 dx_2 \frac{x_1(1-x_1)^\epsilon(1-x_2)^2}{x_1^N\left(1-\frac{x_2}{x_1}\right)^N}$$

$$= \frac{1}{2\pi i}\int_0^1 dx_1 dx_2 \int_C ds\; x_1^{1-N+s}(1-x_1)x_2^{\epsilon-s}(1-x_2)^2(-1)^s\frac{\Gamma(N+s)\Gamma(-s)}{\Gamma(N)}$$

Recall from that the x_i integrals are Beta functions,

$$\frac{1}{2\pi i}\int_C ds\; B(2+s-N,2)B(1+\epsilon-s,3)(-1)^s\frac{\Gamma(N+s)\Gamma(-s)}{\Gamma(N)}$$

$$= \frac{1}{2\pi i}\sum_{s=0}^{\infty} B(2+s-N,2)B(1+\epsilon-s,3)\frac{\Gamma(N+s)}{\Gamma(N)}\frac{1}{s!}$$

$$= B(1+\epsilon,3)B(2-n,2)\Gamma(N)\,{}_3F_2\left[\begin{matrix} -3-\epsilon & 2-N & N \\ -3 & 4-N & \end{matrix};1\right].$$

Producing Sums

General Approach

- The next step would be to find the Laurent expansion around $\varepsilon = 0$.
- However expanding general hypergeometric functions at arbitrary points is unsolved in general. Each function must be handled individually using available techniques.
- A general algorithm to not only compute the sum but also expand in powers of ϵ will be outlined in this talk.

Most approaches, so far, are limited to specific arguments in hypergeometric functions. Here, through summation, one is more general.

Producing Sums

An Example

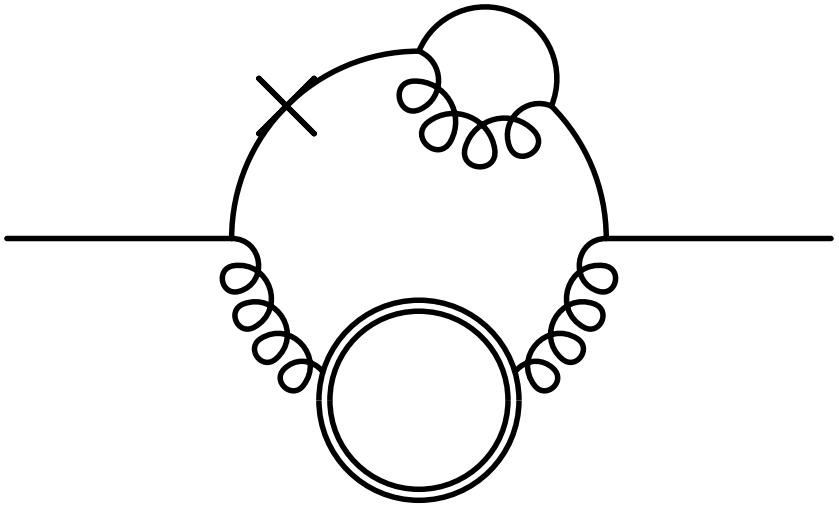
Our method is to give several integration steps that can be automated with computer algebra packages. An example is the 2-bubble diagrams which can be solved using,

1. Perform momentum integrals by introducing Feynman parameters and using textbook formulae (plus recognise some simple sums in the Feynman rules).
2. Recognise the Feynman parameter integrals as special functions; we can even deliver sum free results sometimes. (No Mellin-Barnes integral is needed.)
3. Convert special functions to a sum form that can be expanded in the DREG parameter, ϵ.

(There are many other ways in which sums may arise from Feynman diagrams beyond what is given here.)

