Regularization of IR divergent loop integrals

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Abstract. We report results of a new numerical regularization technique for infrared (IR) divergent loop integrals using dimensional regularization, where a positive regularization parameter $\varepsilon$, satisfying that the dimension $d = 4 + 2 \varepsilon$, is introduced in the integrand to keep the integral from diverging as long as $\varepsilon > 0$. A sequence of integrals is computed for decreasing values of $\varepsilon$, in order to carry out a linear extrapolation as $\varepsilon \rightarrow 0$. Each integral in the sequence is calculated according to the Direct Computation Method (DCM) to handle (threshold) integrand singularities in the interior of the domain. The technique of this paper is applied to one-loop $N$-point functions. In order to simplify the computation of the integrals for small $\varepsilon$, particularly in the case of a threshold singularity, a reduction of the $N$-point function is performed numerically to a set of 3-point and 4-point integrals, and DCM is applied to the resulting vertex and box integrals.

1. Introduction

The integral for an $n$-dimensional $N$-point Feynman diagram with $L$ loops can be represented as

$$ I = (-1)^N \Gamma(N - Ln/2) \int_0^\infty d^N x \frac{\delta(1 - \sum_{j=1}^N x_j)}{x \cdot S^{(N)}(x/2)} \frac{U^{N-(L+1)n/2}}{\mathcal{F}^{N-Ln/2}}. \quad (1) $$

Here the functions $\mathcal{F}$ and $\mathcal{U}$ are polynomials determined by the topology of the corresponding Feynman diagram [1]. A mechanism for the evaluation of infrared (IR) divergent multi-loop integrals of the form (1) by sector decomposition and dimensional regularization is given in [2].

We consider the one-loop $N$-point function, denoted in [3] by

$$ I = I_N^n = (-1)^N \Gamma(N - n/2) \int_0^\infty d^N x \frac{\delta(1 - \sum_{j=1}^N x_j)}{x \cdot S^{(N)}(x/2)} \frac{U^{N-(L+1)n/2}}{\mathcal{F}^{N-Ln/2}}. \quad (2) $$

with

$$ S_{k\ell}^{(N)} = -(r_\ell - r_k)^2 + m_\ell^2 + m_k^2, \quad 1 \leq k, \ell \leq N \quad (3) $$

where $r_\ell = \sum_{j=1}^\ell p_j$; the $p_j$ and $m_j$ are the external loop momenta and the corresponding particle masses, respectively. In order to account for IR divergence, the formalism of dimensional regularization can be applied by setting the dimension $n = 4 + 2 \varepsilon$. The integral in equation (2) then generally diverges as $\varepsilon \rightarrow 0$ ($n \rightarrow 4$). It is expanded with respect to $\varepsilon$, via sector decompositions of the integration domain and expansion of the integrand around $\varepsilon = 0$ in the resulting sector functions.

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The expansion coefficients are calculated in [4] using FORM [5], as sums of multivariate integrals assembled from contributions over the sectors. The coefficients are derived in [6] by expanding the expressions for the integrals directly, based on properties of hypergeometric and related functions. We make use of the asymptotic behavior to compute the coefficients numerically by a linear extrapolation.

We construct a linear system of equations, which incorporates values of the integral for decreasing \( \varepsilon \) in the right hand side of the system. The system is extended by one equation at a time and solved for the leading coefficients of the Laurent expansion of the integral. This gives rise to an extrapolation as \( \varepsilon \) tends to zero. The solutions can be obtained by solving the systems directly or by a recursive method [7].

We will make use of Bulirsch [8] type sequences of the form \( b_\ell = 2, 3, 4, 6, 8, 12, 16, 24, \ldots \), in order to set \( \varepsilon = \varepsilon_\ell = 1/b_\ell \).

