

NEATIBP 1.0, A package generating small-size integration-by-parts relations for Feynman integrals

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Abstract

In this work, we present the package NEATIBP, which automatically generates small-size integration-by-parts (IBP) identities for Feynman integrals. Based on the syzygy and module intersection techniques, the generated IBP identities' propagator degree is controlled and thus the size of the system of IBP identities is shorter than that generated by the standard Laporta algorithm. This package is powered by the computer algebra systems MATHEMATICA and SINGULAR, and the library SPASM. It is parallelized on the level of Feynman integral sectors. The generated small-size IBP identities can subsequently be used for either finite field reduction or analytic reduction. We demonstrate the capabilities of this package on several multi-loop IBP examples.

Keywords: Feynman Integrals, IBP identities, syzygies, module intersection method

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PROGRAM SUMMARY

Manuscript Title: NEATIBP 1.0, A package for generating small-size integration-by-parts relations for Feynman integrals

Authors: Zihao Wu, Janko Boehm, Rourou Ma, Hefeng Xu, Yang Zhang

Program Title: NeatIBP

CPC Library link to program files: (to be added by Technical Editor)

Developer's repository link: <https://github.com/yzhphy/NeatIBP>

Code Ocean capsule: (to be added by Technical Editor)

Licensing provisions(please choose one): GPLv3

Programming language: MATHEMATICA, SINGULAR, C

Computer(s) for which the program has been designed: computers with multiple CPU cores

Operating system(s) for which the program has been designed: Linux

Supplementary material: none

Nature of problem: The difficulty of the IBP reduction of Feynman integrals stems from the large size of the IBP system.

Solution method: We apply the module intersection method to generate IBP relations by algebraic geometry methods, and compare the smaller IBP system we generate with that from Laporta's algorithm. NEATIBP generates the module intersection in SINGULAR [1] and selects relevant and independent IBP relations via an algorithm relying on the library SPASM [2]. The workflow is parallelized by a task manager written in MATHEMATICA [3].

References

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1. Introduction

Feynman integrals are the core objects in perturbative quantum field theory. They are crucial in the theoretical computations, especially which is related to the observations of high energy experiments, such as, in Large

Hadron Collider (LHC) [1, 2, 3, 4]. As the increasing of precision in high-energy experiments, the demand for multi-loop Feynman integral computations going to rise continuously. Typically, for a given scattering process, the computation of scattering amplitude involves numerous Feynman integrals' contribution. One thus performs reductions [5, 6, 7, 8, 9] on the integrals towards smaller sets of integrals which then have to be computed.

Integration-by-Parts (IBP) reduction [6, 7] is a key Feynman integral reduction technique. Laporta's algorithm [10] is the most prevalent IBP reduction algorithm, relying on reducing a linear system of IBP relations. A multitude of other approaches exist for executing IBP reduction, including the use of operators and non-commutative algebra [11, 12, 13, 14, 15, 16, 17, 18], intersection numbers [19, 20, 21, 22], auxiliary mass flow methods [23, 24, 25, 26, 27, 28, 29, 30, 31], finite field methods [32, 33, 34, 35, 36], methods of direct solutions [37], and more. Building on these techniques, there are several packages for IBP reductions available, including AIR [38], FiniteFlow[36], FIRE [39, 40, 41, 42], KIRA [43, 44, 45], LITERED [46], and REDUZE [47, 48].

One of the key factors determining the computational complexity of IBP reduction is the number of initial IBP relations. The syzygy method for IBP reduction [49] is a powerful method to decrease this number of IBP relations. So-called syzygy equations impose constraints on the Feynman integral indices, and thus significantly decrease the number of IBP relations to consider in subsequent computations. Several novel methods have been developed for generating or reformulating syzygy equations, including linear algebra techniques [50, 51], independent syzygy generator selection [52] and module intersection [53, 54, 55]. Moreover, syzygy method can also be used for generating IBP relations of specific type Feynman integrals, such as Feynman integrals with only overall UV divergence [56]. Although there have been numerous advancements in syzygy methods for IBP reduction, it appears that *an automated program employing syzygy method-based IBP techniques is noticeably lacking in the market.*

In this paper, we introduce our package NEATIBP (ver. 1.0). The tool automatically generate small-size IBP systems, relying on syzygy techniques and, in particular, the module intersection method [53, 54].

In our package, we employ the Baikov representation of Feynman integrals [57, 58, 59]. The index restriction condition of Feynman integrals in IBP relations, translates into a module intersection computation over the polynomial ring in the variables of the Baikov representation [53, 54]. The

module intersection in the current version of NEATIBP is determined using the computer algebra system SINGULAR [60]. Then formal IBP relations¹, with restriction of indices, are generated. Based on the formal relations, we introduce sophisticated seeding² and selection algorithms to generate a small size IBP system. During the seeding steps, careful control is exercised over the numerator degree of the generated IBP relations. Using row reduction methods over finite fields³, a small set of sufficient IBP relations is selected. Along our way, the master integrals are determined. The selection step is powered by the finite field linear system reduction package SPASM [61].

The output of NeatIBP is a list of IBP relations, which are sufficient to reduce input integrals to master integrals. This list, which is typically much shorter than the one needed in Laporta’s approach, serves two purposes:

1. Integral reduction over finite fields, with a subsequent reconstruction multi-loop amplitudes.
2. Analytic integral reduction, if required.

The user can use their own programs to finish the above two approach in the current stage. In the future, we will develop corresponding interfaces, feeding NEATIBP results into some mainstream IBP reduction or Gaussian elimination software automatically.

NEATIBP 1.0 is employing parallelization. In the initial step, the zero sectors and symmetric sectors are determined using standard methods [46]. The symmetry maps between sectors are found in a parallelized manner. Subsequently, the module intersection, IBP relation seeding, and selection computations are parallelized across distinct Feynman integral sectors. The status of the computation is visible in our monitor program. Important intermediate results are stored in real-time. Due to this approach, the execution of the program can be interrupted and resumed.

This paper is organized as follows. In Section 2, we provide an overview of the mathematical physics methods used in our program, and briefly outline

¹In this paper, *formal* (IBP) relations refer to IBP relations of integrals with symbolic indices.

²*Seeding* is the procedure of setting symbolic indices in formal IBP relations as specific numbers.

³One should keep in mind that row reduction over finite fields always has risks. An ill-chosen numeric point or prime number could lead to a wrong answer. We will discuss this in Section 3.2.

their implementations in NEATIBP. In Section 3, we present the underlying algorithm of NEATIBP, as well as its parallelization scheme. In Section 4 provides a short guide on how to use NEATIBP, with more details available online. In Section 5, we showcase examples for the usage NEATIBP and give timings. Section 6 summarizes the paper.

We remark that due to graduation requirements of the University of Science and Technology of China necessitating first-author papers, and Wu's significant contribution to this work, the author names ordering of this paper is chosen in the stated way.

