Double Virtual Contributions for Massless $2 \to 3$ Scattering in NNLO QCD

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Abstract

We review the recent advances in the calculation of two-loop QCD corrections for massless five-point scattering that paved the way for their broad phenomenological applications in calculation of NNLO QCD predictions. We first discuss the construction of a transcendental function basis which facilitates derivation of compact analytic representations for two-loop amplitudes and enables their fast and stable numerical evaluation over physical phase space. We then present the recent calculations of the leading-color two-loop corrections for hadroproduction of three photons and three jets.

1 Introduction

Precise theoretical predictions for $2 \to 3$ scattering processes are key ingredients for the precision physics program at the Large Hadron Collider. To obtain predictions accurate to percent level for wide range of observables generally NNLO QCD and NLO EW corrections are required. While NNLO QCD predictions for a variety of important $2 \to 2$ processes became available in the past two decades, extending the NNLO multiplicity frontier further required development of new cutting-edge computational methods. In addition to the growing complexity of handling infrared divergences, the main obstacle is the availability of two-loop scattering amplitudes.

To write down a scattering amplitude, one has to sum together many Feynman integrals. The latter, in turn, can be expressed through a smaller basis of *master* integrals by using integration-by-parts (IBP) identities [1]. This step is highly challenging in cases where number of involved scales and/or loops gets large. The reduction of five-particle amplitudes has been recently extensively studied and several novel techniques have been proposed to tackle this challenge [2–13]. These advances together with the judicious use of functional reconstruction techniques [3, 4, 14] lead to the impressive progress in the computation of massless two-loop five-point scattering amplitudes. The calculation of master integrals for this class of processes have also been under detailed investigation in recent years. The differential equations (DE) [15–19] in their canonical form [20–24], as well as systematization of mathematical properties of special functions that appear in calculations of relevant Feynman integrals [25–29].

These mathematical properties can be used to construct dedicated bases of special functions in which any scattering amplitude with given kinematics can be expressed. Importantly, these bases can be constructed in such a way that the underlying simplicity and mathematical structure of amplitudes is revealed. Indeed, this fact has been fruitfully exploited for high multiplicity two-loop amplitude calculations within the modern analytic reconstruction approaches from numerical finite-field evaluations [3, 4, 12, 30–32]. We constructed such basis set for the case of five-point massless scattering, pentagon functions, in ref. [33]. Furthermore, we showed that highly efficient and stable numerical evaluation of the amplitudes expressed through these bases can be achieved — a prerequisite for large-scale phenomenological applications. We implemented the latter in a public `C++` library [34]. Therefore, the complete set of special functions suitable for NNLO QCD $2 \to 3$ massless cross section calculations is now available.

	Preliminary results	Complete analytic results	Public numerical code	Cross sections
jjj (LC)	[12, 30–32, 35–38]	[39]	[39]	[40]
$\gamma\gamma j$ (LC)		[41, 42]	[41]	[43]
$\gamma\gamma\gamma$ (LC)	[44]	[45, 46]	[45]	[44, 47]
$\gamma\gamma j$		[48]		
$gg \to \gamma\gamma g$ (loop induced)		[49]	[49]	[50]

Table 1: Summary of the known two-loop QCD corrections for massless five-point scattering processes at hardon colliders. All public codes employ `PentagonFunctions++` [33] for numerical evaluation of special functions. (LC) marks the processes in the leading-color approximation.

As a result of increasing understanding of the relevant transcendental functions and the impressive progress in the techniques for taming the complexity of integral reduction, the first calculations of double-virtual corrections to processes involving production of up to three light jets and photons have been successfully completed in the past two years. These calculations are summarized in table 1. Notably, the first complete results without employing the leading-color approximation have started to appear. In the following we will present the results obtained within the framework of numerical unitary [11, 36, 37, 51, 52], namely the complete set of leading-color two-loop contributions required for NNLO QCD corrections to three-jet and three-photon production at hadron colliders.

2 Basis of transcendental functions

Master integrals can be most naturally expressed in terms of *pure* functions order-by-order in the dimensional regulator within the method of differential equations in canonical form. The canonical DEs for integrals $\vec{f}_{\tau,\sigma}$ of the family τ and permutation of external momenta σ read

$$\mathrm{d}\vec{f}_{\tau,\sigma} = \epsilon\, \mathrm{d}A_{\tau,\sigma} \vec{f}_{\tau,\sigma}, \qquad \mathrm{d}A_{\tau,\sigma} = \sum_i a^{(i)}_{\tau,\sigma}\, \mathrm{d}\log W_i\,, \tag{1}$$

where $a^{(i)}_{\tau,\sigma}$ are rational matrices, ϵ is the dimensional regularization parameter, and W_i are letters from the symbol alphabet. For the one-loop pentagon, pentagon-box, double pentagon, and hexagon-box integral topologies the DEs in canonical form were obtained in refs. [53–59].

