The Mathematica package TopoID and its application to the Higgs boson production cross section

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Abstract. We present the Mathematica package TopoID which aims at the automation of several steps in multiloop calculations. The algorithm which lies at the very core of the package is described and illustrated with an example. The main features of TopoID are stated and some of them are briefly demonstrated for NLO or NNLO Higgs boson production.

1. Introduction

With the LHC running in the coming years at 14 TeV, the experimental precision for observables will further improve. Likewise, the theoretical uncertainty needs to be decreased which means higher orders in the perturbation series need to be computed. Some quantities under consideration presently are for example the Higgs boson production cross section at N³LO [1, 2], the four-loop $\overline{\text{MS}}$ -OS relation [3], the four-loop cusp anomalous dimension [4] or the five-loop β -function [5]. All these calculations are based on the evaluation of Feynman diagrams which usually suffers from a factorial growth of complexity with higher orders.

For most of the necessary steps in such a calculation various program packages are already available publically. Color, Lorentz and Dirac algebra (tensorial structures) can be handled, e.g., with FORM [6], FeynCalc [7] or HEPMath [8]. The resulting scalar integrals can then be classified in so-called Feynman integral families or "topologies". TopoID [9, 10] is a package dedicated especially to this task (and others). The integrals within each topology are subject to integrationby-parts identities (IBPs) [11] which allow for a systematic reduction to "master integrals". That is, a large set of integrals can be expressed as linear combinations of only relatively few basis integrals. Public reduction programs include MINCER [12] for three-loop massless propagtors, MATAD [13] for three-loop massive tadpoles or AIR [14], FIRE [15] and Reduze [16] implementing Laporta's approach [17] for generic topologies.

TopoID aims at taming the diagrammatic or "topologic" complexity that arises in a calculation. The complexity involved in algebraic operations on the coefficients of integrals in reduction relations or in the function classes for master integrals, however, is a different and still open subject.

1.1. Example: Higgs boson production at NLO

Let us illustrate the concepts of topology and integral reduction by the single topology needed for the NLO corrections to Higgs boson production due to real radiation:

$$\begin{array}{cccc}
 & & & & & \\ p_1 & & & & \\ d_2 & & & \\ d_3 & & & \\ p_2 & & & \\ p_2$$

The non-planar box topology T in Eq. (1) consists of four scalar propagators $1/d_1, \ldots, 1/d_4$ raised to generic integer powers a_1, \ldots, a_4 ($a_i = 0$ means contraction of line i). Note, this topology is defined in forward scattering kinematics to faciliate the use of the optical theorem (for a detailed discussion see Ref. [10]). Forward scattering means outgoing momenta are fixed by incoming ones ($p_3 = p_1$ and $p_4 = p_2$) and in this sense above topology is non-planar. The double line indicates the Higgs boson, arrows show the momentum flow. Due to the linear dependence of d_1, \ldots, d_4 (with respect to the scalar products $p_1 \cdot k_1$, $p_2 \cdot k_1$ and k_1^2) and since integrals with d_1 or d_2 eliminated do not contribute via the optical theorem, partial fractioning allows to eliminate either d_3 or d_4 in all appearing expressions. This leaves us with two symmetric triangle topologies $T(a_1, a_2, a_3, 0) = T(a_1, a_2, 0, a_3)$. Gauss' theorem in D dimensions gives in this case rise to three IBPs, one for the contraction with either the loop momentum k_1 or one of the external momenta p_1 and p_2 :

$$0 = \int \mathrm{d}^D k_1 \, \frac{\partial}{\partial k_1^{\mu}} \left\{ k_1^{\mu}, p_1^{\mu}, p_2^{\mu} \right\} \frac{1}{d_1^{a_1} d_2^{a_2} d_3^{a_3}}.$$
 (2)

The relations obtained from Eq. (2) by fixing a_1, \ldots, a_3 to integer values then involve integrals with differing denominator powers. Generating a set of such relations for all the needed integrals of a family gives a linear system which can be solved in terms of master integrals. In this case only a single master integral (a bubble with $a_1 = a_2 = 1$, $a_3 = a_4 = 0$) emerges in the end.