2-bubble Class

Example Diagram



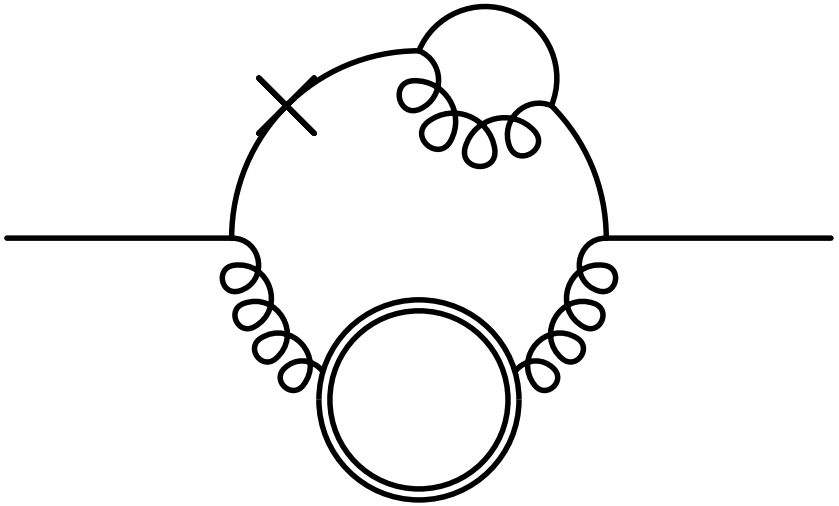
This diagram corresponds, via a dictionary of so-called Feynman rules, to an integral over momenta. Having converted this diagram to a momentum integral several standard steps lead to introducing,

$$x_i \in [0, 1],$$

and an $\epsilon > 0$ that regulates poles.

2-bubble Class

Example Diagram



Here now the diagram consists of an integrand which is 216 terms all of the form,

$$C(\cdots)B\left(2+\frac{\epsilon}{2},-\frac{\epsilon}{2}\right)B\left(3+\frac{\epsilon}{2},-1-\frac{\epsilon}{2}\right)B\left(4+\frac{\epsilon}{2},-\frac{3\epsilon}{2}\right)$$
$$\times\frac{\Gamma(4-\epsilon)}{\Gamma(-1-\frac{\epsilon}{2})\Gamma(3-\frac{\epsilon}{2})\Gamma\left(2+\frac{\epsilon}{2}\right)^3}(1-x_4)^{\frac{\epsilon}{2}}x_4^{1+\frac{\epsilon}{2}}(1-x_6)^{1-ep}x_6^{1-ep}$$
$$\times(1-x_8)^{1+\frac{\epsilon}{2}}x_8(1+x_9)^{\frac{\epsilon}{2}}$$
$$\times(x_8+(1-x_8)x_9)^{N-1}$$

2-bubble Class

Example Diagram

Next one integrates out the x_i over $[0,1]$. For this simple case special function results are sufficient. One can immediately recognise B-functions,

$$C(\cdots)B\left(2+\frac{\epsilon}{2},-\frac{\epsilon}{2}\right)B\left(3+\frac{\epsilon}{2},-1-\frac{\epsilon}{2}\right)B\left(4+\frac{\epsilon}{2},-\frac{3\epsilon}{2}\right)$$
$$\times\frac{\Gamma(4-\epsilon)}{\Gamma(-1-\frac{\epsilon}{2})\Gamma(3-\frac{\epsilon}{2})\Gamma\left(2+\frac{\epsilon}{2}\right)^3}B\left(2-\epsilon,2-\epsilon\right)B\left(2+\frac{\epsilon}{2},1+\frac{\epsilon}{2}\right)$$
$$\times(1-x_8)^{1+\frac{\epsilon}{2}}x_8(1+x_9)^{\frac{\epsilon}{2}}$$
$$\times(x_8+(1-x_8)x_9)^{N-1}$$

In addition one can recognise a hypergeometric function.

2-bubble Class

Example Diagram

Recognising a ${}_2F_1$ one has,

$$C(\cdots)B\left(2+\frac{\epsilon}{2},-\frac{\epsilon}{2}\right)B\left(3+\frac{\epsilon}{2},-1-\frac{\epsilon}{2}\right)B\left(4+\frac{\epsilon}{2},-\frac{3\epsilon}{2}\right)$$
$$\times\frac{\Gamma(4-\epsilon)}{\Gamma(-1-\frac{\epsilon}{2})\Gamma(3-\frac{\epsilon}{2})\Gamma\left(2+\frac{\epsilon}{2}\right)^3}B\left(2-\epsilon,2-\epsilon\right)B\left(2+\frac{\epsilon}{2},1+\frac{\epsilon}{2}\right)$$
$$\times(1-x_9)^{2-\frac{\epsilon}{2}}x_9^{N-3+\epsilon}B\left(2,2+\frac{\epsilon}{2}\right){}_2F_1\left(1-N,2,4+\frac{\epsilon}{2};\frac{x_9-1}{x_9}\right)$$

