Some problems in loop calculations

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We discuss some of the problems that may occur in the calculation of complicated Feynman diagrams. These include the group independent evaluation of color factors, and the summation techniques that are needed for the expansion of diagrams into their Mellin moments.

1. Introduction

The ever increasing accuracy of the high energy experiments forces theorists to calculate perturbative quantities to higher and higher order. For high order graphs there are however not only the integrals to worry about. One of the problems is the organization of calculations with astronomical numbers of diagrams. This we will not discuss here. Another problem concerns the color factors. Traditionally they have been evaluated for QCD with an algorithm that was specific for the SU(N) groups [1] [2]. These results could then be rewritten in terms of Casimir invariants and applied to other groups as well. This procedure works well as long as the only relevant invariants are $C_F$ and $C_A$. Recent calculations (e.g. ref. [3]) however went beyond this and needed additional invariants. Hence new algorithms were needed. We will discuss them here.

Another problem that arises concerns the hadron structure functions in deep inelastic scattering. Here the structure functions can be computed to two loops but for a complete NNLO analysis one will also need the three loop anomalous dimensions. Of these anomalous dimensions only some Mellin moments are known thus far. This raises several points simultaneously. The first is the computation of the Mellin moments, once the exact result in x-space is known. The second problem is that one would like to use these moments for at least a partial analysis. And thirdly one may wonder whether it could be possible to evaluate all moments simultaneously. Or in other words: can one compute these diagrams in Mellin space? This technique has been used in the past for several calculations [3] [5] [6], but each time the calculations were done mainly by hand, in which case one can use many tricks to come to an answer. Additionally these techniques have never been used to the level of complexity one needs for the anomalous dimensions in NNLO. In the case of large numbers of diagrams one will have to solve the problem rather thoroughly. We will discuss some of this and show some progress in at least the first point.

2. Color factors

The evaluation of color factors is a purely mathematical problem. Yet most of the literature about it has been written by physicists. The most widely used paper is the one by
Cvitanovic \[1\]. In this paper explicit properties of the fundamental and adjoint representations of various groups are used to break the traces down and obtain expressions for the traces in terms of \(N\) (for SU\((N)\), SO\((N)\) and Sp\((N)\)) or just numbers (for \(G_2\), \(F_4\), \(E_6\) and \(E_7\)). The algorithms for the exceptional groups are difficult to implement and for \(E_8\) no algorithms are given. But if one constructs a program for SU\((N)\) it can be rather fast, and for ‘simple’ QCD calculations this is all one needs, because the quarks are in the fundamental representation and the gluons are in the adjoint representation. Such programs can be quite short in any symbolic manipulation language (see for instance ref. \(2\)). For most calculations thus far this is all one needs because for QED and SU\((2)\times U(1)\) the group theory is completely trivial. Nowadays however there is much activity concerning what lies beyond the standard model, and a much larger variety of groups can occur. Hence it would be wise to present perturbative calculations in such a way that the group and the representation(s) have not been fixed yet. Yet one would like to have a compact result. The essence of such an endeavor is of course to utilize no group or representation specific information, and to express the result in terms of as few invariants as possible. These invariants then can be either tabulated for different groups and representations, or there should be easy algorithms to evaluated them. What we are going to show here is a very short version of a recent paper \(4\) on this subject. For more details the reader should consult the original paper.

First we take

\[
[T^a_R, T^b_R] = i f^{abc} T^c_R
\]  

(1)

Of special interest are two quadratic Casimir operators:

\[
(T^a_R T^a_R)_{ij} = C_R \delta_{ij}
\]

(2)

\[
f^{acd} f^{bcd} = C_A \delta^{ab}
\]

(3)

The index \(R\) in \(T_R\) and \(C_R\) labels the representation. The next set of invariants we consider are symmetrized traces.

\[
\text{Str } T^{a_1} \ldots T^{a_n} \equiv \frac{1}{n!} \sum_\pi \text{Tr } T^{a_{\pi(1)}} \ldots T^{a_{\pi(n)}}
\]

(4)

For each representation one may define a symmetric invariant tensor \(d_R\) with

\[
d^{a_1 \ldots a_n}_R \equiv \text{Str } T^{a_1}_R \ldots T^{a_n}_R
\]

(5)

This does overparametrize the problem, but if we manage to express all color factors in terms of contractions of such objects we have made an enormous simplification.