In the standard approach to the calculation of master integrals, one attempts to use eq. (1) to find solutions in terms of a class of functions known as *multiple polylogarithms* (MPLs) [25, 60]. This has been a remarkably successful strategy for the problems with few scales, but its generalization to multi-scale problems is not straightforward due to the presence of algebraic letters in the alphabet. In this case finding explicit MPL solutions frequently becomes impractical, the number of MPLs required to write the solution explodes, and spurious branch cuts typically have to be introduced. This leads to unacceptably slow evaluation in the physical region, even in the simplest five-point massless case.

To address these issues, we study the relevant space of transcendental functions and identify a minimal basis set of pentagon functions. This is advantageous both for examining the analytic structure of scattering amplitudes and for their efficient numerical evaluation. Our approach is constructive and directly uses the information provided by the canonical DEs. First, we write the solutions of DEs from an initial point X_0 in the physical scattering region in all 5! permutations of external momenta through Chen's iterated integrals [28],

$$\vec{f}^{(w)}(X) = \sum_{w'=0}^{w} \sum_{i_1,\dots,i_{w'}=1}^{31} \vec{\kappa}^{(w-w')}_{i_1,\dots,i_{w'}} \, [W_{i_1},\dots,W_{i_{w'}}]_{X_0}(X)\,. \tag{2}$$

where $\kappa^{(w-w')}$ are transcendental constants of weight $w-w'$,

$$\kappa^{(w-w')}_{i_1,\dots,i_{w'}} = a^{(i_1)} a^{(i_2)} \dots a^{(i_{w'})} \vec{f}^{(w-w')}(X_0)\,, \tag{3}$$

and the iterated integrals of weight w along the path γ are defined recursively as

$$[W_{i_1},\dots,W_{i_w}]_{X_0}(X) = \int_\gamma \mathrm{d}\log W_{i_w}(X') \; [W_{i_1},\dots,W_{i_{w-1}}]_{X_0}(X'), \quad []_{X_0} = 1\,. \tag{4}$$

The values of the master integrals at an initial point X_0 were partially presented in refs. [61,62]. We complete the results of [61,62] and derive the initial values of the DEs at X_0 in all permutations of external momenta by demanding the absence of unphysical singularities. We identify 19 algebraically-independent transcendental constants whose polynomials span all the initial values. In the next step, we construct sets of algebraically-independent transcendental *functions* recursively weight-by-weight, up to weight four. The algebraic identities at each weight are linearized by the shuffle product of iterated integrals, and the basis of the vector space spanned by all functions, modulo products of lower weight functions, is identified through linear algebra. For numerical evaluation of pentagon functions we derive their explicit representations in terms of dilogarithms up to weight two, and we derive representations through one-fold integrals [53, 63] at weight three and four. The number of pentagon functions that we obtain by following this procedure is shown in table 2. We observe that, starting from the 1917 topologically-independent master integrals, our analysis reveals a considerably smaller basis of transcendental functions.

The pentagon functions can be efficiently evaluated over the whole physical phase space. We demonstrate this by evaluating all pentagon functions on a sample of 90000 phase-space points, drawn from a typical distribution employed in computations of differential cross sections for processes with five massless particles. More specifically, we use the phase space definition from ref. [47]. Given a quantity x and its evaluation with double precision x_{double} and quadruple precision x_{quad}, we estimate the relative error of the former by the number of "correct digits" d,

$$d_x = -\log_{10}\left|1 - \frac{x_{\text{double}}}{x_{\text{quad}}}\right|, \tag{5}$$

Weight	Linearly independent	Irreducible
1	10	10
2	79	24
3	482	111
4	1462	472

Table 2: Counting of the master integral components at each transcendental weight (ϵ order). The second column corresponds to the number of the $\mathbb{Q}$-linearly independent components. The third column shows the number of irreducible components, i.e. the number of pentagon functions.