Then one can perform a Pfaff transformation,

$${}_2F_1\left(1-N,2,4+\frac{\epsilon}{2};\frac{x_9-1}{x_9}\right)=(1-x_9)^{1-N}{}_2F_1\left(1-N,2+\frac{\epsilon}{2},4+\frac{\epsilon}{2};x_9\right)$$

2-bubble Class

Example Diagram

Then immediately one can apply Euler's transformation,

$$C(\cdots)B\left(2+\frac{\epsilon}{2},-\frac{\epsilon}{2}\right)B\left(3+\frac{\epsilon}{2},-1-\frac{\epsilon}{2}\right)B\left(4+\frac{\epsilon}{2},-\frac{3\epsilon}{2}\right)$$
$$\times\frac{\Gamma(4-\epsilon)}{\Gamma(-1-\frac{\epsilon}{2})\Gamma(3-\frac{\epsilon}{2})\Gamma\left(2+\frac{\epsilon}{2}\right)^3}B\left(2-\epsilon,2-\epsilon\right)B\left(2+\frac{\epsilon}{2},1+\frac{\epsilon}{2}\right)$$
$$B\left(2,2+\frac{\epsilon}{2}\right)\Gamma\left(3-\frac{\epsilon}{2}\right)\frac{\Gamma\left(\epsilon-1\right)}{\Gamma\left(2+\frac{\epsilon}{2}\right)}{}_3F_2\left[\begin{array}{c}1-N,2+\frac{\epsilon}{2},3-\frac{\epsilon}{2}\\4+\frac{\epsilon}{2},2+\frac{\epsilon}{2}\end{array};1\right]$$

All integration has been done, it remains to understand the pole structure in ϵ. This is a special case that can be solved by other packages like HypExp2.

2-bubble Class

Example Diagram

To compute a Laurent expansion the Γ-functions are no problem but there is no simple and general formula to expand a ${}_3F_2$,

$$ {}_3F_2\left[\begin{array}{c} P_1(\epsilon), P_2(\epsilon), P_3(\epsilon) \\ P_4(\epsilon), P_5(\epsilon) \end{array};1\right] $$

for $P_i(\epsilon)$ a degree-1 polynomial in ϵ. However one can use the sum form,

$$ {}_3F_2\left[\begin{array}{c} 1-N, 2+\frac{\epsilon}{2}, 3-\frac{\epsilon}{2} \\ 4+\frac{\epsilon}{2}, 4+\frac{\epsilon}{2} \end{array};1\right] = \sum_{i=0}^{\infty} \frac{(1-N)_i \left(2+\frac{\epsilon}{2}\right)_i \left(3-\frac{\epsilon}{2}\right)_i}{\left(4+\frac{\epsilon}{2}\right)_i \left(4+\frac{\epsilon}{2}\right)_i} \frac{1}{i!} $$

however the sum is ill-posed! Notice that $(1-N)_r$ vanishes when $r > N-1$. E.g. $(-3)_2 = 6$ while $(-3)_4 = 0$. Thus the upper bound of the sum must be corrected,

$$ {}_3F_2\left[\begin{array}{c} 1-N, 2+\frac{\epsilon}{2}, 3-\frac{\epsilon}{2} \\ 4+\frac{\epsilon}{2}, 4+\frac{\epsilon}{2} \end{array};1\right] = \sum_{i=0}^{N-1} \frac{(1-N)_i \left(2+\frac{\epsilon}{2}\right)_i \left(3-\frac{\epsilon}{2}\right)_i}{\left(4+\frac{\epsilon}{2}\right)_i \left(4+\frac{\epsilon}{2}\right)_i} \frac{1}{i!} $$