For a reduction into invariants we first deal with all generators that are not in the adjoint representation. If there are still open indices we multiply with appropriate projection operators. This gives complete traces and we have to find an expression for them in terms of symmetrized traces. Of course one can eliminate contracted indices inside the same trace as one does with traces over gamma matrices. Here this is more complicated though. Writing the expression in terms of symmetrized traces can either be done by recursion or with a closed formula which is a bit messy to write here. The formula gives much faster results, but in both cases the expressions become rather long when there are many generators in the trace.
Next one has an expression with invariants $d_R$ and ‘structure constants’ $f$ which can be considered as proportional to generators of the adjoint representation. These do not necessarily occur in loops. If they do, they can be written also in terms of invariants $d_A$. After this step we are left with combinations of invariants and structure constants in which the structure constants cannot be arranged in terms of loops. At this point we start using Jacobi identities. For a computer this is not easy, but the program we constructed can do this for color traces that contain (at the beginning) up to 14 generators without any problem and for 16 it works almost always. This manages to reduce all such traces to contractions between invariants $d$ with the exception of one combination of three tensors $d_R$ and two structure constants $f$ when we started with 14 generators, and three similar objects at the 16 generator level. In some cases these objects can be reduced (like if at least two of the three invariants $d$ belong to the adjoint representation, or for groups for which some identities hold which includes almost, but unfortunately not all groups). The resulting objects are considered as fundamental by the program. It is possible to express them in terms of an even smaller set of independent objects, but unfortunately this will not make the expressions shorter, because the constants in such a reduction are not simple. Hence the program gives its answers in these objects and one can evaluate these contractions afterwards for any given group. The paper presents also the formalism on how to do this for each group and for any given representation. Here we just give some examples of some rather complicated color traces. All examples use an experimental version of the program FORM which will be released later this year.

We first look at the following trace:

\[
R_{nn} = Tr[T^{i_1}_R \cdots T^{i_n}_R T^{i_1}_R \cdots T^{i_n}_R]
\]

which gives some type of maximal complexity. For $n = 7$ we obtain:

\[
R_{77} = 112/3 \ d_R^{abcdef} \ d_A^{abcdef} \ d_A^{abcdef} - 328/9 \ d_R^{abcdef} \ d_A^{abcg} \ d_A^{abcdef}
+ d_R^{abcdef} \ d_A^{abcdef} (-56 \ C_R + 296/3 \ C_A)
+ d_R^{abcdef} \ d_A^{abcdef} (42 \ C_R - 749/10 \ C_A) + 67/15 \ I_2(R) d_A^{abcdef} d_A^{abcdef}
+ d_R^{abcdef} d_A^{abcdef} (35 \ C_R^3 - 357/2 \ C_R^2 C_A + 868/3 \ C_R C_A^2 - 2695/18 \ C_A^3)
+ I_2(R) d_A^{abcdef} d_A^{abcd} (7 \ C_R^2 - 1603/60 \ C_R C_A + 497/20 \ C_A^2)
+ N_A I_2(R) (+C_R^6 - 21/2 \ C_R^5 C_A + 175/4 \ C_R^4 C_A^2 - 280/3 \ C_R^3 C_A^3
+ 52015/48 \ C_R^2 C_A^4 - 19075/288 \ C_R C_A^5 + 43357/2592 \ C_A^6)
\]

(6)

in which $N_A$ is the dimension of the adjoint representation and $I_2(R)$ is the second index of the representation $R$ and it can also be written as $I_2(R) = (N_RC_R)/N_A$ with $N_R$ the dimension of the representation $R$. This computation took less than 35 sec on a PP200 running NeXTstep.

If the representation $R$ in the above example is taken to be the adjoint representation things are much simpler and much quicker:

\[
A_{77} = 8 \ d_A^{abcdef} \ d_A^{abcdef} \ d_A^{abcdef} + 53 \ C_A \ d_A^{abcdef} \ d_A^{abcdef} \ d_A^{abcdef} - 5/648 \ N_A C_A^7
\]

(7)

and the computer time needed is less than 1 sec. Finally a topologically complicated example: It is called the Coxeter graph. It contains 14 vertices and the smallest loop in it has 6 vertices.

\[
G_6(n = 14) = 16 \ d_A^{abcdef} d_A^{abcg} d_A^{abcdef} - 8 \ C_A \ d_A^{abcdef} d_A^{abcdef} d_A^{abcdef} + 1/648 \ N_A C_A^7
\]

(8)
This took 1.6 sec.