2. Review of methods and their implementations

2.1. IBP reduction

IBP reduction refers to reducing given scalar integrals in a Feynman integral family to a finite number of linearly independent integrals. A Feynman integral family, for a given Feynman diagram, is a set of Feynman integrals of the form

$$G_{\alpha_1, \dots, \alpha_n} = \int \prod_{j=1}^L \frac{d^D l_j}{i\pi^{D/2}} \frac{1}{D_1^{\alpha_1} \dots D_n^{\alpha_n}}, \quad (1)$$

where the D_i are the propagators associated to the Feynman diagram, α_i 's are the power indices, usually taking integer values. The IBP relations originate from the vanishing boundary term in dimensional regularization, such that

$$0 = \int \prod_{j=1}^L \frac{d^D l_j}{i\pi^{D/2}} \frac{\partial}{\partial l_k^\mu} \frac{v^\mu}{D_1^{\alpha_1} \dots D_n^{\alpha_n}}, \quad (2)$$

where v^μ is a vector formed by loop or external momenta. The right hand side of (2) can be expanded as a linear combination of multiple Feynman integrals in this family. Thus, (2) generates infinite number of linear constrains on the Feynman integrals in the family. Constrained by the relations, only finite [62] number of Feynman integrals in the family are independent. They can be chosen to form a linear basis. Any integral I in the family can be represented as

$$I = \sum_i c_i I_i, \quad (3)$$

where I_i 's are called *master integrals*, c_i 's are the reduction coefficients. In order to reduce some target integrals toward a chosen master integral basis,

we usually follow the following steps. Firstly, we generate enough IBP relations from (2). We then need to solve the linear equation system, with the target integrals treated as the unknown and master integrals as the known. Finally we will get the reduction result (3).

Usually, (2) generates IBP relations with the indices α_i 's (for denominators) increased, for a generally chosen v^μ . This phenomenon will significantly increase the size of the IBP system, since the integrals with increased indices are often irrelevant to the reduction target. Fortunately, new methods can avoid this the appearance of such unneeded integrals, by solving syzygy equations [49, 52, 63, 64, 50, 53, 54, 55]. In NEATIBP, we use IBP relations from Baikov representation, with the help of syzygy equations and the module intersection method[53, 55]. We will introduce them in the subsequent sections.

2.2. IBP relations from the Baikov representation

The Baikov representation of Feynman integrals is

$$G_{\alpha_1, \dots, \alpha_n} = C \int dz_1 \cdots dz_n P^\gamma \frac{1}{z_1^{\alpha_1} \cdots z_n^{\alpha_n}}, \quad (4)$$

where C is a constant irrelevant to the IBP relations, $\gamma = \frac{D-L-E-1}{2}$, with L and E the number of independent loop and external momenta respectively, and

$$P = P(z_1, \dots, z_n) = \det G(l_1, \dots, l_L, p_1, \dots, p_E), \quad (5)$$

standing for the Gram determinant of loop and external momenta.

In the Baikov representation, IBP relations are generated from the total derivative expression as

$$0 = C \int dz_1 \cdots dz_n \sum_{i=1}^n \frac{\partial}{\partial z_i} \left(a_i(z) P^\gamma \frac{1}{z_1^{\alpha_1} \cdots z_n^{\alpha_n}} \right), \quad (6)$$

where $a_i(z)$'s are some chosen polynomials of z_j 's. If one can find such a_i 's that there exist corresponding polynomials $b(z)$ and $b_i(z)$'s satisfying

$$b(z)P + \sum_{i=1}^n \left(a_i(z) \frac{\partial P}{\partial z_i} \right) = 0, \quad (7)$$

and

$$a_i(z) = b_i(z)z_i, \quad \text{for } i \in \{j | \alpha_j > 0\}, \quad (8)$$

(6) yields,

$$0 = C \int dz_1 \cdots dz_n \left(\sum_{i=1}^n \left(\frac{\partial a_i}{\partial z_i} - \alpha_i \frac{a_i}{z_i} \right) - \gamma b \right) P^\gamma \frac{1}{z_1^{\alpha_1} \cdots z_n^{\alpha_n}}, \quad (9)$$

which generates IBP relations via the Baikov representation, keeping the *non-negative* indices from being increased. We call these IBP relations *formal IBP relations* if the indices α_i are symbolic.

The equations (7) are the syzygy equations of the set of generators $\langle P, \frac{\partial P}{\partial z_1}, \dots, \frac{\partial P}{\partial z_n} \rangle$. Considering Baikov kernel P is defined as the determinate of certain matrix, which let us call as P_{ij} , we have such a Laplace expansion [53] as

$$\sum_j P_{ij} \frac{\partial P}{\partial P_{kj}} - \delta_{ik} P = 0. \quad (10)$$

The matrix entries, P_{ij} , are scalar products of the momenta, thus being linear combinations of the propagators z_i 's and kinematic variables. Consequently, from the Laplace expansion (10), the solutions of the syzygy equation (7) can be directly read, using the chain rule of derivative. The completeness of those syzygy generators are proved in [53].

Given a Baikov kernel P , the solutions of (7), which are vectors of polynomials, (b, a_1, \dots, a_n) , are not unique. All the solutions form an algebraic structure called *module*. Call the solution module of (7) M_1 . Similarly, the solutions of (8) also form a module, M_2 . In order to find the common solutions of (7) and (8), we perform *module intersection* [55]

$$M = M_1 \cap M_2. \quad (11)$$

In the current version of NEATIBP, the module intersection problem is solved using syzygy method. Let us denote the generators of M_1 and M_2 as f_i and g_i , respectively. We solve the syzygy equation of $\langle f_i \rangle \cup \langle g_i \rangle$ to get

$$\sum_i s_i f_i + \sum_j r_j g_j = 0. \quad (12)$$

Then, $\sum_i s_i f_i$ is both in M_1 and M_2 , serving as a generator of $M_1 \cap M_2$.

From the module intersection (11), we get the generators of module M . They can be used in (9) to generate formal IBP relations in the following form,

$$0 = \sum_{\{\vec{\beta}\}} c_{\{\vec{\beta}\}}(\alpha_1, \dots, \alpha_n) I_{\alpha_1 + \beta_1, \dots, \alpha_n + \beta_n}. \quad (13)$$

With the power indices α_i in the formal IBP relations as integers, specific IBP relations are obtained. This process is called *seeding*, and the specific integer value for α_i 's is called a *seed*.

Seeding is a key step for many IBP reduction algorithms. For syzygy or module intersection-based IBP reduction, the seeding process would be more sophisticated since the syzygy/module intersection generators may provide IBP relations with different numerator degrees. The details of seeding in NEATIBP v1.0 is described in the next section.