We evaluate all pentagon functions with double and quadruple precision at each phase space point. We define the *minimal* logarithmic relative error among all pentagon functions at each kinematical point X as

$$R(X) = \min_i [r_i(X)], \qquad i \in \{\text{all pentagon functions}\}. \tag{6}$$

We display the distribution of $R(X)$ over a physical phase space of ref. [47] in fig. 1. We observe excellent numerical stability in the bulk of the phase space and average evaluation time of several seconds.

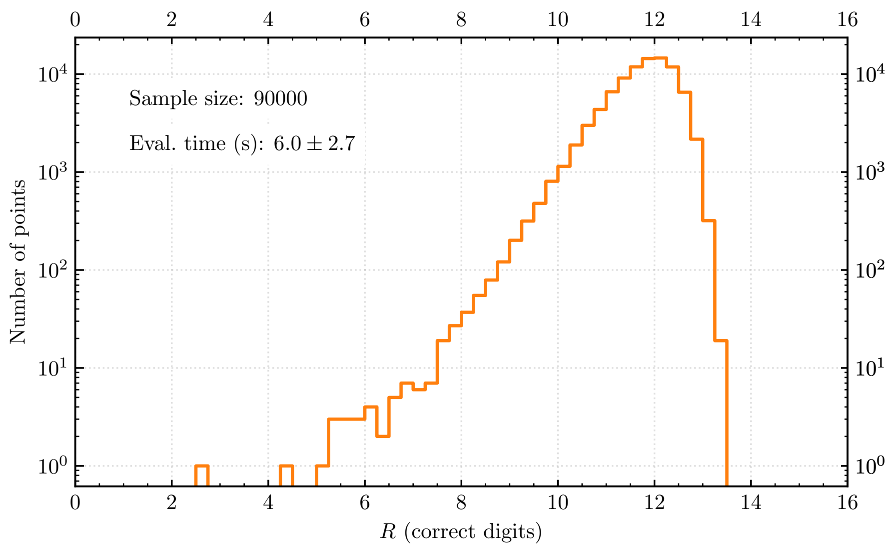

Figure 1: Logarithmic distribution of minimal correct digits (see eq. (6)) of pentagon functions evaluated on a sample of 90000 phase-space points. The average evaluation time of all pentagon function in double precision on a single thread is estimated on a server with *Intel(R) Xeon(R) Silver 4216 CPU @ 2.10GHz*. This figure is from ref. [33] licensed under *CC-BY 4.0*.

The pentagon functions have been already used in numerous "real-world" applications (see references in table 1), showcasing excellent performance. We therefore conclude that the numerical bottleneck of double-virtual contributions caused by the evaluation of transcendental functions is completely eliminated.

3 Rational coefficients

Let us now turn to the discussion of the rational (algebraic) functions of external kinematics which are the coefficients of transcendental functions.

Any calculation of a multi-loop scattering amplitude begins by considering its integrand which schematically takes the form of

$$\mathcal{A}(\ell_l) = \sum_{\Gamma\in\Delta}\sum_i c_{\Gamma,i}\frac{m_{\Gamma,i}(\ell_l)}{\prod_{j\in P_\Gamma}\rho_j}\,, \tag{7}$$

where ℓ_l denotes the loop momenta of the problem, Δ is the set of distinct propagator structures Γ, and P_Γ is the multiset of inverse propagators ρ_j in Γ. $m_{\Gamma,i}(\ell_l)$ are polynomials in loop momenta and rational functions of external kinematics $\boldsymbol{s}$ and ϵ. The goal of integral reduction is to bring the amplitude's integrand to the form

$$\mathcal{A} = \sum_i c_i(\boldsymbol{s},\epsilon)\,\mathcal{I}_i\,, \tag{8}$$

where $\mathcal{I}_{\Gamma,i}$ are the master integrals and $c_i(\boldsymbol{s},\epsilon)\in\mathbb{Q}(\boldsymbol{s},\epsilon)$. Upon expressing the master integrals in a basis of special functions (pentagon functions in this case) until the required order in ϵ, one can subtract the UV and IR divergences analytically and derive the finite quantity of interest, the finite remainder

$$\mathcal{R} = \sum_{\mathrm{i}} r_{\mathrm{i}}(\boldsymbol{s})\,\boldsymbol{g}^{\mathrm{i}} + \mathcal{O}(\epsilon), \tag{9}$$

where $\boldsymbol{g}^{\mathrm{i}}$ are the relevant monomials of pentagon functions in the multi-index notation. Given a good choice of transcendental functions, the rational coefficients $r_{\mathrm{i}}(\boldsymbol{s})$ are remarkably simple. However, their derivation starting from the amplitude's integrand in eq. (7) is hindered by intermediate expression swell and is the key challenge in the calculation of multi-scale two-loop amplitudes. This is especially pronounced at the step of employing the IBP identities.