3. Sums

The method of evaluating structure functions in Mellin space dates back to the origins of QCD [5]. It has been used [6] to obtain the anomalous dimensions of the deep inelastic structure functions at the two loop level. Kazakov and Kotikov [7] used it for obtaining the ratio $R = \sigma_L/\sigma_T$ of deep inelastic structure functions at the two loop level. A complete program for all two loop calculations has however not been constructed thus far. Hence there is a challenge here. The main prize would of course be a program that can compute the three loop anomalous dimensions. We will address here a project in which first a program is constructed to evaluate all relevant two loop coefficient functions in Mellin space. Then one has to look at the inverse Mellin transform to obtain results in $x$-space. Next would be the study of three loop anomalous dimensions. Thus far we cannot say much of this.

Let us have a look at a typical two loop diagram.

\[
\frac{1}{(p_1^2)^a((P+p_1)^2)^A(p_2^2)^b((P+p_2)^2)^B(p_3^2)^c(p_4^2)^d(p_5^2)^e} \]

We can attack this diagram in a variety of ways. The method one might prefer is the ‘brute force’ method. One decides to compute the $N$-th moment in which we keep $N$ symbolic. Therefore the two denominators are expanded, which results in a single symbolic sum. The resulting integral can be attacked with the standard techniques, but one has to introduce 4 more sums. The only good news is that no individual term has more than 4 nested sums. Amazingly enough these sums can be solved, although one has to do quite some work teaching the computer summation. The summation packages of the big computer algebra programs are almost useless here. One runs however immediately into trouble when trying to solve a similar topology . Thus far the brute force method has failed on this diagram.

Hence one has to be a bit smarter. If one looks in the Kazakov and Kotikov paper one can see a number of reduction schemes by which relations between the various topologies are derived. Two of them can then be marked as the simplest ones. These are then evaluated. They need only a single sum if enough preparatory work is done. Then a next level of topologies can be done which gives sums that involve these simpler topologies. But because the whole scheme is properly built up, the sums do not mix in such a way that we run into very complicated sums. Still one may need a number of sums that are not readily available and hence quite some attention has to go into the construction of a program that can handle all available sums. Because the complete program is still under construction I cannot show too many details here but yet, some may be interesting.

The class of functions that we run into is called ‘harmonic series’. What is shown here about them can be found in a more complete version in ref [8]. There exists a variety of notations for them. Because the more conventional notation is not very useful for computer
programs we use a slight modification of this notation. The basic function is

\[ S_m(n) = \sum_{i=1}^{n} \frac{1}{i^m} \quad m > 0 \]  
\[ = \sum_{i=1}^{n} \frac{(-1)^i}{i^m} \quad m < 0 \]

and higher functions are defined by recursion:

\[ S_{m_1, \ldots, m_k}(n) = \sum_{i=1}^{n} \frac{1}{i^{m_1}} S_{m_2, \ldots, m_k}(i) \quad m_1 > 0 \]
\[ = \sum_{i=1}^{n} \frac{(-1)^i}{i^{m_1}} S_{m_2, \ldots, m_k}(i) \quad m_1 < 0 \]

These functions appear, among others, when Γ-functions are expanded in terms of \( \epsilon \). But they also pop up in sums of the type

\[ \sum_{i=1}^{n} \frac{(-1)^i}{n} \cdot \frac{1}{i} = -S_{1,1,1}(n) \]

which are rather common in these calculations. Certain classes of sums can be evaluated to any complexity of the participating harmonic series. An example is combinations of \( S_{\ldots}(n-i) \), \( S_{\ldots}(i) \) and powers of \( 1/i \) as in