2.3. The sectors of a Feynman integral family

The integrals in an integral family can be categorized by the propagators that appear in the denominator of the integrand. Such a category is called a *sector* in the integral family. An integral $G_{\alpha_1, \dots, \alpha_n}$ is in a sector (s_1, \dots, s_n) , if,

$$s_i = \begin{cases} 1, & \alpha_i > 0 \\ 0, & \alpha_i \leq 0 \end{cases}, \quad (14)$$

Changing one or more “1” to “0” in the sector expression (s_1, \dots, s_n) of a certain sector A , we get another sector B which is called a *sub sector* of sector A . Accordingly, sector A is called a *super sector* of sector B . Sometimes, one can label a sector by the set $\{i | s_i = 1\}$. For example, sector $(0, 1, 0, 0, 1, 0, 1, 0, 0)$ can be labeled as $\{2, 5, 7\}$.

Among the 2^n sectors in an integral family with n propagators, there are many of them called *zero sectors*, in which all integrals are zero. NEATIBP applies Lee’s zero sector criteria to determine zero sectors [46]. This method is based on Lee-Pomeransky representation [46, 65, 15]. It is shown in [46] that for a given sector S , if there exist constants t_i 's such that

$$\sum_i t_i x_i \frac{\partial G}{\partial x_i} = G, \quad (15)$$

where G denotes the Lee-Pomeransky polynomial on sector S , then S is a zero sector.

2.4. The symmetries of Feynman integrals

Symmetries between Feynman integrals are important for the integral reduction.

It is well-known that the symmetries of Feynman integrals can be found from the polynomial symmetry of their parameterized representations. The

polynomial symmetries can be found by Pak's algorithm [66]. In this way, the symmetry between Feynman integrals via swapping propagators is determined.

Furthermore, the propagator permutation can be reformulated to a momentum map, which is found by the following ansatz,

$$l_i \mapsto A_{ij}l_j + B_{ik}p_k, \quad \text{where } \det(A_{ij}) = \pm 1, \quad p_i \mapsto C_{ij}p_j. \quad (16)$$

corresponding to the permutation,

$$D_i \rightarrow D_{\sigma(i)}, \quad \text{for } i \in \{j | \alpha_j > 0\}, \quad (17)$$

where σ stands for a certain permutation. We call a symmetry relation a *symmetry inside a sector*, if the permutation rule σ map integrals in one sector to integrals in the same sector. We call it a *symmetry between sectors* otherwise. The coefficients in the ansatz (16) are determined by the propagator matching and the invariance of the Gram matrix of external legs.

We remark that, a momentum map is stronger than the polynomial symmetry. For a polynomial symmetry, in some cases, the corresponding momentum map does not exist. There may be other cases that it does exist, but some efforts are needed to derive it. For instance, NEATIBP will search symmetry relations in lower sectors by redefining external momenta.

2.5. Propagator cuts

For complicated integrals family, frequently one would like to carry out the IBP reduction with propagator cuts. For integrals with Dirac delta functions in the integrand, IBP relations with cuts are also necessary. In NEATIBP v1.0, computation with propagator cut is also included. For the conceptual introduction of the propagator cuts and the related generalized unitarity methods, we refer to the ref. [67][68][69][63].

In this version of our package, we implement the propagator cut convention in the Baikov representation as [63]. Suppose that \mathcal{C} is the set of propagator indices on the cut, then the Baikov integral kernel becomes,

$$P \mapsto P|_{z_j \rightarrow 0}, \quad j \in \mathcal{C}. \quad (18)$$

and the IBP relation can be found by the following module intersection,

$$(M_1|_{z_j \rightarrow 0}) \cap (M_2|_{z_j \rightarrow 0}), \quad j \in \mathcal{C}. \quad (19)$$

The resulting IBP relations have no increase of the uncut indices of propagators. Usually, with a cut, the module intersection computation and the IBP seeding would be much easier. For complicated Feynman integral family, it makes sense to consider all the spanning cuts of the IBP reduction and then construct the full IBP reduction.

In this version of NEATIBP, we only deal with the Feynman integrals with the propagator index lower than 2 *on the cut*. The integrand for double propagators on the cut in the Baikov representation, which contains the derivative of the kernel P is more complicated. We leave this case for the future versions.

We also remark that the choice of propagator cuts usually breaks the symmetry between sectors. So, in this version of our package, if the propagator cut is imposed then the symmetry searching should be turned off.

3. Algorithms

In this section, we will introduce the main ideas of the algorithm of NEAT-IBP.

3.1. Generating IBP relations referring to sectors

In NEATIBP, the IBP reduction relations are generated by seeding process referring to the sector structure of an integral family. We apply the similar idea “tail mask” as that in the Laporta algorithm. For each sector, we just accumulate IBP relations which can reduce the target integrals to the master integrals of this sector, and the (unreduced) integrals in the sub sectors. The integrals from the sub sectors are also called *tail integrals*⁴.

Generating IBP relations in a family is divided into sub tasks which correspond to the sectors. The family can be visualized as a web structure with each sector as a node, (see Fig. 1). The input of each node is a set of the target integrals of the current sector, consisting user input and tail integrals from its super sectors. The output of each node includes master integrals and IBP relations generated from the current sector. Tail integrals in these IBP relations would become the input of the corresponding sub nodes.

The web structure enables us to distribute the computation in parallel. In our parallelization scheme, a task immediately starts once all its super tasks are finished. In NEATIBP v1.0, the parallel tasks are arranged by a mission status registration table and a task manager. Logically, such a parallelization

⁴In the following discussions, we call integrals from the current sectors as *head integrals*.

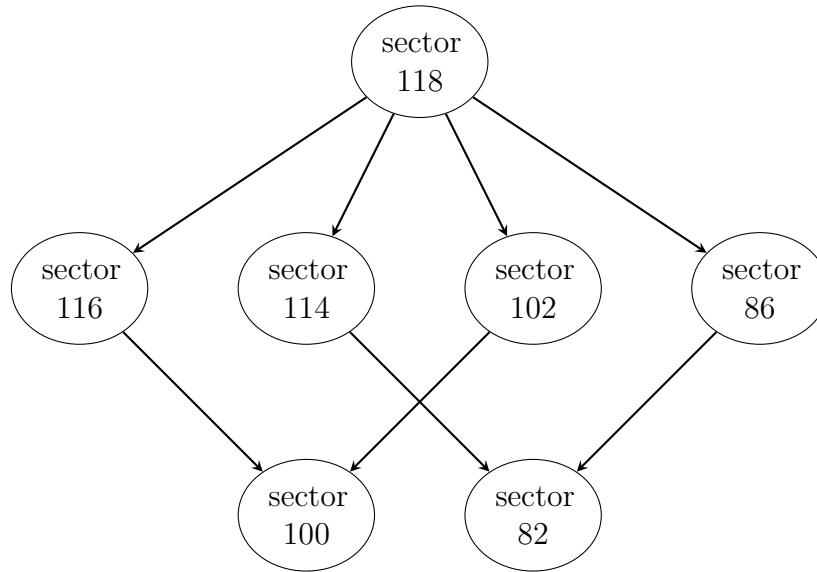


Figure 1: An example of a web structure of the sectors in a slashed box family, as a sub family of the double box.

scheme is built in a way shown in Fig. 2. In the registration table, the mission statuses have four cases . They are *waiting*, *ready to compute*, *computing* and *finished*. The task manager is in charge of the evolving of the registration table in the following ways,

- At the beginning, all mission statuses are initialized as *waiting*.
- The manager reads the registration table periodically.
- Once the manager detects that a *waiting* mission has no unfinished super mission, it modifies its status to *ready to compute*.
- Once the manager expects that there are available computation resources, it modifies the statuses of certain number of missions with *ready to compute* status to *computing* status, and, at the same time, send a message to workers to start the computing of those missions.
- Once a worker finished computing, it reports to the registration table to modify the status of the mission as *finished*.

