STEPS TOWARDS A SUBTRACTION FORMALISM AT NNLO

Massimiliano Grazzini (INFN, Florence)

Les Houches, may 2005

Outline

- Introduction
- The subtraction method
 - Subtraction at NLO
 - Subtraction at NNLO
 - An application: the $C_F T_R$ contribution to $e^+e^- \rightarrow 2$ jets
- Conclusions

The subtraction method

Let us consider an n-jet observable in e^+e^- at NLO accuracy

$$d\sigma = \int r d\Phi_{n+1} + \int v \, d\Phi_n$$

real: singularities appear after integration over unresolved parton virtual: singularities explicit as poles in $1/\epsilon^n$ n = 1, 2

Add and subtract a local counterterm $\tilde{r}d\tilde{\Phi}$ with the same singularity structure of the real contribution that can be integrated analytically over the phase space of the unresolved parton

$$d\sigma = \int (rd\Phi_{n+1} - \tilde{r}d\tilde{\Phi}_{n+1}) + \int \tilde{r}d\Phi_{n+1} + \int vd\Phi_n$$

$$d\sigma = \int (rd\Phi_{n+1} - \tilde{r}d\tilde{\Phi}_{n+1}) + \int \tilde{r}d\tilde{\Phi}_{n+1} + \int vd\Phi_n$$

This term can now be integrated numerically The singularities cancel in the sum

The method has been first introduced to compute $e^+e^- \rightarrow 3$ jets observables to NLO R.K. Ellis, D.A.Ross, A.E.Terrano (1981)

Later it was realized that it can be generalized in a process independent manner

Key observation: the soft and collinear limits of the QCD matrix element are universal

The counterterm $\tilde{r}d\tilde{\Phi}$ can be constructed by using the kernels that control the singular limits

General algorithms now available

S.Frixione, Z.Kunszt, A. Signer (1995) S.Catani, M. Seymour (1996)

Anatomy of subtraction at NLO

At NLO IR singularities originate from the following configurations:

- C: two partons become collinear
- S : one gluon becomes soft
- SC : two partons become collinear and one of them is soft

Let us introduce an operator \mathcal{E} such that

 $\mathcal{E}(f) = f - f(C) - f(S) - f(SC)$

where f(L) is the form of fin the singular limit L

The operator \mathcal{E} is not able to subtract all the divergences because soft and collinear limits overlap

To eliminate overlapping divergences we define the following formal rules (\mathcal{E} -prescription)

- I) Apply \mathcal{E} to f;
- 2) Apply \mathcal{E} to each of the resulting terms;
- 3) Iterate the procedure until no further term is generated;

The first step gives f - f(C) - f(S) - f(SC)

The second step gives

 $f - (f(C) - f(C \oplus S)) - (f(S) - f(S \oplus C)) - f(SC)$ = f - f(C) - f(S) + f(SC)

where we have used commutativity of soft and collinear limits

All the implementations of the subtraction method are based on this procedure

Apply the \mathcal{E} prescription to $rd\Phi$: the counterterm takes the form: $\tilde{r}d\tilde{\Phi} = r(C)d\Phi(C) + r(S)d\Phi(S) - r(SC)d\Phi(SC)$

Frixione-Kunszt-Signer (FKS): partition of phase space to have one soft and collinear singularity at most and then define $d\Phi_{n+1} = d\Phi_n(\tilde{i}j)d\Phi_2(i, j, L)$

where $d\Phi_2(i, j, L)$ is an approximation of $d\Phi_2$ in the limit L and \tilde{ij} is the on-shell parton obtained from *i* and *j*

Catani-Seymour (dipole): partial fractioning through eikonal identity $\frac{1}{p_i \cdot p_j p_i \cdot p_k} = \frac{1}{p_i \cdot p_j p_i \cdot (p_j + p_k)} + \frac{1}{p_i \cdot p_k p_i \cdot (p_j + p_k)}$

Then introduce *exact* phase-space parametrization keeping the reduced matrix element on shell without approximations