\[ \sum_{i=1}^{n-1} \frac{1}{i^2} S_{2}(n-i)S_{-2,1}(i) = -3S_{2,-4,-1}(n) - 4S_{2,-3,-2}(n) + 4S_{2,-3,-1,1}(n) - 3S_{2,-2,-3}(n) + 2S_{2,-2,-1,2}(n) + 2S_{2,-2,-1,1}(n) + 2S_{2,3,-1,1}(n) + 4S_{3,-3,-1}(n) - 4S_{3,-2,-2}(n) + 4S_{3,-2,-1,1}(n) + 2S_{3,1,-2,-1}(n) - 3S_{4,-2,-1}(n) \]

and so on. There are also complicated sums that have thus far resisted generalization. This means that we cannot put in arbitrary harmonic series. An example is

\[ \sum_{j=0}^{n} \binom{n}{j} \binom{n+j}{2+j} \frac{(-1)^j}{(j+2)^2} S_1(n+j) = \frac{1}{(n+1)(n+2)}(2S_1(n)S_1(n-2) - S_2(n-2) - S_{-2}(n+2) - S_{-2}(n-2) + (-1)^n(n^2+n+3) \binom{n-2}{n+2}) \]

\[ -S_1(n-2)(1 + \frac{1}{n-1} + \frac{1}{n} - \frac{1}{n+1} - \frac{1}{n+2}) \]

The sums become also much more difficult when only a ‘partial range’ is considered as in

\[ \sum_{i=1}^{m} (-1)^i \binom{n}{i} \frac{1}{i^3} = ??? \]
One solution would be the introduction of a new type of functions with two variables. One would then construct the proper relations for these functions and hopefully, at the end of the complete calculation most or all would cancel. This approach may be necessary for the three loop anomalous dimension. At the two loop level it is not needed.

The sums that occur in the evaluation of diagrams in Mellin space are of course closely related to the sums that one runs into when making Mellin transforms of complete results in $x$-space. However, in the case of the transforms there is an extra class of sums: sums to infinity. These are in principle easier, but we need to derive some extra relations for them if we would like to be able to do them to a sufficient depth. Additionally one needs to know the values of the harmonic series at infinity. These values give us a number of constants that do not enter the problem if we calculate the diagrams directly in Mellin space. Hence their cancellation serves as a good check. For instance, the Mellin transform of $c_2$ in ref. [9] results in a formula with 154 terms. Because this is a new result it is shown in the appendix. It does take the program however only a few seconds to evaluate it. There is however an interesting spin-off. From the calculations in Mellin space, we know which classes of functions can occur in the Mellin transform. We can construct a basis in the space of these functions. If we have an equal number of functions in $x$-space of which the Mellin transforms span the space formed by this basis, we can do the inverse Mellin transform by just solving a linear set of equations. Additionally it tells us that there cannot be any relations between the functions in $x$-space that we used. Let us have a look at this basis. First we define the ‘level’ of a term that involves an harmonic series. This level is the sum of the absolute value of its indices and to that we add the number of powers of denominators in the term. Hence the level of the argument of the sum in eq. 15 is $2 + 2 + 3 = 7$. This is also the level of the terms on the right hand side of the equation. For two loop calculations we will need only functions of a level up to four. At level one there are only two functions: $S_1(n)$ and $S_{-1}(n)$. The function $1/n$ can be written as $S_1(n) - S_1(n-1)$. The two terms in this expression correspond to the same function in $x$-space except for an overall factor $1/x$ for the second term. Hence we will not consider $1/n$ as an independent function. Additionally we do not have to worry about products of harmonic series with identical arguments. These can always be expressed in terms of sums of terms that have only single harmonic series as is shown in an example:

$$S_{1,2}(n) S_{-1,1}(n) = -S_{-2,1,2}(n) - S_{-2,2,1}(n) + S_{-2,3}(n) + 2 S_{-1,1,1,2}(n) + S_{-1,1,2,1}(n) - S_{-1,1,3}(n) - S_{-1,2,2}(n) - S_{1,-3,1}(n) + S_{1,-1,1,2}(n) + S_{1,-1,2,1}(n) - S_{1,-1,3}(n) + S_{1,2,-1,1}(n)$$

(18)