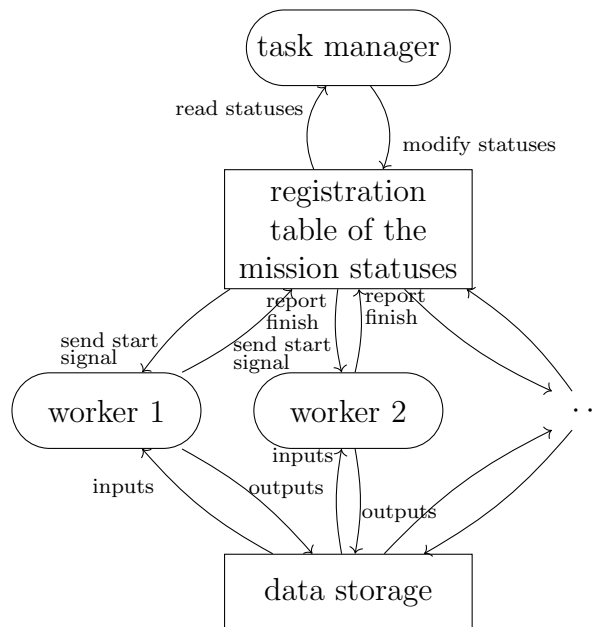


Figure 2: Distributed computation based on registration table.

In NEATIBP, we inserted a mission status monitor to show the contents of the registration table in real time, which describes status of all the missions. We will show this in Section 4.3.

3.2. Generating IBP relations in one sector

In this section, the IBP generation in our program is introduced. IBP relations can be generated via a seeding process introduced in Section 2.2 from the formal IBP relations derived in the Baikov representation. Note that unlike Laporta algorithm, given a fixed seed, IBPs from the module intersection or syzygy can have quite uneven numerator degrees. Therefore, for the given maximal numerator degree, we use different seeds for each formal IBP in eqn. (9) to make sure that the resulting IBP relations have the same maximal numerator degree. We call this seeding process *Zurich seeding*⁵.

⁵One of the authors of this paper used the process frequently when he was working in Zurich.

The IBP relations can be expressed as a linear system as follows

$$0 = \sum_j c_{ij}^h I_j^h + \sum_k c_{ik}^t I_k^t \quad (20)$$

where I_j^h and I_k^t stands for head and tail integrals relevant to the IBP system generated from the current sector.

To make sure the IBP system can reduce the target integrals to master integrals in this sector and the tail integrals, row reduction operations on the matrix of the coefficients c_{ij}^h would be applied. For the row reduction, the ordering of the integrals in (20) should be arranged by our preference.

The master integrals of the current sector are also determined during the row reduction. On the other hand, We find that the foreknow information on the master integral can sometimes reduce the size of IBP seeds⁶, and thus reduce the memory usage. For this purpose, we use Lee’s critical counting [65] and also the maximal cut syzygy method in AZURITE [70]. Specifically, in NEATIBP v1.0, we embed a minimal version of AZURITE, named as AZURITINO, to determine the master integrals as a running option.

We remark that, we use Lee’s critical point counting here as an “order of magnitude” estimation of the number of master integrals, to set up the initial seeding range for AZURITINO.

By a standard linear algebra computation, a column reduction of c_{ij}^h matrix selects independent IBP relations on the current sector. Here we prefer IBP relations with lower tail integral degrees in the selection. Schematically, after removing the linearly dependent relations, we have

$$0 = \sum_j \tilde{c}_{ij}^h I_j^h + \sum_k \tilde{c}_{ik}^t I_k^t \quad (21)$$

Furthermore, from the linearly independent IBPs, we can select IBP relations that are actually needed to reduce the target integrals. Specifically, considering a row reduction,

$$R_{ik} = \sum_j L_{ij} \tilde{c}_{jk}^h, \quad (22)$$

⁶Because we do not need to add more seeds to verify whether the set of master integrals is stable when numerator degree increases.

where the matrix R is a row echelon form. Suppose that the i -th row corresponds to an input integral, the set

$$\{j | L_{ij} \neq 0\}, \quad (23)$$

corresponds to the indices of used IBPs to reduce this particular input integral. In this manner, we can further select used IBPs from the independent IBP set.

We remark that the above row reduction operations are just for IBP relation selections. Therefore, we use generic kinematic values and finite field methods to speed up these steps. However, this could be a bit risky if the numeric point is not “generic” enough or prime number associated with the finite field hits a singular case in the linear operators. In NEATIBP v1.0, we added a check process to check the IBP relations, with other numeric kinematic points. Multiple kinematic points and prime numbers, and a majority vote process may make the selection more stable. However, this approach would change the parallelization scheme and hence we leave it for the future versions of NEATIBP.

In this version of NEATIBP, we implement the row reduction over finite field by using the open-source package SPASM [61].

NEATIBP allows input integrals with or without multiple propagators. For integrals with multiple propagators, NEATIBP serves as an IBP generator which avoids higher propagator indices and reduces the IBP system size as well. With NEATIBP v1.0, we suggest to run tasks for input integrals with or without multiple propagators separately. One may avoid a large number of seeds by doing this.

We remark that, in NEATIBP, while solving module intersection problems in SINGULAR, a degree bound is frequently used. Once the total degree of an intermediate result reaches the given `degBound`, an early termination of Buchberger’s algorithm is triggered. This results in a faster computation, but possibly yields an incomplete basis, and thus incomplete generating system of the module intersection. We observe that there are cases, where the module intersection result obtained with degree bound, together with seeds without increased indices, may lead to a larger irreducible integral set than the set of master integrals. In these cases, NEATIBP v1.0 can automatically search⁷ for certain seeds with increased denominator power indices, to

⁷We describe the strategy of how to search for them in a footnote in Section 4.2 around

further reduce the irreducible integral set. This mechanism is designed for complicated diagrams where we have to use low degree bounds in SINGULAR to make the module intersection computation less time-consuming.