In previous work [9, 10] we applied the dimensional extrapolation to infrared cases where the integrand denominator does not vanish in the interior of the integration domain. In [11] we dealt with vanishing denominators for vertex (triangle) integrals. At present we target one-loop \( N \)-point functions after their reduction to vertex and box integrals according to [3, 12], and sector decompositions to disentangle overlapping singularities along multiple coordinate axes. These will allow for an efficient numerical computation of integrals which suffer from both threshold singularities inside the domain, and IR divergence causing singular behavior at the boundaries of the integration region.

All computations are numerical and performed with automatic integration code after reduction and sector decompositions, as implemented using QUADPACK in [13] for non-IR divergent \( N \)-point functions through the polygon. The basic vertex and box functions are computed with techniques of the Direct computation method (DCM) [10, 14, 15]:

- **iterated multivariate integration**, which uses one-dimensional or low-dimensional integration techniques repeatedly [14, 16, 17];
- **nonlinear extrapolation** by the \( \epsilon \)-algorithm [18, 19], to handle singularities inside the domain.

DCM relies on the one-dimensional QUADPACK [20] numerical methods DQAG and DQAGS, which are deterministic and adaptive. DQAGS also uses a nonlinear extrapolation internally, for treating algebraic and algebraic-logarithmic integrand singularities. DCM introduces a term \( i \delta \) with finite \( \delta > 0 \) in the integrand denominator, and extrapolates a sequence of integral values for decreasing values of \( \delta \).

It is our goal in this paper to extend DCM to IR divergent integrals which may have threshold singularities, in particular for the basic triangle and box elements in the decomposition, by resorting to a double extrapolation or regularization (with respect to \( \delta \) and \( \varepsilon \)) if needed.

In section 2 we review the reduction and sector decomposition formalism of one-loop \( N \)-point functions into triangles and boxes. Section 3 explains the dimensional extrapolation by solving a linear system, or by using a recursive method developed for Vandermonde type systems in [7]. The use of the linear extrapolation is validated by the underlying asymptotic expansions for the vertex and box subproblems, which leads to the double extrapolation for IR divergent problems where the denominator also vanishes in the interior of the integration domain. Numerical results of the procedures are given for sample problems in section 4.

### 2. Reduction overview

Through the reduction formalism applied in [3], the \( n \)-dimensional hexagon, pentagon and box functions are expressed in terms of \( n \)-dimensional triangle and \( (n+2) \)-dimensional box functions.

Assuming \( \text{det}(S) \neq 0 \),

\[
I_N^n = \sum_{k=1}^{N} B_k I_{N-1,k} + (N - n - 1) \frac{\text{det}(G)}{\text{det}(S)} I_N^{n+2}, \tag{4}
\]

where \( S \) is defined by equation (3), \( G \) is the Gram matrix, \( G_{k\ell} = 2 r_k r_\ell \), \( k, \ell = 1, \ldots , N \); and the reduction coefficients \( B_k = -\sum_{i=1}^{N} S_{ki}^{-1} \) can be obtained by solving the system of linear equations...
\[ \sum_{l=1}^{N} S_{kl}B_l = -1, \quad k = 1, \ldots, N. \] Infrared singularities emerge through poles in the integral expansions as a function of \( \varepsilon \) where \( n = 4 + 2\varepsilon \). Thus the \( n \)-dimensional \( N \)-point function is decomposed as a linear combination of \( n \)-dimensional \((N - 1)\)-point functions, and a remainder term which involves a \((n + 2)\)-dimensional \( N \)-point function. It is noted in [3] that the latter is IR finite, even in the massless case. In particular, denoting the Mandelstam variables \( s_j = p_j^2 \) and \( s_{ij} = (p_i + p_j + \ldots)^2 \), the IR behavior in

\[
I_4^n(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2) =
\begin{align*}
&+ B_1 I_3^n(s_{12}, s_4, m_3, m_4, m_1) \\
&+ B_3 I_3^n(s_{12}, s_3, m_4, m_1, m_2) \\
&+ (n - 3)(B_1 + B_2 + B_3 + B_4) I_4^{n+2}(s_{12}, s_{23}, s_1, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2)
\end{align*}
\]

is confined to the triangle integrals.