At any given level $k$ greater than 1 there are three times as many functions than at the previous level. For each function at level $k - 1$ one can construct a function at level $k$ by adding at the left an index 1, an index -1, or by raising the leftmost index by one (in absolute value). Hence at level 4 there are 54 independent functions. Because we also need the lower functions one has to consider 80 functions in $x$-space before one can make a full inverse Mellin transform. An example is:

$$S_{-1,1,2}(n-1) \rightarrow \frac{\text{Li}_3(1-x)}{1+x} - \frac{\ln(1-x)}{1+x} \zeta_2 - \frac{1}{1+x} \zeta_3$$

$$+ \delta(1-x)\left(-\frac{1}{8} \zeta_4 + \frac{1}{8} \zeta_3 \ln(2) - \frac{1}{24} (\ln(2))^4 - \text{Li}_4\left(\frac{1}{2}\right)\right)$$

(19)
There is one case in which the basis of single higher harmonic series is not practical. This is when one has to evaluate these series at infinity. In that case some of these objects can be infinite and one would like to cancel the infinities between the various terms. In principle one has to evaluate these series at infinity. In that case some of these objects can be infinite and one would like to cancel the infinities between the various terms. This is a rather soft divergence which can be regularized rather easily by replacing the infinity temporarily by a large integer $N$. In some cases one has to worry then about whether objects go to infinity like $\frac{1}{N}$ or like $2N$ in which case one gets additional finite contributions as in $S_1(2N) \to S_1(N) + \ln 2$. These things are rather straightforward though.

### A. Two loop moments

The Mellin transform of the coefficient functions $c_2$ from Zijlstra and van Neerven

$$c_2 = +\theta(N-3) S_{1,-2}(N-3) \left(8/5C_F C_A - 16/5C_F^2\right)$$

$$+\theta(N-3) S_{1,-2}(N-2) \left(-8/5C_F C_A + 16/5C_F^2\right)$$

$$+\theta(N-2) \zeta_3 \left(12/5C_F C_A - 24/5C_F^2\right)$$

$$+\theta(N-2) \left(+S_1(N-2) \left(8/5C_F C_A - 16/5C_F^2\right)ight)$$

$$+S_2(N-2) \left(8/5C_F C_A - 16/5C_F^2\right)$$

$$+S_{-4}(N-1) \left(12C_F C_A - 24C_F^2\right) + S_{-3,1}(N-1) \left(-8C_F C_A + 16C_F^2\right)$$

$$+S_{-2}(N-1) \left(8C_F C_A - 16C_F^2\right) + S_{-2,2}(N-1) \left(-24C_F C_A + 48C_F^2\right)$$

$$+S_1(N-1) \left(1585/54C_F C_A - 89/27C_F n_f + 5/2C_F^2\right)$$

$$+S_{1,-3}(N-1) \left(-24C_F C_A + 48C_F^2\right)$$

$$+S_{1,-2}(N-1) \left(36C_F C_A - 72C_F^2\right) + S_{1,-2,1}(N-1) \left(8C_F C_A - 16C_F^2\right)$$

$$+S_{1,1}(N-1) \left(311/9C_F C_A - 26/9C_F n_f - 43C_F^2\right)$$

$$+S_{1,1,1}(N-1) \left(22/3C_F C_A - 4/3C_F n_f + 8C_F^2\right)$$

$$+S_{1,-2}(N-1) \left(24C_F C_A - 48C_F^2\right) + S_{1,1,1,1}(N-1) \left(24C_F^2\right)$$

$$+S_{1,2}(N-1) \left(-22/3C_F C_A + 4/3C_F n_f - 4C_F^2\right)$$

$$+S_{1,2,1}(N-1) \left(4C_F C_A - 32C_F^2\right) + S_{1,2,1}(N-1) \left(-4C_F C_A - 24C_F^2\right)$$

$$+S_2(N-1) \left(-212/5C_F C_A + 4C_F n_f + 189/5C_F^2\right)$$

$$+S_{1,3}(N-1) \left(12C_F C_A + 4C_F^2\right) + S_{2,-2}(N-1) \left(-8C_F C_A + 16C_F^2\right)$$

$$+S_{2,1}(N-1) \left(-44/3C_F C_A + 8/3C_F n_f + 8C_F^2\right)$$

$$+S_{2,1,1}(N-1) \left(-24C_F^2\right) + S_{2,2}(N-1) \left(20C_F^2\right)$$

$$+S_3(N-1) \left(55/3C_F C_A - 10/3C_F n_f - 18C_F^2\right)$$

$$+S_{3,1}(N-1) \left(8C_F C_A + 8C_F^2\right) + S_4(N-1) \left(-12C_F C_A + 14C_F^2\right)$$