2-bubble Class

Example Diagram

The sum is now precisely of the form solved by ρSum and indeed it returns that,

$$\sum_{i=0}^{N-1} \frac{(1-N)_i \left(2+\frac{\epsilon}{2}\right)_i \left(3-\frac{\epsilon}{2}\right)_i}{\left(4+\frac{\epsilon}{2}\right)_i \left(4+\frac{\epsilon}{2}\right)_i} \frac{1}{i!} = \frac{6}{N(1+N)(2+N)}$$

to constant order in ϵ. Taking the product of the above Laurent series with the relevant ones for the Γ-functions gives the correct expansion for the diagram.

Alternatively one could have introduced a binomial expansion for $(x_8 + (1-x_8)x_9)^{N-1}$ which would give precisely the same sum.

2-bubble Class

Physical Meaning

- Using the special function techniques described, all the diagrams in the 2-bubble class were reduced to a sum form which were solved using refined holonomic summation.
- This represents $\sim 13\%$ of the 1-mass 3-loop diagrams that contribute to the heavy flavour Wilson coefficients needed for parton distribution studies, see previous talks in this session.

Now change gears to mathematics...

Statement of Problem

Informal Statement

Any given Feynman diagram (with atmost one mass) can be expressed as a definite nested multi-sum,

$$F_n(\epsilon) = \sum_{i_1=\alpha_1}^{L_1(n)} \cdots \sum_{i_m=\alpha_m}^{L_m(n,i_1,\ldots i_m)} \sum_{j_1=\beta_1}^{\infty} \cdots \sum_{j_N=\beta_N}^{\infty} f(\epsilon, n, i_1, \ldots, i_m, j_1, \ldots, j_N).$$

In this talk frequently $\epsilon = 0$ to simplify slides however the method certainly includes $\epsilon \neq 0$!

Aim

Given a definite nested multi-sum find, in terms of indefinite nested multi-sums, another (simpler) representation.

Definition of Summand

Formal Statement

Definition

Let $\{f(n,k)\}_{n\geq 0, k\geq 0}$ be a multivariate (here bivariate) sequence over a field $\mathbb{F}$. f is hypergeometric in n and k if $\exists d \in \mathbb{Z}^+$ and $r_1(x,y), r_2(x,y) \in \mathbb{F}(x,y)$ such that $f(n+1,k)/f(k) = r_1(n,k)$ and $f(n,k+1)/f(n,k) = r_2(n,k) \, \forall n,k \geq d$.

Definition

Restrict to sequences where:
$\exists d \in \mathbb{Z}^+$, $a_i, b_i, m_i \in \mathbb{Z}$ and $c_i \in \mathbb{F}$ for $i \in [1,r]$ where $a_i n + b_i k + c_i \notin \mathbb{Z}^- \forall n,k \geq d$ and $\exists \, p(x,y), q(x,y) \in \mathbb{F}[x,y]$ where $q \neq 0$ factors linearly over $\mathbb{F}$:
$f(n,k) = p(n,k)/q(n,k) \prod_{i=1}^{r} \Gamma(a_i n + b_i k + c_i)^{m_i} \, \forall n,k \geq d$.

n.b. $\mathbb{Z}^{\pm}$ both include zero.

Statement of Problem

Summary

Allow the summand to be as defined, times harmonic numbers and linear combinations of such terms.

$$F_n(\epsilon) = \sum_{i_1=\alpha_1}^{L_1(n)} \cdots \sum_{i_m=\alpha_m}^{L_m(n,i_1,\ldots i_m)} \sum_{j_1=\beta_1}^{\infty} \cdots \sum_{j_N=\beta_N}^{\infty} f(\epsilon, n, i_1, \ldots, i_m, j_1, \ldots, j_N)$$

where $n \in \mathbb{N}$ and $n \geq n_0 \in \mathbb{N}$, all the upper bounds, L_k, are integer-linear in n, $\{i\}$ and $\{j\}$. All the lower bounds are specified constants, $\{\alpha\}, \{\beta\} \in \mathbb{N}$. The summand, F, is hypergeometric with respect to n, $\{i\}$ and $\{j\}$.