3.3. Additional remarks

The whole process of NEATIBP is in three steps, the initialization, the parallel missions between sectors and the summary.

In the initialization step, we determine all sectors that are relevant to the missions according to the target integrals the user input. Among the sectors, there are some zero sectors. We treat all target integrals in these zero sectors as 0 in the whole process.

NEATIBP allows the user to choose whether the symmetry is needed. If so, we need to consider both symmetries inside sectors and between sectors. The symmetries between sectors are found in the initialization step. Through this, some nonzero sectors⁸ can be mapped to its *image sector*. We select a set of nonzero sectors, called *unique sectors*, such that all other nonzero sectors can be mapped to a unique sector, and a unique sector cannot be mapped to another unique sector. NEATIBP converts all integrals in the non-unique sectors to their images after symmetry mapping, which are combinations of integrals from unique sectors.

In the second step, the symmetries inside a sector can be derived using methods stated in Subsection 2.4. We treat these symmetry relations in the same way as IBP relations and put them together to form a linear system after seeding.

4. Manual

In this section, we provide a manual describing the installation and usage of NEATIBP. Note that this manual is based on the most recent version (v1.0.2.4) at the time that this paper is finished. This version is complete in the sense that it implements the basic functions introduced in the previous sections. NEATIBP will be continually updated with further improvement. For this, users can refer to the NEATIBP GitHub repository.

the discussion on the option `StrictDenominatorPowerIndices`.

⁸In this context, they are called the *source sector* of its image sector.

4.1. Installation

NEATIBP is a MATHEMATICA/SINGULAR package. One can obtain NEATIBP from the following GitHub repository link, which also provides installation instructions.

<https://github.com/yzhphy/NeatIBP>

The user can install NEATIBP by

```
git clone https://github.com/yzhphy/NeatIBP.git
```

following the `Readme.md` document of the repository. The dependencies of NEATIBP are SINGULAR [60] and SPASM [61], so these have to be installed before usage. If SPASM is not present on the machine yet, we recommend to install it using or along the lines of script provided in the NEATIBP repository.

As an alternative way of installation, we also provide a package for the supercomputing package manager SPACK [71], which installs NEATIBP along with all of its dependencies. Please follow the respective section of the `Readme.md` document.

4.2. Preparing inputs

To utilize NEATIBP for a Feynman integrals reduction task, the following three files are required in the working directory in order to run the program:

1. A configuration file named “`config.txt`” containing the necessary settings.
2. A kinematics file, which by default is named “`kinematics.txt`”, containing the kinematic information for the Feynman diagram.
3. A target integral file, which by default is named “`targetIntegrals.txt`”, containing the target integrals which are supposed to be reduced.

The input files should be prepared in form of Mathematica readable files using the command `Get`. In the configuration file, settings that control the execution of NEATIBP are specified. If an option value is not given, the program refers to default values given in `NeatIBP/default_settings.txt`. We list some of the settings which are frequently used:

1. `kinematicsFile` and `targetIntegralsFile`: These variables contain the names of the `txt` files which specify the kinematics of the Feynman

diagram and the target integrals, respectively. Please make sure that the file names are given with absolute paths. To do so, one can use `workingPath` which points to the working directory (the directory of the configuration file).

2. `SingularApp`: This variable tells NEATIBP how to run Singular. Its value is a string with the command running SINGULAR in the shell.
3. `SparseRREF`SpaSMLibrary`: This variable tells NEATIBP where to find SPASM. Its value is a string containing the absolute path to the file “`libspasm.so`”.
4. `ReductionOutputName` and `outputPath`: If `outputPath` is set to the value `Automatic` (default value), the output of NEATIBP will be written to the subfolder with name `ReductionOutputName` inside the subfolder `outputs` in `workingPath`. If the output should be written to a different location, `outputPath` can be set.⁹
5. `OptionSimplification`: This is an integer value selecting the simplification mode used to simplify the results of the module intersection in SINGULAR. The simplification mode is explained in the SINGULAR documentation, see

https://www.singular.uni-kl.de/Manual/4-3-2/sing_349.htm.

6. `FiniteFieldModulus`: The finite field modulus used in SPASM for NeatIBP. This value should be a prime number not larger than 46337.
7. `AzuritinoIntersectionDegreeBound` specifies the degree bound for module intersection computations via SINGULAR in AZURITINO, while `NeatIBPIntersectionDegreeBound` gives the degree bound for the formal IBP generation step in NEATIBP. For more details on how to specify degree bounds, please refer to

https://www.singular.uni-kl.de/Manual/4-3-2/sing_399.htm.

⁹If `outputPath` is set to `Automatic` and the output path already exists, then NEATIBP will ask the user whether to overwrite the contents. If the folder is user-specified, it is the user’s responsibility to delete data from previous runs.

8. **IntegralOrder**: A variable controlling the ordering of Feynman integrals. It can take the values **MultiplePropagatorElimination**, **ISPElimination**, or **Global**. The three options correspond to different preferences of ordering, respectively reducing the degree of denominators, numerators, or both (the total absolute degree), as priority. Note that, when **AZURITINO** is enabled (which is by default), since it finds master integrals without double propagators, **IntegralOrder** must be set to **MultiplePropagatorElimination**.
9. **NeedSymmetry**: A Boolean type variable, which determines whether symmetries of Feynman integrals are considered.
10. **CutIndices**: A list containing the indices of the cut propagators.
11. **SeedingAdditionalDegree**: The maximum of the additional numerator degree considered relative to the degree of the target integrals.
12. **MIFromAzuritino**: A Boolean type variable, which determines whether to use **AZURITINO** to find master integrals.
13. **CriticalPointInAzuritino**: A Boolean type variable determining whether to use Lee's critical point counting method [65] to estimate the amount of master integrals before using **AZURITINO**.
14. **StrictMI**: If this Boolean type variable is set to **True**, then **NEAT-IBP** terminates with an error if the **IBP** relations generated are not sufficient to reduce the target integrals to the pre-determined master integrals. Otherwise, **NEATIBP** uses a (typically slightly) redundant integral basis.
15. If **StrictDenominatorPowerIndices** is **False**, **NEATIBP** will try to introduce a minimally necessary set of seeds with increased indices for denominators, in case the generated **IBP** system cannot reduce the target to master integrals¹⁰.

¹⁰This function is called **AdditionalIBPs** in **NEATIBP**. It firstly tries to add seeds with only one denominator index increased at each position and test if these seeds generate a complete linear system. Otherwise, according to the value of **AllowedDenominatorPowerLift**, the function adds seeds with multiple increased indices for denominators. For example, if **AllowedDenominatorPowerLift** is set to 2, there may be index increase of type $(+1, +1, 0, 0, \dots)$ or $(+2, 0, 0, 0, \dots)$.