The integrals \( I_3^n \) and \( I_4^{n+2} \) are split into sector functions of the form

\[
I_3^n(s_{1,2,3}, s_{12}, s_3, m_1^2, m_2^2, m_3^2) = -\Gamma(3 - n/2) \sum_{\mathcal{P}_{(1,2,3)}} S^n_{\mathcal{P}}(s_{1,2,3}, s_{12}, s_3, m_1^2, m_2^2, m_3^2)
\]

where \( \mathcal{P}_{(1,2,3)} \) is the set of the cyclic permutations of \((1, 2, 3)\), and

\[
I_4^{n+2}(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2) = -\Gamma(4 - n/2) \times
\]

\[
(S_{\text{Box}}^n(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2) + S_{\text{Box}}^{n+2}(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2) + S_{\text{Box}}^{n+2}(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2))
\]

The basic triangle and box functions satisfy the integral representations

\[
S^n_{\mathcal{P}}(s_{1,2,3}, s_{12}, s_3, m_1^2, m_2^2, m_3^2) = \int_0^1 dt_1 dt_2 \frac{(1 + t_1 + t_2)^{3-n}}{(D_{\mathcal{P}})^{3-n/2}}
\]

\[
S^{n+2}_{\text{Box}}(s_{12}, s_{23}, s_{1}, s_2, s_3, s_4, m_1^2, m_2^2, m_3^2, m_4^2) = \int_0^1 dt_1 dt_2 dt_3 \frac{(1 + t_1 + t_2 + t_3)^{2-n}}{(D_{\text{Box}})^{3-n/2}}
\]

where the functions \( D_{\mathcal{P}} \) and \( D_{\text{Box}} \) are quadratics,

\[
D_{\mathcal{P}} = \frac{\sum \mathcal{P}(s_{1,2,3}, s_{12}, s_3, m_1^2, m_2^2, m_3^2, m_4^2) \sim 0,}
\]

The functions (8) and (9) will be computed with the integration technique of DCM, and a nonlinear extrapolation will be performed when denominators vanish within the integration region. This calculation will be carried out for each value of \( \varepsilon \) needed in the dimensional extrapolation as \( \varepsilon \to 0 \).

3. Linear extrapolation

Consider a function \( S(\varepsilon) \) which satisfies an asymptotic expansion

\[
S(\varepsilon) \sim S + a_1 \varphi_1(\varepsilon) + a_2 \varphi_2(\varepsilon) + \ldots, \quad \varepsilon \to 0,
\]

where the functions \( \varphi_j(\varepsilon) \) are known and in decreasing order, in the sense that \( \lim_{\varepsilon \to 0} \frac{\varphi_{j+1}(\varepsilon)}{\varphi_j(\varepsilon)} = 0 \).
Then for a linear extrapolation we construct a sequence $S(\varepsilon_\ell), \ell = 0, 1, \cdots$, and solve linear systems of the form

$$a_0 + \varphi_1(\varepsilon_\ell) a_1 + \cdots \varphi_\nu(\varepsilon_\ell) a_\nu = S(\varepsilon_\ell), \quad \ell = 0, \ldots, \nu,$$

in the unknowns $a_j, j = 0, \cdots, \nu$, of order $(\nu + 1) \times (\nu + 1)$, for increasing values of $\nu$ and for decreasing $\varepsilon_\ell$.