$$+S_1(N) \left(-4639/45C_F C_A + 110/9C_F n_f + 337/5C_F^2\right)$$

$$+S_1(N) \zeta_3 \left(72C_F C_A - 144C_F^2\right) + S_{1,-3}(N) \left(24C_F C_A - 48C_F^2\right)$$

$$+S_{1,-2}(N) \left(-56C_F C_A + 112C_F^2\right) + S_{1,1,-2}(N) \left(-48C_F C_A + 96C_F^2\right)$$
\[ +S_{1,1}(N) \left( -68C_FC_A + 4C_Fn_f + 84C_F^2 \right) + S_{1,1,1}(N) \left( -8C_F^2 \right) \\
+ S_{1,3}(N) \left( -24C_FC_A + 48C_F^2 \right) + S_{2,-2}(N) \left( -16C_FC_A + 32C_F^2 \right) \\
+ S_2(N) \left( 74C_FC_A - 4C_Fn_f - 74C_F^2 \right) + S_{2,1}(N) \left( 16C_F^2 \right) \\
+ S_3(N) \left( -20C_FC_A + 28C_F^2 \right) + S_{3,1}(N) \left( -8C_FC_A + 16C_F^2 \right) \\
+ S_4(N) \left( 12C_FC_A - 24C_F^2 \right) \\
+ S_1(N+1) \left( 3914/27C_FC_A - 488/27C_Fn_f - 121C_F^2 \right) \\
+ S_3(N+1) \left( -84C_FC_A + 144C_F^2 \right) \\
+ S_{1,-3}(N+1) \left( -40C_FC_A + 80C_F^2 \right) \\
+ S_{1,-2}(N+1) \left( 20C_FC_A - 40C_F^2 \right) + S_{1,-1}(N+1) \left( 8C_FC_A - 16C_F^2 \right) \\
+ S_{1,1}(N+1) \left( 668/9C_FC_A - 68/9C_Fn_f - 68C_F^2 \right) \\
+ S_{1,1,1}(N+1) \left( 22/3C_FC_A - 4/3C_Fn_f + 36C_F^2 \right) \\
+ S_{1,1,2}(N+1) \left( 56C_FC_A - 112C_F^2 \right) + S_{1,1,1,1}(N+1) \left( 24C_F^2 \right) \\
+ S_{1,2}(N+1) \left( -22/3C_FC_A + 4/3C_Fn_f - 32C_F^2 \right) \\
+ S_{1,1,2}(N+1) \left( 4C_FC_A - 32C_F^2 \right) + S_{1,2,1}(N+1) \left( -4C_FC_A - 24C_F^2 \right) \\
+ S_{1,3}(N+1) \left( 28C_FC_A - 28C_F^2 \right) \\
+ S_2(N+1) \left( -1909/15C_FC_A + 38/3C_Fn_f + 646/5C_F^2 \right) \\
+ S_{2,1}(N+1) \left( -44/3C_FC_A + 8/3C_Fn_f - 48C_F^2 \right) \\
+ S_{2,1,1}(N+1) \left( -32C_F^2 \right) + S_{2,2}(N+1) \left( 28C_F^2 \right) \\
+ S_3(N+1) \left( 115/3C_FC_A - 10/3C_Fn_f - 4C_F^2 \right) \\
+ S_{3,1}(N+1) \left( 8C_FC_A + 24C_F^2 \right) + S_4(N+1) \left( -12C_FC_A - 6C_F^2 \right) \\
+ \left( -S_1(N+3) + S_{1,-2}(N+3) \right) \left( 72/5C_FC_A - 144/5C_F^2 \right) \\
+ \left( S_2(N+2) + S_3(N+2) \right) \left( 72/5C_FC_A - 144/5C_F^2 \right) \\
+ S_{1,-2}(N+3) \left( -72/5C_FC_A + 144/5C_F^2 \right) \\
+ S_{3,1}(N+3) \left( -72/5C_FC_A + 144/5C_F^2 \right) \\
- 5465/72C_FC_A + 457/36C_Fn_f + 331/8C_F^2 \\
+ \zeta_3 \left( 54C_FC_A - 72C_F^2 \right) \]

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