`AllowedDenominatorPowerLift` is the allowed total denominator degree increase in the additional seeds. Note that setting the variable `AllowedDenominatorPowerLift` to 0 is equivalent to setting the variable `StrictDenominatorPowerIndices` to `True`.

16. `MemoryUsedLimit`: The limit for memory usage specified in megabytes. NEATIBP will try to estimate the memory usage of newly scheduled parallel tasks, and try to control (but not to guarantee) the memory usage below this limit.
17. `ThreadUsedLimit`: The maximum number of NEATIBP parallel computation. This value is used in two circumstances. First, when finding symmetries between sectors, NEATIBP by default uses `ParallelTable`. This value is the kernel it launches using `LaunchKernels` (if it is not larger than `$ProcessorCount`). Second, in the IBP relation generation step, this value is the maximum number of sectors that are synchronously computed. Note that, in this step, the task manager also needs to occupy a MATHEMATICA kernel. So, the maximum kernel usage in this step is `ThreadUsedLimit+1`. Also, if you turn on a monitor, since it also occupies a kernel, the number of kernels you may use is `ThreadUsedLimit+2`.
18. Using the Boolean type variables `DeleteSingularScriptFiles` and `DeleteSingularResultFiles`, one can determine whether NEATIBP deletes on completion of the computation the temporary SINGULAR input and output files, respectively.

The user can also request in the configuration file various additional outputs. For details, see the section “additional outputs” in the default configuration file `NeatIBP/default_settings.txt`.

In the kinematics file, the user shall provide the following variables:

1. `LoopMomenta`: A list for the loop momenta of the Feynman diagram.
2. `ExternalMomenta`: A list containing all external momenta of the Feynman diagram.
3. `Propagators`: A list with the propagators of the Feynman diagram.

4. **Kinematics**: A list containing replacement rules for the kinematic conditions of the external momenta.
5. **GenericPoint**: A list containing replacement rules corresponding to a general numeric point (with rational coordinates) for scalar kinematic variables appearing in **Kinematics** and **Propagators**.
6. **GenericD**: A replacement rule corresponding to a general numeric value (rational number) for the spacetime dimension d .

In the target integral file, the user shall prepare a list of the target integrals. Here, the integral $G_{\alpha_1, \dots, \alpha_n}$ is expressed as $\mathbf{G}[\alpha_1, \dots, \alpha_n]$.

4.3. Running NEATIBP

After preparing the above-mentioned input files in the working directory, the user can execute NEATIBP to generate the IBP relations. Assuming the user has installed NEATIBP in the directory `/SomePath/NeatIBP/`, it can be run by changing directory to the working path and executing the command

```
/SomePath/NeatIBP/run.sh
```

While NEATIBP is running, the user can execute in a separate terminal window in the working path the command

```
/SomePath/NeatIBP/monitor.sh
```

to launch a monitor which shows the current status of the parallel missions.

An example of a monitor output is

```
-----
2023.4.10 23:17:53
42 sector(s) waiting super sector(s): 244,241,236,233,229,205...
0 sector(s) ready to compute.
14 sector(s) computing: 245,237,218,217,211,206...
81 sector(s) finished: 255,254,253,251,247,239...
-----
```

In the output, the sector numbers are the binary ids of the sectors.

Note that, in case a worker process terminates unexpectedly during computation, this will not be reported to the registration table and the management system will consider the job to still be computing. To recognize this, the monitor has a process detection, which will report in case of an unexpected termination of a process a warning of the form

```

-----
2023.3.17 15:32:25
128 sector(s) waiting super sector(s): 252,250,249,246,245,243...
0 sector(s) ready to compute.
7 sector(s) computing: 254,253,251,247,239,223...
2 sector(s) finished: 255,127.
*****
Warning:
1 sector(s) lost: 191.
The corresponding process(es) cannot be detected. Maybe they terminated
unexpectedly.
-----

```

In the above example, the computing process of sector 191 was terminated manually while computing, resulting in the warning.

NEATIBP supports to resume computation if a process is terminated by hand or unexpectedly. To do this, make sure the execution of NEATIBP in the respective working path is stopped, then run the following command in the working path

```

/SomePath/NeatIBP/continue.sh

```

NEATIBP will restart the sectors that have not been finished yet.

In the Github repository of NEATIBP, we provide some examples for how to use NEATIBP. In the current version, one of the examples (dbox) include the output results. User can refer to this manual and try the examples by themselves. Note that, in the examples, we provided some convenient scripts to apply the operations, which again are called `run.sh`, `monitor.sh`, and `continue.sh`. User can modify the file `packagePath.txt` such that it contains the absolute path where NEATIBP was installed. Then, open a terminal in these example working folders, and use

```

./run.sh

```

to run NEATIBP, use

```

./monitor.sh

```

to turn on a monitor, or use

```

./continue.sh

```

to continue an unfinished computation. For computation in other directories, the user can copy the file `packagePath.txt` along with respective three scripts from the example's directory to the working directory and them do the same.

4.4. Output generated

After NEATIBP has finished running, its output will be exported into three sub directories of the output path, namely `inputs`, `results`, and `tmp`. The `inputs` folder will contain the three input files described in Subsection 4.2. The `results` folder will contain four files, and a minimum of two sub folders. The file `IBP_all.txt` lists all IBP relations generated by NEATIBP. The file `MI_all.txt` lists all master integrals. The file `OrderedIntegrals.txt` lists all integrals occurring in the IBP relations, in an integral ordering from high to low. The file `summary.txt` is a log file containing a summary of the computation. The sub folders `results/IBP/` and `results/MI/` contain txt files with IBP relations and master integrals on each sector, respectively. If the user requested additional outputs in the configuration file, there will be sub folder `additional_outputs` containing the requested additional outputs. The folder `tmp`, contains some temporary files created during runtime.

As discussed in Subsection 3.2, the finite field row reduction in NEATIBP using a numeric point may hit singularities. Thus, after NEATIBP finished running, it is recommended to check the results on further different numeric points. In NEATIBP, we provide an automatic checker to test if the IBP relations generated can reduce the target integrals to master integrals. To do this, open a terminal in any folder and run

```
math -script /SomePath/NeatIBP/CheckIBP.wl [path]
```

where `[path]` is the output path of the NEATIBP results. The program will perform a row reduction on a different random numeric point to see if the IBP system is sufficient to reduce the target integrals. It is recommended to execute the check several times to sufficiently reduce the probability of a mistake.

4.5. Row reduction using SPASM

As mentioned before, this version of NEATIBP relies on SPASM [61] for row reduction over finite fields. To connect SPASM to MATHEMATICA, we use `LIBRARYLINK`, a component of MATHEMATICA, which can connect to C libraries and supply an interface. For communication, specific data structures are used in our C code, which then is packaged as a library called `SparseRREF.so`, and an interface file called `SparseRREF.m`. In NEATIBP, this interface to SPASM is included and automatically used.