2. Canonical ordering

The most important capability of TopoID is the fast and efficient IDentification of isomorphic Topologies. This is essential since the routing of loop momenta and the order of propagators in the definition of a topology are ambiguous. The basic idea is to use the sum $\mathcal{U} + \mathcal{F}$ of the Symanzik polynomials appearing in the Feynman representation, which is independent of loop momenta, as an identifier. Therefore, the Feynman parameters $\{\alpha_j\}$ (corresponding to scalar propagators) are permuted in a unique algorithmic way. See also Ref. [18].

The task of the algorithm can be stated without reference to Feynman integrals: bring the polynomial P with m terms into a unique form \hat{P} by renaming the n variables $\{x_j\}$. This can be achieved by the following steps:

- (i) Convert P into a $m \times (n+1)$ matrix $M^{(0)}$. Each row corresponds to a term, the first column to constant coefficients and the remaining columns to powers of the $\{x_j\}$ in the monomial.
- (ii) Start with the above $M^{(0)}$ and in the second column (k = 1).
- (iii) Compute for all considered matrices $M^{(k),\sigma}$ all transpositions of columns k and $k+1,\ldots,n$ where the index σ collects all applied permutations.
- (iv) Sort rows in each matrix lexicographically by the first k columns.
- (v) Extract the lexicographically largest vector from columns k of all matrices.
- (vi) Keep only matrices with this maximal vector. If k < n-1, increment k and go to step (iii).
- (vii) Each remaining matrix encodes the same unique \hat{P}_{σ} and a corresponding permutation of variables σ .

2.1. Example: a simple polynomial in two variables

We demonstrate the above algorithm in a simple example where equation labels indicate the respective step and iteration:

$$P = x_1^2 + 2x_1x_2 + x_2^2 + x_3^2 \to M^{(0)} = \begin{pmatrix} 1 & 2 & 0 & 0 \\ 2 & 1 & 1 & 0 \\ 1 & 0 & 2 & 0 \\ 1 & 0 & 0 & 2 \end{pmatrix}.$$
 (i)

$$S^{(1)} = \left\{ M^{(0)(123)} = M^{(0)} \right\}, \ k = 1.$$

$$S^{\prime(1)} : M^{\prime(1)(123)} = \begin{pmatrix} 1 & 2 & | & 0 & 0 \\ 2 & 1 & | & 1 & 0 \\ 1 & 0 & | & 2 & 0 \\ 1 & 0 & | & 0 & 2 \end{pmatrix}, \ M^{\prime(1)(213)} = \begin{pmatrix} 1 & 0 & | & 2 & 0 \\ 2 & 1 & | & 1 & 0 \\ 1 & 2 & | & 0 & 0 \\ 1 & 0 & | & 0 & 2 \end{pmatrix}, \ M^{\prime(1)(321)} = \begin{pmatrix} 1 & 0 & | & 0 & 2 \\ 2 & 0 & | & 1 & 1 \\ 1 & 0 & | & 2 & 0 \\ 1 & 2 & | & 0 & 0 \end{pmatrix}.$$
(iii-1)

$$S^{\prime\prime(1)}: M^{\prime\prime(1)(123)} = \begin{pmatrix} 1 & \mathbf{0} & 0 & 2\\ 1 & \mathbf{0} & 2 & 0\\ 1 & \mathbf{2} & 0 & 0\\ 2 & \mathbf{1} & 1 & 0 \end{pmatrix}, \ M^{\prime\prime(1)(213)} = \begin{pmatrix} 1 & \mathbf{0} & 2 & 0\\ 1 & \mathbf{0} & 0 & 2\\ 1 & \mathbf{2} & 0 & 0\\ 2 & \mathbf{1} & 1 & 0 \end{pmatrix}, \ M^{\prime\prime(1)(321)} = \begin{pmatrix} 1 & 0 & 0 & 2\\ 1 & 0 & 2 & 0\\ 1 & 2 & 0 & 0\\ 2 & 0 & 1 & 1 \end{pmatrix}.$$
(iv-1)