By doing so they are able to combine r(C), r(S) and r(SC)in r(D) = r(S) + r(C) - r(SC)

At NNLO we have to consider:

• Double virtual contribution with n resolved partons

$$|\mathcal{M}_n^{(1)}|^2 + \langle \mathcal{M}_n^{(2)} | \mathcal{M}_n^{(0)} \rangle + \mathrm{c.c.}$$

• Real-virtual contribution: one parton is unresolved

$$\langle \mathcal{M}_{n+1}^{(1)} | \mathcal{M}_{n+1}^{(0)} \rangle + \text{c.c.}$$

• Tree-level double real contribution: two partons are unresolved $|\mathcal{M}_{n+2}^{(0)}|^2$

The singularity structure of the three contributions has been basically understood S. Catani (1998); J.Campbell, N. Glover (1998)

S. Catani, MG (1999); Z.Bern, V. Del Duca, W. Kilgore, C. Schmidt (1999), D. Kosower, P. Uwer (1999), S. Catani, MG (2000)

...but a concrete subtraction scheme did not emerge yet

Results for $e^+e^- \rightarrow 2$ jets available + C_F^3 for $e^+e^- \rightarrow 3$ jets

A.Gehrmann- De Ridder, T.Gehrmann, E.W.N.Glover (2004)

Is an NNLO general subtraction formalism really needed ?

The number of two-loop amplitudes computed so far is limited

A new powerful method based on sector decomposition has been recently introduced C. Anastasiou, K.Melnikov, F.Petriello (2004)

It already allowed to compute the NNLO corrections to $e^+e^- \rightarrow 2$ jets and Higgs production at hadron colliders C. Anastasiou, K.Melnikov, F.Petriello (2004) But...

Sector decomposition could show problems when dealing with more complicated processes A general NNLO subtraction formalism would be interesting in itself and would help elucidating the pattern of cancellation of infrared singularities

How to formulate a subtraction formalism at NNLO?

The Catani-Seymour dipole approach appears to be the most advanced form of subtraction method to NLO but....

Can it be extended to NNLO ? Up to now only partial results available

S.Weinzierl (2002) D. Kosower (2002)

The price to pay to enforce exact phase space factorization are complicated expressions of the momenta appearing in the reduced matrix element

Spurious singularities appear when taking collinear limits of NLO kernels

Our proposal

S. Frixione, MG (2004)

We propose a method that retains some of the features of both dipole and FKS approaches:

- Explicit Lorentz invariance
- No exact phase-space factorization but...
- IR singularities combined in universal kernels factorizing the same reduced ME
- This is achieved by suitably extending the \mathcal{E} prescription to NNLO

We have successfully applied it to the calculation of the $C_F T_R$ contribution to $e^+e^- \rightarrow 2$ jets We first consider the double real contribution The new singular configurations are:

J.Campbell, E.W.N. Glover (1998) S. Catani, MG (1999)

- SC: two partons are collinear and a third parton is soft;
- SS :two partons become soft;
- CC[1]: : three partons become collinear;
- CC[2]: two parton pairs become independently collinear;
- SSC: two partons are soft and collinear, or one of them is collinear to a third parton;
- SCC[1]: three partons are collinear and one of them is also soft;
- SCC[2]: two parton pairs are collinear and one of the parton is soft;
- SSCC[1]: three partons are collinear and two of them are soft;
- SSCC[2]: two parton pairs are collinear and two of them are also soft;

Define $\mathcal{E}_{NNLO}(f) = \mathcal{E}_{NLO}(f)$ -f(SC) - f(SS) - f(CC) - f(SCC) - f(SSC) - f(SSCC)

The claim is that applying the \mathcal{E} -prescription to the double real contribution we can systematically subtract its singularities

Up to four iterations are necessary to define the counterterm At NNLO there are two distinct topologies that need be considered:





We understand that the singular terms, before being combined, have to be manipulated in order to make their contribution in the two topologies manifest Let us focus on $e^+e^- \rightarrow n$ jets