Aim

Find an expression for a definite nested multi-sum, using the outlined summand, in terms of indefinite nested multi-sums.

Statement of Problem

Illustration ($<$ 10 minutes of CPU time)

$$\sum_{i=2}^{n+1}\sum_{j=2}^{n+2-i}\sum_{a=0}^{\infty}\sum_{b=0}^{\infty}\frac{\binom{n+2}{i}\binom{n+2-i}{j}(-1)^{i+j}B(i,j)(j+i-1)}{(j+i+a+b)(i+j+a+b-1)(j+b)(i+b)}$$

$$\begin{aligned}
= \quad & \frac{2n^3+5n^2+4n-2}{n+1}S_2+\left[\frac{5}{2}S_2-\frac{n^2+2n+2}{n+1}\right]S_1^2-2nS_{2,1} \\
- \quad & 2n(n+1)\zeta_3-S_1^3+\frac{1}{4}S_1^4-\frac{1}{4}S_2^2+2(n+1)S_3-\frac{1}{2}S_4-2S_{3,1} \\
+ \quad & \left[4\zeta_3+(2n-1)S_2+2S_3-2(n+1)-4S_{2,1}\right]S_1+2S_{2,1,1}
\end{aligned}$$

where $S_{a,\ldots,b}=S_{a,\ldots,b}(n)$ for convenience.

- We have gone from a tough to simple, if long, expression.

Existing Tools

Creative Telescoping

For a definite sum one may use Zeilberger's algorithm which exploits creative telescoping,

Creative Telescoping (Zeilberger)

Given a bivariate hypergeometric sequence $f(N, i)$ find $c_j(N)$ for $j = 1, \ldots, d$ and $g(N, i)$ such that,

$$g(N, i+1) - g(N, i) = c_0(N)f(N, i) + \ldots + c_d(N)f(N+d, i).$$

Summing over the equation one obtains a recurrence for the sum,

$$S_N(a) = \sum_{i=1}^{a} f(N, i),$$

$$g(N, a+1) - g(N, 1) = c_0(N)S_N(a) + \ldots + c_d(N)S_{N+d}(a)$$

Colloquially, one finds a linear combination of shifted summands that telescope.

To go to the refined holonomic summation approach there are several generalisations. First recall holonomic sequences,

Holonomic sequence

A sequence a_n is holonomic if there exist polynomials $p_0(x), \ldots, p_r(x) \in \mathbb{F}[x]$ $p_0, p_d \neq 0$ such that,

$$p_0(n)a_n + \ldots + p_d(n)a_{n+d} = 0,$$

for all $n \in \mathbb{N}$.

yet we go further and allow for inhomogeneous recurrences. It is for this reason one uses the term refined holonomic summation.

Existing Tools

Refined Holonomic Summation

One extends to allowing a summand to be defined by a system of such inhomogeneous recurrences.

- In addition one allows field extensions that are 'intelligently' constructed by the algorithm Schneider '05.
- For example the algorithm, by input parameters, can construct a single extension or several extensions offering many different output recurrences for a problem, example later.

Understanding all these ideas is beyond the scope of this talk! We will see examples that give a feel for what is happening.

Existing Tools

Sigma

- To solve summation problems for hundreds of Feynman diagrams one must use software.
- Of the examples available, we will use a collection of algorithms found in Schneider '04, '05... related to Karr '81 & Chyzak '00. A Mathematica package, Sigma, is available that implements the algorithms.
- Sigma exploits the mathematical frame work of refined difference field theory where the refined construction can be defined constructively.
- More simply, note that Sigma computes linear recurrences with polynomial coefficients.