This process can be related to the Neville algorithm as follows (see, e.g., [7]). The interpolating polynomial $P_{k,d}(x)$ of degree $d$ for a function $f(x)$ is defined as the polynomial of degree $d$ which interpolates at the points $x_\ell$, so that

$$P_{k,d}(x_\ell) = f(x_\ell), \quad \text{for } \ell = k - d, k - d + 1, \ldots, k.$$  \hfill (12)

Denoting the polynomial coefficients by $c_{k,d}^{(j)}$, the value of the polynomial at a particular point $x$,

$$P_{k,d}(x) = \sum_{j=0}^{d} c_{k,d}^{(j)} x^j,$$  \hfill (13)

can be calculated recursively with the Neville algorithm, using

$$P_{k,0}(x) = f(x_k),$$

$$P_{k,d}(x) = \frac{(x_k - x)P_{k-1,d-1}(x) - (x_k - d)P_{k,d-1}(x)}{x_k - x_k - d}, \quad d = 1, \ldots, k.$$  \hfill (14)

Furthermore, by substituting the formula $P_{k,d}^{(j)}(0) = c_{k,d}^{(j)} j!$ into equation (14), formulas are obtained for the coefficients,

$$c_{k,0}^{(j)} = f(x_k),$$
$$c_{k,d}^{(j)} = \frac{x_k c_{k-1,d-1}^{(j)} - x_k - d c_{k,d-1}^{(j)} + c_{k-1,d-1}^{(j)} - c_{k-1,d-1}^{(j-1)}}{x_k - x_k - d}, \quad d = 1, \cdots, k \quad \text{and} \quad j = 1, \ldots, d - 1.$$  \hfill (15)

This gives rise to an extrapolation table, where the values for $j = 0$ and $j = d$ can be included by setting $c_{k,d}^{(-1)} = c_{k,d}^{(d+1)} = 0$. The table allows calculating the coefficients of the interpolating polynomial $P_{k,k}(x)$ of degree $k$, coinciding with $f(x)$ at the points $x = x_0, \cdots, x_k$. Note that $f$, $x$ and $k$ can play the role of $S$, $\varepsilon$ and $\nu$ in equation (11) above, for $\varphi_j(\varepsilon) = \varepsilon^j$. In this case, the system of equation (12) combined with equation (13), or equation (11) is a Vandermonde type system, and (15) yields an algorithm for its solution.

4. Asymptotics

This section establishes the underlying asymptotic expansions which validate the linear (dimensional) extrapolation for various classes of vertex and box diagrams, and gives results for sample problems.

4.1. Vertex diagrams

Kurihara [6] derives expansions with respect to $\varepsilon$ for the tensor integral of the massless one-loop 3-point integral of rank $M \leq 3$,

$$T_{\mu_1 \cdots \mu_k}^{(3)} = \sum_k C_{k}^{k} f_3(p_1, p_2, p_3, n_x) p_1^{(k)} p_2^{(k)} p_3^{(k)} n_x^{(k)}.$$  


with
\[
J_3^b(p_1^2, p_2^2, p_3^2; n_x^{(k)}, n_y^{(k)}) = \frac{1}{(4\pi)^2 (4\pi \mu_R^2)^{\varepsilon}} \int_0^1 dx \int_0^{1-x} dy \frac{x_n^{(k)} y_n^{(k)}}{D^{1-\varepsilon}},
\]
(16)
\[
D = (p_1 x - p_2 y)^2 - p x y - p_1^2 x - p_2^2 y - i 0,
\]
\[
\rho = p_3 - (p_1 + p_2)^2.
\]
In the case \(p_1^2 = p_2^2 = 0\) and \(p_3^2 \neq 0\) with \(n_x = n_y = 0\), (16) gives
\[
J_3(0, 0, p_3^2; 0, 0; \varepsilon) = \frac{1}{(4\pi)^2 (4\pi \mu_R^2)^{\varepsilon}} \int_0^1 dx \int_0^{1-x} dy \frac{1}{(-p_3^2 x y - i 0)^{1-\varepsilon}}.
\]
(17)
where \(\mu_R\) is the renormalization energy scale. As \(\varepsilon \to 0\), \(J_3\) of equation (17) satisfies an expansion of the form
\[
J_3(0, 0, p_3^2; 0, 0; \varepsilon) \sim \frac{C_{\varepsilon = 2}}{\varepsilon^2} + \frac{C_{\varepsilon = 1}}{\varepsilon} + C_0 + \mathcal{O}(\varepsilon).
\]
(18)
The linear extrapolation method of section 3 can be applied to the system of equation (11) with \(S(\varepsilon) = \varepsilon^2 J_3(0, 0, p_3^2; 0, 0; \varepsilon)\). We gave numerical results for the coefficients \(C_{\varepsilon = 2}, C_{\varepsilon = 1}\) and \(C_0\) of equation (18) in [10].