$$\hat{M}^{\prime\prime(1)} = (0, 0, 2, 1)^{\mathrm{T}}.$$
(v-1)
$$S^{(2)} = \left\{ M^{\prime\prime(1)(123)}, M^{\prime\prime(1)(213)} \right\}, k = 2.$$
(vi-1)

$$S'^{(2)} : M'^{(2)(123)} = \begin{pmatrix} 1 & 0 & 0 & | & 2 \\ 1 & 0 & 2 & | & 0 \\ 1 & 2 & 0 & | & 0 \\ 2 & 1 & 1 & | & 0 \end{pmatrix}, M'^{(2)(132)} = \begin{pmatrix} 1 & 0 & 2 & | & 0 \\ 1 & 0 & 0 & | & 2 \\ 1 & 2 & 0 & | & 0 \\ 2 & 1 & 0 & | & 1 \end{pmatrix},$$

$$M'^{(2)(213)} = \begin{pmatrix} 1 & 0 & 2 & | & 0 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & | & 2 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 \\$$

$$\begin{pmatrix}
1 & 2 & 0 & 0 \\
2 & 1 & 1 & 0
\end{pmatrix}^{\prime} \qquad \begin{pmatrix}
1 & 2 & 0 & 0 \\
2 & 1 & 0 & 1
\end{pmatrix}$$

$$S''^{(2)}: M''^{(2)(123)} = \begin{pmatrix}
1 & 0 & 0 & 2 \\
1 & 0 & 2 & 0 \\
1 & 2 & 0 & 0 \\
2 & 1 & 1 & 0
\end{pmatrix}, M''^{(2)(132)} = \begin{pmatrix}
1 & 0 & 0 & 2 \\
1 & 0 & 2 & 0 \\
1 & 2 & 0 & 0 \\
2 & 1 & 0 & 1
\end{pmatrix},$$

$$M''^{(2)(213)} = \begin{pmatrix}
1 & 0 & 0 & 2 \\
1 & 0 & 2 & 0 \\
1 & 2 & 0 & 0 \\
2 & 1 & 1 & 0
\end{pmatrix}, M''^{(2)(231)} = \begin{pmatrix}
1 & 0 & 0 & 2 \\
1 & 0 & 2 & 0 \\
1 & 2 & 0 & 0 \\
2 & 1 & 0 & 1
\end{pmatrix}.$$
(iv-2)

$$\hat{M}^{\prime\prime(2)} = (0, 2, 0, 1)^{\mathrm{T}} \,. \tag{v-2}$$

$$S^{(2)} = \left\{ M^{\prime\prime(2)(123)}, M^{\prime\prime(2)(213)} \right\}.$$
 (vi-2)

$$\hat{P} = P = x_3^2 + x_2^2 + x_1^2 + 2x_1x_2, \ \hat{\sigma} = \{(123), (213)\}.$$
(vii)

We observe, P was already in its unique form \hat{P} (apart from the order of terms) and the algorithm resulted in two permutations (123) and (213) which correspond to the apparent symmetry in exchanging x_1 and x_2 . In the context of Feynman integrals this means the algorithm gives not just a unique identifier $\hat{\mathcal{U}} + \hat{\mathcal{F}}$ but also its symmetries.