Existing Tools

Sum by Sum Approach

$$F_n = \sum_{i_1=\alpha_1}^{L_1(n)} \cdots \sum_{i_m=\alpha_m}^{L_m(n,i_1,\ldots i_m)} \sum_{j_1=\beta_1}^{\infty} \cdots \sum_{j_N=\beta_N}^{\infty} f(n,\{i\},\{j\})$$

$\downarrow$

Zoom to the innermost sum

$$\hat{F}_n = \sum_{j_N=\beta_N}^{\infty \text{ or } L_N} f(n,\{i\},\{j\})$$

$\downarrow$

Find a recurrence for the inner sum,

$$g_0(n)\hat{F}_n + \ldots + g_r(n)\hat{F}_{n+r} = G(n)$$

Solve Recurrence and substitute in solution

Refined Holonomic Approach

For Multi-sums

$$F_n = \sum_{i_1=\alpha_1}^{L_1(n)} \cdots \sum_{i_m=\alpha_m}^{L_m(n,i_1,\ldots i_m)} \sum_{j_1=\beta_1}^{\infty} \cdots \sum_{j_N=\beta_N}^{\infty} f(n,\{i\},\{j\})$$

$\downarrow$

Zoom to the innermost sum

$$\hat{F}_n = \sum_{j_N=\beta_N}^{\infty \text{ or } L_N} f(n,\{i\},\{j\})$$

$\downarrow$

Find a recurrence for the inner sum,

$$g_0(n)\hat{F}_n + \ldots + g_r(n)\hat{F}_{n+r} = G(n)$$

Replace innermost sum with the sequence and its recurrences

A Worked Example

Consider the following definite nested multi-sum,

$$F_n = \sum_{i_1=0}^{n-2} \sum_{i_2=0}^{n-i_1-2} \frac{4 i_1!(-1)^{i_2}(n-i_1-1)(1+i_2)!}{(1+i_1+i_2)^2(2+i_1+i_2)^2(i_1+i_2)!} \binom{n-i_1-2}{i_2}$$

To find a recurrence for F_n, first re-write the sum,

$$4 \sum_{i_1=0}^{n-2} i_1!(n-i_1-1) a_{i_1,n}$$

$$a_{i_1,n} = \sum_{i_2=0}^{n-i_1-2} \frac{(-1)^{i_2}(1+i_2)!}{(1+i_1+i_2)^2(2+i_1+i_2)^2(i_1+i_2)!} \binom{n-i_1-2}{i_2}$$

now apply a recurrence finding algorithm, e.g. Sigma.

A Worked Example

One finds that,

$$\begin{aligned}(2+i_1+n+i_1n)a_{i_1,n}-(2+i_1-n)(1+i_1+n)a_{i_1+1,n} &= \frac{1}{(1+i_1^2)i_1!},\\ -(1+i_1-n)(1+2i_1+i_1n)a_{i,n}-(1+n)(1+i_1+i_1n)a_{i,n+1} &= -\frac{1}{(1+n)i_1!}.\end{aligned}$$

- The two recurrences plus initial conditions specify the summand — a holonomic sequence. This is an example of the system of recurrences mentioned earlier.
- The right-hand sides are non-zero and represented inside a difference field — which necessitates the name refined approach.

Combining them one finds, for example, a zero-order recurrence,

$$F_n = \frac{4n}{2+n} - \frac{8S(n)}{(1+n)(2+n)}, \quad S_1(n) = \sum_{i=1}^{n} \frac{1}{i}.$$

Conceptual Advantages

- Consider a sum, in the refined approach, defined by a zeroth-order recurrence. It has the most complicated rhs possible. Essentially that is the sum-by-sum approach!
- At the other extreme, the class of Feynman diagram sums studied obey homogeneous (rhs $=0$) recurrences of order ~ 35.
- The refined approach allows the structure of the problem to be distributed between the order of the recurrence and the complexity of the recurrence right-hand side.

This freedom is a motivating concept to explore the refined approach. Again rigorously explaining how these ideas work is a significant excursion. It is the ability to construct 'intelligent' extensions that gives freedom.

Conceptual Advantages

- Using the sum-by-sum approach one must expand the summand in ϵ as a first step. Such an expansion blows up the size of the summand quickly.
- By holding the epsilon expansion inside the recurrence one can compute, with a small extra overhead, all the coefficients in an expansion at once.
- One is motivated to propose that at higher and higher orders in ϵ the refined approach will become increasingly quicker than the sum-by-sum approach.
  This scaling is a second motivating concept to explore the refined approach.