The interface component can also be used individually for other purposes. To do this, one can run the following command in MATHEMATICA

```
Get["SomePath/NeatIBP/SparseRREF/SparseRREF.m"]
```

and use the command

```
SRSparseRowReduce[M, Modulus->p]
```

to obtain the RREF (reduced row echelon form) from an sparse input matrix M (which should be a `SparseArray`) given over the rational numbers which is reduced to the finite prime field \mathbb{F}_p modulo the prime p in case of co-prime denominators. The output will be a sparse echelon-form modulo p of MATHEMATICA type `SparseArray`.

5. Examples

In this section, we provide examples to illustrate the performance of NEATIBP. This section gives details on three different examples: a 2-loop 5-point massless planar diagram, a 2-loop 4-point non-planar diagram with internal and external massive lines, and a 3-loop 4-point planar diagram with one external massive line. The input files of these examples can be found in the Github repository, in folder “examples/examples_in_the_papers/”. The input and output files can be found in the Dropbox links shown later.

5.1. A pentagon-box diagram example

In this subsection, we consider the two-loop five-point diagram as depicted in Figure 3. The paper [49] which originally introduced the syzygy IBP method used this diagram as an example, but did not cover all the sub sectors.

The propagators of this diagram are

$$\begin{aligned} D_1 &= l_1^2, & D_2 &= (l_1 - p_1)^2, & D_3 &= (l_1 - p_{12})^2, & D_4 &= (l_1 - p_{123})^2, \\ D_5 &= l_2^2, & D_6 &= (l_2 + p_{1234})^2, & D_7 &= (l_2 + p_{123})^2, & D_8 &= (l_1 + l_2)^2, \\ D_9 &= (l_1 - p_{1234})^2, & D_{10} &= (l_2 + p_1)^2, & D_{11} &= (l_2 + p_2)^2, \end{aligned}$$

where $p_{i\dots j} := p_i + \dots + p_j$. The last three propagators are irreducible scalar products (ISPs). The external kinematic conditions are

$$\begin{aligned} p_1^2 &= p_2^2 = p_3^2 = p_4^2 = 0, & p_1 \cdot p_2 &= \frac{s_{12}}{2}, \\ p_1 \cdot p_3 &= \frac{-s_{12} - s_{23} + s_{45}}{2}, & p_1 \cdot p_4 &= \frac{-s_{15} + s_{23} - s_{45}}{2}, \\ p_2 \cdot p_3 &= \frac{s_{23}}{2}, & p_2 \cdot p_4 &= \frac{s_{15} - s_{23} - s_{34}}{2}, & p_3 \cdot p_4 &= \frac{s_{34}}{2} \end{aligned}$$

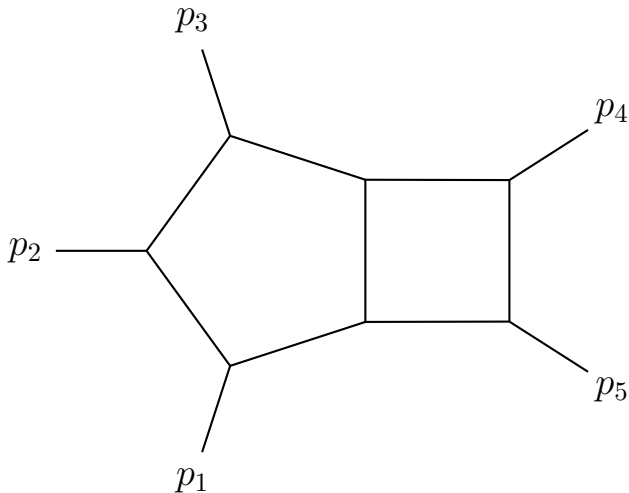


Figure 3: A two-loop five-point diagram example

The momentum conservation condition in this diagram is $p_1 + p_2 + p_3 + p_4 + p_5 = 0$.

We demonstrate this example using two sets of target integrals as inputs. The first set of target integrals is to show the performance on numerator reduction. It consists of 2483 randomly chosen integrals from sector $\{1, 2, 3, 4, 5, 6, 7, 8\}$ and its subsectors. They have maximum numerator degree 5, and are free of multiple denominators. Using NEATIBP (v1.0.2.3), we find 61 master integrals and get an IBP system with 14120 IBP identities, which are enough to reduce all the target integrals to master integrals.

The above computation was carried out using 10 CPU cores and 128GB RAM. The computation took about 27 minutes. The input and some output files can be obtained at the following link:

<https://www.dropbox.com/s/rrwillc0xyv30pf/pb.tar.gz>

As a reference, FIRE6 [42] used 11207942 IBP identities in the reduction of the same target integrals. In the computation, we ran FIRE6 with kinematic variables set to be rational numbers.

The second set of targets contains 880 integrals, which come from the derivatives of the 61 master integrals. This set shows the performance of NEATIBP for integrals with multiple propagators. By generating 3313 IBP identities, NEATIBP relates the given 880 integrals to the 61 master integrals.

The computation finishes in 17 minutes on 10 CPU cores and 128GB RAM. As a reference, FIRE6 reduced those target integrals using 1010236 IBP identities. The input and relevant output files can be downloaded at the following link:

https://www.dropbox.com/s/vhzilt837nhn118/pb_D.tar.gz

5.2. A non-planar two-loop massive diagram example

In this subsection, we discuss an example from the top quark phenomenology. The diagram is given in Figure 4. This nonplanar diagram is one of the most complicated two-loop diagrams contributing to the NNLO corrections for tW production at hadron colliders in [72] (and the references therein).

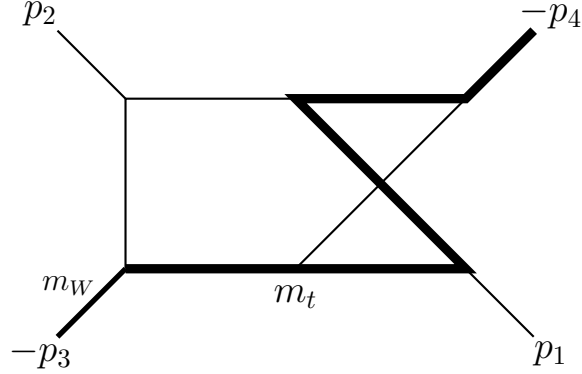


Figure 4: A nonplanar two-loop diagram for the tW production

The propagators of this diagram are

$$\begin{aligned}
 D_1 &= -m_t^2 + l_1^2, & D_2 &= -m_t^2 + l_2^2, & D_3 &= (l_1 + l_2)^2, \\
 D_4 &= -m_t^2 + (l_1 + p_1)^2, & D_5 &= -m_t^2 + (l_1 + l_2 + p_1 + p_2 - p_3)^2, \\
 D_6 &= (l_2 + p_2 - p_3)^2, & D_7 &= (l_2 - p_3)^2, & D_8 &= (l_1 - p_1 + p_3)^2, \\
 D_9 &= (l_2 - p_1 - p_2 + p_3)^2.
 \end{aligned}$$

Its external kinematic conditions are

$$\begin{aligned}
 p_1^2 = p_2^2 = 0, & \quad p_3^2 = m_W^2, & p_1 \cdot p_2 &= \frac{m_t^2 + m_W^2 - t - u}{2}, \\
 p_1 \cdot p_3 &= \frac{m_W^2 - t}{2}, & p_2 \cdot p_3 &= \frac{m_W^2 - u}{2}
 \end{aligned}$$

The momentum conservation condition in this example is $p_1 + p_2 = p_3 + p_4$.