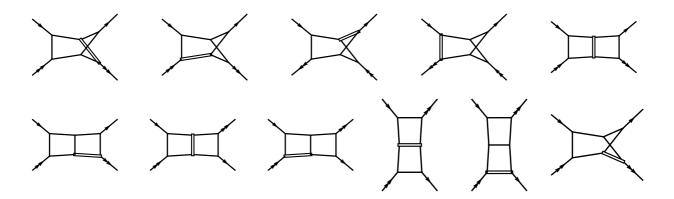


Figure 1. Minimal set of topologies needed for the real corrections to the Higgs boson production cross section at NNLO. This set is sufficient for the calculation of all 2946 appearing diagrams.

3. Features of TopoID

TopoID is written in Mathematica and assists in obtaining results for the amplitude of a given process in terms of a minimal set of master integrals. However, for the computationally expensive parts of a calculation, much faster FORM code is generated that does not demand for a Mathematica license. The main input for this task are the Feynman diagrams which can be generated, e.g., by QGRAF [19].

Starting from the diagrams, TopoID identifies a minimal set of topologies. That is, by contraction and permutation of propagators all scalar integrals arising from the diagrams can be mapped to at least one of the topologies in the minimal set. See Fig. 1 for a minimal set sufficient for the real contributions to NNLO Higgs boson production.

In case the topologies identified in a first step expose linearly dependent propagators, see Sec. 1.1, linear independent subtopologies are detected and partial fractioning relations are generated automatically. The algorithm described in Ref. [18] which employs Gröbner bases is used. For Eq. 1 the following set of rules is generated whose repeated application is guaranteed to terminate:

$$d_{4} \rightarrow -m_{H}^{2} + s + d_{1} + d_{2} - d_{3},$$

$$d_{3}/d_{4} \rightarrow \left(-m_{H}^{2} + s + d_{1} + d_{2} - d_{4}\right)/d_{4},$$

$$d_{2}/(d_{3}d_{4}) \rightarrow \left(m_{H}^{2} - s - d_{1} + d_{3} + d_{4}\right)/(d_{3}d_{4}),$$

$$d_{1}/(d_{2}d_{3}d_{4}) \rightarrow \left(m_{H}^{2} - s - d_{2} + d_{3} + d_{4}\right)/(d_{2}d_{3}d_{4}),$$

$$1/(d_{1}d_{2}d_{3}d_{4}) \rightarrow (d_{1} + d_{2} - d_{3} - d_{4})/(\left(m_{H}^{2} - s\right)d_{1}d_{2}d_{3}d_{4}).$$
(3)

It is of course understood that TopoID is capable of dealing with various properties of topolgies, such as completeness with respect to scalar products involving loop momenta, distinct and scaleless subtopologies and symmetries. Also graphs corresponding to a set of propagators can be reconstructed and unitarity cuts (used extensively in connection with the optical theorem and forward scattering) can be revealed in a very efficient way.

Finally, let us mention that also relations among master integrals (emerging from different topologies) can be found using TopoID (usually in conjunction with a Laporta algorithm). These relations emerge by identifying equivalent integrand denominators and transforming possible numerators accordingly. Such relations can simplify a calculation tremendously or are very useful cross-checks. An example for such a relation from NNLO Higgs boson production can be

sketched as follows:

$$= + c_1 + c_2 + c_2$$
 (4)

Here, the integral from the left-hand side stems from the fitfth and the first integral on the right-hand side from the ninth topology of Fig. 1, and the coefficients c_i are rational functions in the kinematic invariants m_H^2 and s and the space-time dimension D.

4. Conclusion

The package TopoID is a generic, process independent tool for multiloop calulations, useful especially when many topologies are involved. Until now it has been applied successfully to the qq'-channel in Higgs boson production at N³LO [2] and to the NNLO soft-virtual corrections to Higgs boson pair production [20]. It can also handle the classification of the massless five-loop propagator topologies, including all their symmetries. Along with this proceedings contribution, a first public version can be obtained from the web page https://www.ttp.kit.edu/~jens/ where also future versions, a detailed documentation and additional material will be provided.

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