Conceptual Advantages

Example Sum

Consider the following double sum,

$$F_n(\epsilon) = \sum_{j_0=0}^{n-5} \sum_{j1=0}^{n-3-j_0} \frac{(-1)^{j_1}(1+j_1)(j_0+j_1)!\,\left(1-\frac{\epsilon}{2}\right)_{j_0}\left(3-\frac{\epsilon}{2}\right)_{j_1}}{(4-\epsilon)_{j_0+j_1}\left(4+\frac{\epsilon}{2}\right)_{j_0+j_1}} \binom{n-j_0-2}{j_1+1}$$

This is the appropriate input for the refined approach. For the sum-by-sum approach one must expand the summand.

$$F_n(\epsilon) = F_n^0(\epsilon) + \epsilon F_n^1(\epsilon) + \ldots$$

Conceptual Advantages

Example Sum

$$F_n^0(\epsilon) = \sum_{j_0=0}^{n-5} \sum_{j1=0}^{n-3-j_0} \frac{(-1)^{j_1}(1+j_1)(j_0+j_1)!\,(1)_{j_0}\,(3)_{j_1}}{(4)_{j_0+j_1}\,(4)_{j_0+j_1}} \binom{n-j_0-2}{j_1+1}$$

$$F_n^1(\epsilon) = \sum_{j_0=0}^{n-5} \sum_{j1=0}^{n-3-j_0} \frac{3(-1)^{j_1} j_0!(2+j_1)!(1+j_1)(j_0+j_1)!}{((3+j_0+j_1)!)^2} \binom{n-j_0-2}{j_1+1}$$

$$\times\left(1 + \frac{3}{1+j_1} + \frac{3}{2+j_1} - \frac{3}{1+j_0+j_1} - \frac{3}{2+j_0+j_1} - \frac{3}{3+j_0+j_1}\right.$$

$$\left. +3S_1(j_0) + 3S_1(j_1) - 3S_1(j_0+j_1)\right)$$

Worked Example

Sigma Session

Now an example showing the technical side of how recurrences are controlled,

$$\sum_{i=0}^{N-10} \sum_{j=0}^{2i} (-1)^j \binom{2i}{j} \binom{N}{i} S_1(j)^2$$

Here classical summation techniques succeed for the inner sum,

```
In[1]:= << Sigma.m
In[2]:= sum3 = SigmaSum[(-1)^j Binomial[2i, j] Binomial[N, i] S[1, j]^2, j, 0, 2i]
In[3]:= Prec3 = GenerateRecurrence[sum3, i, SimplifyByExt-> None];
```

Worked Example

Sigma Session

The returned recurrence is inhomogeneous and with no field extensions. However the resulting recurrence is 4th order and too big to show. One can find something more compact by asking Sigma to use refined theory,

```
In[4]:= Prec3DN = GenerateRecurrence[sum3, i, SimplifyByExt->
        DepthNumber];
```

Sigma computes a 3rd order recurrence with two field-extensions,

$$s_1 = \sum_{j=0}^{2i} \frac{(-1)^j \binom{2i}{j}^2}{1+2i-j}, \qquad s_2 = \sum_{j=0}^{2i} \frac{(-1)^j \binom{2i}{j}^2}{2+2i-j}.$$

Worked Example

Sigma Session

The 'price' of using refined difference theory is that both extension sums represent separate summation problems. One can find with Sigma for example,

$$s_1 = \frac{(-1)^i (2i)!}{(1+2i)(i!)^2}, \qquad s_2 = \frac{(-1)^i (2i)!(1+4i+2i^2)}{2(1+i)^2(1+2i)(i!)^2}.$$

One can substitute back into the recurrence and obtain something still quite large,

Worked Example

Sigma Session

$$
\begin{aligned}
&2(i+1)\left(32i^3+116i^2+130i+43\right)\mathrm{iSUM}(i+1)(i-N+1)\\
&-4(2i+1)^2(8i+13)\mathrm{iSUM}(i)(i-N)(i-N+1)\\
&-(i+1)(8i+5)(i+2)^3\mathrm{iSUM}(i+2)\\
&=r(i,N)\binom{N}{i}
\end{aligned}
$$

for $r(i,N)$ a large rational expression in i and N. Now we go to the outer sum which requires a shifted recurrence to build up a system,

In[5]:= **Srec3 = GenerateRecurrence[sum3, i, OneShiftIn− > N]**

Out[5]= $(1+N)iSUM[i]+(-N+i-1)iSUM[1+N,i]==0$

Worked Example

Sigma Session

There are now quite a few options to compute the final recurrence.