The 597 target integrals for the two-loop scattering amplitudes $pp \rightarrow tW$, are from sector $\{1, 2, 3, 4, 5, 6, 7\}$ and its subsectors. Using NEATIBP (v1.0.2.3), we generated 7169 IBP relations which are sufficient to reduce all the target integrals to 90 master integrals.

The computation was performed using 20 CPU cores and 128GB RAM. The computation took about 1.5 hours. The input and relevant output files can be obtained at the following link:

<https://www.dropbox.com/s/6wnfwfn0he47ztk/214pNP7.tar.gz>

We remark that for this diagram the syzygy computation is rather expensive. Using the degree bound 5 for the computation in SINGULAR, we observe that we do not obtain a sufficiently large set of syzygies, and hence the number of resulting irreducible integrals is slightly larger than the expected 90. Increasing the degree bound to 6 makes the syzygy computation significantly more expensive. NEATIBP then obtains a sufficient set of IBPs and finds 90 master integrals by automatically seeding on some extra integrals with double propagators.

5.3. A three-loop example

In this subsection, we present a three-loop four point example shown in Figure 5. Note that master integrals in related families are calculated in [73].

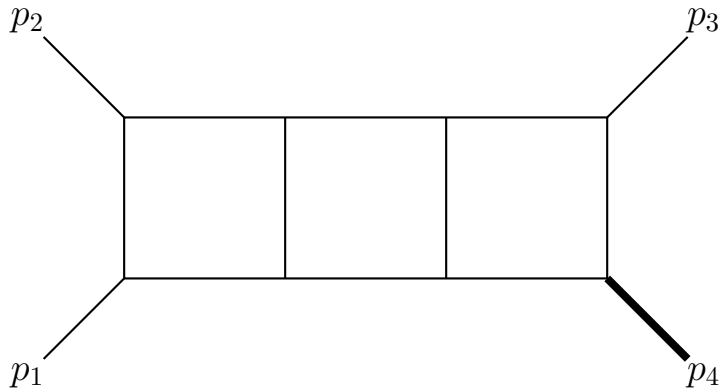


Figure 5: The planar triple box diagram with an external massive leg

The propagators of this diagram are

$$\begin{aligned}
D_1 &= l_1^2, & D_2 &= (l_1 - p_1)^2, & D_3 &= (l_1 - p_{12})^2, & D_4 &= l_3^2, \\
D_5 &= (l_3 + p_{12})^2, & D_6 &= (l_1 + l_3)^2, & D_7 &= (l_2 - l_3)^2, & D_8 &= l_2^2, \\
D_9 &= (l_2 - l_4)^2, & D_{10} &= (l_2 + p_{12})^2, & D_{11} &= (l_1 + p_4)^2, & D_{12} &= (l_2 + p_1)^2, \\
D_{13} &= (l_3 + p_1)^2, & D_{14} &= (l_3 + p_4)^2, & D_{15} &= (l_1 + l_2)^2.
\end{aligned}$$

The external kinematic conditions are

$$\begin{aligned}
p_1^2 = p_2^2 = 0, & \quad p_4^2 = m^2, & p_1 \cdot p_2 &= \frac{s}{2}, \\
p_2 \cdot p_4 &= -\frac{s+t}{2}, & p_1 \cdot p_4 &= \frac{t-m^2}{2}.
\end{aligned}$$

The momentum conservation condition for this diagram equals $p_1 + p_2 + p_3 + p_4 = 0$.

We randomly pick 21185 integrals as our target. They are in the sector $\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$ and its subsectors. The most complicated integral has the numerator degree 6 in the top sector. Using NEATIBP (v1.0.2.3), we found 83 master integrals and acquired 200074 IBP relations, which are sufficient to reduce all given target integrals to master integrals.

This computation was carried out on a computer with 50 CPU cores and 1.5TB RAM and took about 6 hours. The input and relevant output files can be downloaded at the link:

<https://www.dropbox.com/s/8mabbgauxpmxzrb/314p1m.tar.gz>

6. Summary

In this paper, we present the package NEATIBP v1.0, for generating an IBP system which are sufficient to reduce the input target Feynman integrals to master integrals. The module intersection method, which is a contemporary variant of the original syzygy approach [49], is used to restrict the growth of propagator indices in the IBP generation. We expect that the size of this IBP system is of orders of magnitude smaller than that obtained from Laporta's algorithm. The resulting IBP system can be used for either finite field reduction with subsequent reconstruction of physical quantities, or for analytic reduction.

In this version of NEATIBP, the module intersection computation is powered by the open-source computer algebra system SINGULAR, while IBP generation, workflow control and the I/O operations are controlled by MATHEMATICA. The selection of linearly independent and sufficient IBP relations is carried out using the C-library SPASM. NEATIBP v1.0 incorporates parallelization across different Feynman integral sectors. The execution is controlled by MATHEMATICA code, and the status of the computation is recorded in a registration table on disk. The status can be monitored by the user in the terminal. In the event that the execution of NEATIBP is interrupted, it is possible to resume the computation using the saved temporary files stored on disk.

We anticipate the following updates in the future versions:

1. Migrate the code to rely only on open-source software.
2. Introduce advanced massive parallelization. This includes the introduction of an additional layer of parallelization within a single sector for concurrent execution of the seeding process. Further parallelization could arise from the different cuts of one Feynman integral family. A promising approach to effectively manage and intertwine the multiple levels of parallelism is to realize the workflow management through the open source SINGULAR/GPI-SPACE framework [74, 75], which relies on the workflow management system GPI-SPACE [76], incorporates the computer algebra system SINGULAR, which is used by NEATIBP for module intersection computations, and offers convenient installation using the SPACK package manager [77].
3. Incorporate alternative approaches for module intersection or syzygy computation. In the current version of NEATIBP, we apply the available general functionality of SINGULAR for computing module intersections. In future versions, we might consider to customize this implementation for our specific setting. Moreover, further methods, like linear algebra techniques [50] and the dual conformal symmetry method for syzygy generation [78] will be considered in future versions.
4. It is well known that the syzygy/module intersection method is very effective on cuts. NEATIBP v1.0 can easily generate IBP relations on cuts. Future versions will find all spanning cuts automatically and build the rules for combining the results for the cuts.

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