If, in (16) with \(p_1^2 = p_2^2 = 0\), \(p_3^2 \neq 0\), one of \(n_x\) and \(n_y\) is zero and the other is not, e.g., \(n_x = \eta > 0\) and \(n_y = 0\), then the asymptotic behavior is given by
\[
J_3(0, 0, p_3^2; \eta, 0; \varepsilon) \sim \frac{1}{(4\pi)^2 p_3^2} \left( \frac{C_{\varepsilon = 1}}{\varepsilon} + C_0 + \mathcal{O}(\varepsilon) \right),
\]
(19)
with coefficients
\[
C_{\varepsilon = 1} = \frac{1}{\eta}, \quad C_0 = -\frac{2}{\eta^2} + \frac{1}{\eta} \left( \log(-p_3^2) - \sum_{j=1}^{\eta-1} \frac{1}{j} \right).
\]
Values for the coefficients obtained in double precision for (generating and solving) the system of equation (11) with \(S(\varepsilon) = \varepsilon^2 J_3(0, 0, p_3^2; \eta, 0; \varepsilon)\) were reported in [10] for \(n_x = \eta = 2\), \(n_y = 0\) and \(p_3^2 = 100\), a tolerated relative error of \(10^{-13}\) for (repeated) integration with the QUADPACK program DQAGS, using a sequence of \(\varepsilon = \varepsilon_\ell = \frac{1}{2^\ell}\) where \(\{b_\ell\}\) is a Bulirsch type sequence. The reported integration times ranged between 0.03s and 0.09s, for \(b_\ell = 12, 16, 24, \ldots, 384\). The contribution of the times for the actual extrapolation procedure were found to be negligible. Table 1 lists results for the coefficients of equation (19) obtained in a quadruple precision run for this problem.

For \(p_1^2 = 0\), \(p_2^2 \neq 0\) and \(p_3^2 \neq 0\) in equation (16), IR divergence occurs when \(n_x = n_y = 0\) or \(n_x \neq 0, n_y = 0\), leading to
\[
J_3(p_1^2, p_2^2, p_3^2; \eta, 0; \varepsilon) \sim \frac{1}{(4\pi)^2 p_3^2} \left( \frac{C_{\varepsilon = 1}}{\varepsilon} + C_0 + \mathcal{O}(\varepsilon) \right).
\]
(20)
with coefficients given in [6]. Apart from the IR divergence as indicated by the \(\varepsilon\)-dependence in (20), a singularity may appear inside the integration region through a zero denominator function \(D\) in (16). For each value of \(\varepsilon\) in the sequence, the interior singularity can be handled in DCM, by replacing \(i 0\) in \(D\) by \(i \delta\) and performing a nonlinear extrapolation as \(\delta \to 0\). Results of the double extrapolation procedure are given in [11] for a diagram with \(n_x = n_y = 0\) and \(p_2^2 = 40, p_3^2 = -100\).
relative integration error tolerance and is expressed in [6] using dimensional regularization as

\[ J_{\mu...\nu} = \sum_k C_{\mu...\nu}^{(k)} J_{4}^{(k)}(p_1^2, p_2^2, p_3^2; n_x, n_y, n_z) \]