1. Using the 4th order inner sum recurrence one can obtain a 10th order recurrence with no extensions (classical approaches) in 110s.
2. Or, using SimplifyByExt$-$ $>$Full, a 4th order recurrence with 8 extension sums in 64s.
3. Using the 3rd order recurrence classical theory now finds an 8th order recurrence in 38s.
4. Finally, using SimplifyByExt$-$ $>$Full there is a 4th order recurrence with 5 extension sums that an be found in 15s.

These choices are automated by ρSum into an Mathematica package which chooses how to compute recurrences using heuristics.

Worked Example

Sigma Session

The 5 extension sums found in the last configuration are,

$$\sum_{i=0}^{N-10} \frac{\binom{N}{i}}{1+N-i}, \qquad \sum_{i=0}^{N-10} \frac{\binom{N}{i}}{1+2i},$$

$$\sum_{i=0}^{N-10} \frac{(-1)^i (2i)!}{(1+N-i)(i!)^2} \binom{N}{i}, \qquad \sum_{i=0}^{N-10} \frac{(-1)^i i (2i)!}{(1+N-i)(2i-1)(i!)^2} \binom{N}{i},$$

$$\sum_{i=0}^{N-10} \frac{(-1)^i (2i)!}{(2i+1)(i!)^2} \binom{N}{i}.$$

All of these sums are hypergeometric and so a parallel application of Sigma or Zeilberger's algorithm etc can simplify these sums.

Computing Recurrences

Handling Right-hand Sides with ϵ

Passing Sigma a sum, defined in terms of recurrences accurate to some order in ϵ, one obtains a recurrence to the requested order in ϵ. Schematically one has,

$$g_d(\epsilon, j, n)a_{j+d} + \ldots + g_0(\epsilon, j, n)a_j = \sum_{k=a}^{b} c_k(j, n)\epsilon^k$$

where in the g_i the ϵ is exact (unexpanded) while on the right one computes a Laurent expansion to the appropriate order in ϵ.

- The right-hand side of the recurrence may contain definite nested multi-sums which should be simplified as already seen. (Unprocessed right-hand sides are extremely slow to work with.)
- Processing the right-hand side can be trivial or tough, as previous examples show.

In practice finding and simplifying a recurrence take similar amounts of time due to optimisation.

Illustrative Result

It is not correct to think of one method as quickest in general.
Take our example sum,

$$S = \sum_{i_1=0}^{n-2} \sum_{i_2=0}^{n-i_1-2} \frac{4 i_1!(-1)^{i_2}(n-i_1-1)(1+i_2)!}{(1+i_1+i_2)^2(2+i_1+i_2)^2(i_1+i_2)!} \binom{n-i_1-2}{i_2}$$

The refined approach is 4 times faster than the current 'state-of-the-art' algorithm and some examples can be as much as 10 times faster.

Uses of ρSum

There have already been numerous uses of Refined HOlonomic SUMmation (ρSum) in particle physics publications. The most important being,

1. PoS RADCOR2013 (2013) 058, PoS LL2012 (2012) 050, PoS LL2012 (2012) 050.
2. Nucl.Phys. B886 (2014) 733-823, Nucl.Phys. B885 (2014) 280-317 and Nucl.Phys. B882 (2014) 263-288.

In particular the Nuclear Physics B papers are a major contribution to the long standing problem in QCD phenomenology of heavy flavour Wilson coefficients.

Summary

- A special function problem was expressed in terms of summation.
- The simple example of a 3-loop bubble diagram was outlined.
- Various approaches and the new refined approach to multi-summation were explained. Both of which can solve expansions of hypergeometric functions.
- An illustration of the potential improvement of the refined algorithm was given. Although one should not think about 'best and worst' but a toolkit of algorithms.