A key idea that opened the possibility of calculating two-loop five-point amplitudes in QCD is to bypass the complexity of intermediate expressions with exact numerical evaluations over finite fields [3, 14]. The analytic expressions are then reconstructed from numerical samples. The complete frameworks of numerical reduction of scattering amplitudes over finite fields, `FiniteFlow` [4, 32, 61] and two-loop numerical unitary [11, 36, 37, 51, 52, 64], have been developed and applied successfully to complete a number of previously unimaginable calculations. The developments in IBP reduction techniques using insights from algebraic geometry [10, 11, 65–68] proved to be highly effective in further reducing the complexity.

The framework of analytic reconstruction from finite-field evaluations can be significantly enhanced if the constraints on the analytic structure of scattering amplitudes from physics are integrated. For instance, it was realized in ref. [37] that the possible denominators of the rational coefficients r_{i} are the symbol letters. Furthermore, the reconstruction of analytic expressions can be seriously simplified by judicious ansatzing [30, 49, 69]. Another important observation is that the rational coefficients are amenable for dramatic simplification by multivariate partial fractioning [5, 30, 70, 71], which leads to compact analytic amplitudes and their efficient numerical evaluation. Some of these ideas found their application also in more traditional approaches [46, 48, 70].

3.1 Numerical unitarity

The two-loop numerical unitarity framework [11, 12, 36, 37, 51, 64] is particularly suitable for taking advantage of the analytic reconstruction framework. We begin by constructing a special parametrization of the integrand in eq. (7) in terms of master integrands, which integrate to master integrals, and surface terms, which integrate to zero [11]. In order to determine the coefficients $c_{\Gamma,i}$ we rely on the factorization properties of the integrand. Specifically, we consider $\mathcal{A}(\ell_l)$ on loop-momentum configurations ℓ_l^Γ where the propagators are on-shell, that is $\rho_j(\ell_l^\Gamma)=0$ iff $j \in P_\Gamma$. Taking such a limit, the leading contribution to eq. (7) behaves as

$$\sum_{\text{states}} \prod_{i\in T_\Gamma} \mathcal{A}_i^{(0)}(\ell_l^\Gamma) = \sum_{\Gamma' \geq \Gamma, i \in M_{\Gamma'} \cup S_{\Gamma'}} \frac{c_{\Gamma',i}\, m_{\Gamma',i}(\ell_l^\Gamma)}{\prod_{j\in(P_{\Gamma'}\setminus P_\Gamma)} \rho_j(\ell_l^\Gamma)} \,. \tag{10}$$

On the left-hand side of this equation, we denote by T_Γ the set of tree amplitudes associated with the vertices in the diagram corresponding to Γ, and the sum is over the physical states propagating through the internal lines of Γ. On the right-hand side, we sum over the propagator structures which contribute to the limit, denoted Γ', for which $P_\Gamma \subseteq P_{\Gamma'}$. The coefficients $c_{\Gamma,i}$ can be determined numerically by sampling eq. (10) over a sufficient number of values of ℓ_l^Γ. We evaluate the tree amplitudes through off-shell recursion. In this way, we build a constraining system of cut equations for the $c_{\Gamma,i}$. We solve the cut equations numerically. Therefore, the knowledge of the analytic integrands or individual Feynman diagrams is not required in the numerical unitarity approach.

4 Leading-color two-loop QCD corrections for three-photon and three-jet production

We now present the complete set of leading-color two-loop contributions required to obtain next-to-next-to-leading-order (NNLO) QCD corrections to three-jet and three-photon production at hadron colliders. We obtain analytic expressions for a generating set of helicity finite remainders using the two-loop numerical unitarity approach. We employ CARAVEL [64] to generate all the required numerical data, and the analytic reconstruction techniques developed in refs. [12, 30]. In both cases we derive compact analytic expressions that are suitable for phenomenological applications and we present a public C++ library [72] for their efficient and stable numerical evaluation.

The typical evaluation time for the considered squared helicity- and color-summed two-loop finite remainders, which we denote $H^{(2)}$, is given in table 3. We observe that even for the most complicated partonic channel, namely the five-gluon channel, the squared remainder can be evaluated in only a few seconds on a single CPU core.