and is expressed in [6] using dimensional regularisation as

\[ J_{4}^{(k)}(s, t, p_1^2, p_2^2, p_3^2; n_x^{(k)}, n_y^{(k)}, n_z^{(k)}) = \Gamma(2-\varepsilon) \] 

\[ \frac{1}{(4\pi)^2 (4\pi\mu_R^2)^\varepsilon} \int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} dz \frac{z^{n_x^{(k)}-1} y^{n_y^{(k)}-1} z^{n_z^{(k)}+1}}{D^{2-\varepsilon}} \] (21)

where

\[ D = -s x z - t y (1 - x - y - z) - p_1^2 x y - p_2^2 y z - p_3^2 z (1 - x - y - z) - p_1^2 x (1 - y - z) - i0. \]

We consider the case where \( p_1^2 = p_2^2 = p_3^2 = 0 \) (all particles on-shell) and \( n_x = n_y = n_z = 0 \). The integral of the form \( J_{4}^{(k)} \) in equation (2), is IR divergent, and its asymptotic behavior is captured in

\[ \left(4\pi\right)^2 (4\pi\mu_R^2)^\varepsilon \frac{\Gamma(2-\varepsilon)}{\Gamma(2-\varepsilon)} J_{4}(s, t; 0, 0, 0, 0; 0, 0; \varepsilon) \]

\[ = \int_0^1 dx \int_0^{1-x} dy \int_0^{1-x-y} dz \frac{1}{(-s x z - t y (1 - x - y - z) - i0)^{2-\varepsilon}}, \] (22)

\[ \sim \frac{c_{-2}}{\varepsilon^2} + \frac{c_{-1}}{\varepsilon} + c_0 + O(\varepsilon) \] (23)

For \( s = t = -1 \), the integrand denominator of of equation (22) does not vanish in the interior of the integration region, so that only the dimensional regularization is performed (\( \delta = 0 \)). Note that, for example, only one of the Mandelstam variables occurring in the parameter list of the triangle functions \( J_{3}^{(k)} \) of equation (5) is -1 and the other two are 0. The same holds for the Mandelstam parameters of the triangle denominator \( S_{3n}^{(k)} \) in equation (8).

Table 2 gives coefficient values resulting from the numerical reduction according to (4), applied for \( N = 4 \). The linear (Bulirsch type) extrapolation sequence is started at \( \varepsilon = 1/8 \). Thus the first \( (3 \times 3) \) system is solved at \( \varepsilon = 1/16 \). The requested accuracy was set to about 10 digits for the triple integration of the \( (n+2) \)-dimensional box function in equation (5), whereas the triangle integrations were performed to a tolerated error of about 12 digits. Note that the \( (n+2) \)-dimensional box function is IR finite; thus
it is integrated with $\varepsilon = 0$. The time incurred in the triple integrations dominates the total computation time. The computation to produce table 2 takes about 13s (user execution time) on a MacBook Pro laptop (Intel Core Duo processor, 3.06 GHz).

The integrand denominator of the box function in equation (22) vanishes in the interior of the integration region for $s = 123, t = -200$; thus a double extrapolation is required. However, in this case, the triangle function denominator in equation (8) does not vanish in the interior of the integration domain. Results for the real parts of the coefficients in (23) are given in table 3. The computation for table 3 takes about 406s.

5. Concluding remarks
In this contribution we reported on a new numerical regularization technique for infrared (IR) divergent loop integrals using dimensional regularization. This method relies on a numerical extrapolation to derive the behavior of the integral around four-dimensions.

In order to achieve this, a double extrapolation is required, to deal with singular integrand behavior inside the integration domain as well as IR divergence. We resort to a reduction and sector decompositions, applied numerically, where the Direct Computation Method (DCM) is applied on the basic box and triangle levels. Since the method is fully numerical, it is viable without change for various problem types.

Many integrals result, rendering the procedure a good candidate for parallel/distributed implementations. For difficult box calculations we are developing a multi-core parallelization on the (outer) function evaluation levels in the iterated integration procedure.

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