Process	Typical timing (s)
$q\bar{q} \to \gamma\gamma\gamma$	0.8
$gg \to ggg$	1.6
$q\bar{q} \to ggg$	1.0
$q\bar{q} \to Q\bar{Q}g$	0.7
$qg \to qq\bar{q}$	1.0

Table 3: Typical evaluation time of squared two-loop finite remainders contributing to three-photon and three-jet production at hadron colliders. The timings are measured on *Intel(R) Core(TM) i7-7700 CPU @ 3.60GHz*.

A more refined assessment of the numerical performance of our results is given in fig. 2, where we show the distribution of correct digits in the evaluation of the five-gluon squared remainder $H^{(2)}_{gg\to ggg}$ over a physical phase space defined in ref. [39]. We find that double precision is sufficient for the vast majority of phase-space points, and have implemented a

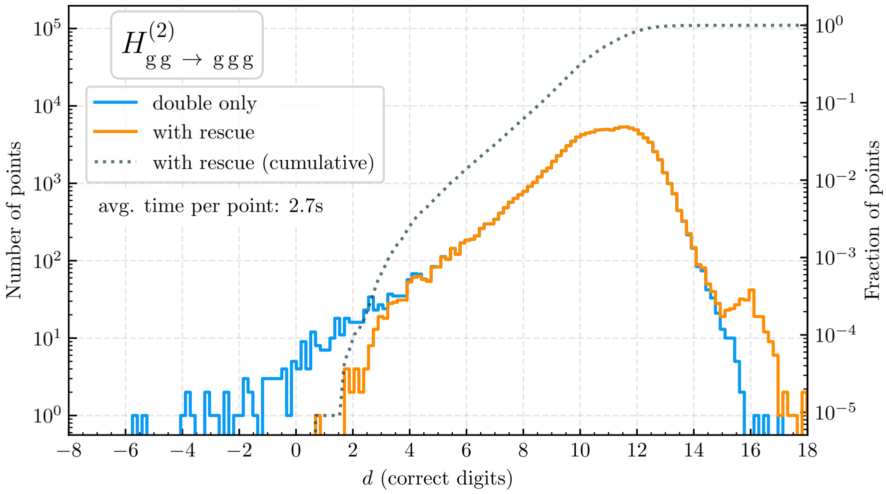

Figure 2: Logarithmic distribution of correct digits (see eq. (5)) of the five-gluon two-loop squared finite remainder on a sample of 110k points. The blue line corresponds to evaluation with double precision. The orange line represents evaluation with the rescue system enabled. The gray dashed line is the cumulative distribution of the latter. Average core time for evaluation on a single phase-space point with rescue system enabled as measured when evaluating all sample points in parallel using all 32 threads of `Intel(R) Xeon(R) Silver 4216 CPU @ 2.10GHz`. This figure is from ref. [39] licensed under *CC-BY 4.0*.

rescue system which detects unstable points and reevaluates them with quadruple precision. With the rescue system enabled, we find very good overall numerical stability. This shows that our results and the numerical library we provide are ready to be used in phenomenological studies.

5 Conclusion

The progress in calculation of massless two-loop five-point amplitudes in the past two years has resulted in availability of the first double-virtual contributions for the NNLO QCD corrections for a number of key $2 \to 3$ processes involving production of photons and light jets. The recurring theme that made this progress possible has been exploiting the remarkable simplicity and special properties of scattering amplitudes, both obscured at the intermediate stages of calculations. The availability of the complete set of pure Feynman integrals, and the construction of a basis of the relevant transcendental functions for five-point massless scattering, pentagon functions presented here, are one of the main prerequisites. The application of finite field arithmetic, analytic reconstruction and ansatzing, together with the advancements in the IBP-reduction techniques, then allow one to bypass the intermediate expression swell and access the simpler results directly. Strikingly compact analytic results can finally be derived thanks to the development of multivariate partial fractioning techniques. As a result, public codes for efficient numerical evaluation of the double-virtual contributions to three-jet, triphoton, and diphoton+jet production are now available. Here we presented the former two in the leading color approximation.

Thanks to the advancements in handling the real-radiation contributions and infrared divergences at NNLO QCD, the first proof-of-principle phenomenological studies involving NNLO QCD corrections to $2 \to 3$ production processes have been recently reported. We therefore expect that NNLO QCD predictions for this class of processes will become broadly available in the near future.

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