We write the three contributions to the NNLO cross-section as

$$d\sigma = \int rrd\Phi_{n+2} + \int rvd\Phi_{n+1} + \int vvd\Phi_n$$
$$= d\sigma_{rr} + d\sigma_{rv} + d\sigma_{vv}$$

We start by applying the \mathcal{E} - prescription to rr

$$d\sigma_{rr} = \int \left(rrd\Phi_{n+2} - \tilde{rr}_{-2} d\tilde{\Phi}_{n+2}^{-2} - \tilde{rr}_{-1} d\tilde{\Phi}_{n+2}^{-1} \right) \quad \longrightarrow \quad$$

Finite: to be integrated numerically

$$+\int \tilde{rr}_{-2}d\tilde{\Phi}_{n+2}^{-2}$$

$$+\int \tilde{rr}_{-1}d\tilde{\Phi}_{n+2}^{-1}$$

To be integrated analytically over the phase space of unresolved partons

Can be integrated over NLO phase space but it is still divergent because there is one unresolved parton Combine $\int \tilde{r}r_{-1}d\tilde{\Phi}_{n+2}^{-1}$ with rv and define: $rv^{(s)} = rv + \int \tilde{rr}_{-1} d\Phi_2^{-1}$ which is now finite for $\epsilon \to 0$ as in a NLO calculation We can define a subtraction for $rv^{(s)}$ as before In summary we end up with $d\sigma = \int \left(rrd\Phi_{n+2} - \tilde{r}r_{-2}d\tilde{\Phi}_{n+2}^{-2} - \tilde{r}r_{-1}d\tilde{\Phi}_{n+2}^{-1} \right)$ + $\int \left(rv^{(s)} d\Phi_{n+1} - \tilde{rv}^{(s)} d\tilde{\Phi}_{n+1} \right)$ + $\int \tilde{rr}_{-2} d\tilde{\Phi}_{n+2}^{-2} + \int \tilde{rv}^{(s)} d\tilde{\Phi}_{n+1} + \int vv d\Phi_n$,

where the phase spaces have to be properly defined and the appropriate measurement functions are understood

An application: the $C_F T_R$ contribution of $e^+e^- \rightarrow 2$ jets

This is certainly a simple example but we find in it many of the complications of a NNLO calculation:



rr : CC, SS, CSS, CCSS, C singular configurations

rv: singularities explicit from loop and implicit when the gluon becomes collinear to q or \bar{q}

The three-parton kernel $K_{q'_1\bar{q}'_2q_3}^{(3)}$

According to the \mathcal{E} -prescription the counterterm \tilde{rr}_{-2} is

$$\widetilde{rr}_{-2} = rr(CC) + rr(SS) - rr(CC \oplus SS)$$
$$-rr(C \oplus C) - rr(C \oplus SS) + rr(C \oplus C \oplus SS)$$

and is controlled by a kernel which is in general a matrix in colour $\widetilde{rr}_{a} = \langle \mathcal{M}_{a}^{(0)} | \mathbf{K}_{a'\bar{a}'a}^{(3)} | \mathcal{M}_{q...a_{n+2}}^{(0)} \rangle$ space

$$TT_{-2} = \langle \mathcal{M}_{q...a_{n+2}} | \mathbf{\Lambda}_{q_1' \bar{q}_2' q_3} | \mathcal{M}_{q...a_{n+2}} | \mathbf{\Lambda}_{q...a_{n+2}} | \mathbf{\Lambda}_{q_1' \bar{q}_2' q_3} | \mathcal{M}_{q...a_{n+2}} | \mathbf{\Lambda}_{q...a_{n+2}} | \mathbf{\Lambda}_{q_1' \bar{q}_2' q_3} | \mathbf{\Lambda}_{q...a_{n+2}} | \mathbf{\Lambda}_{q...$$

However it turns out that

 $rr(SS) = rr(C \oplus SS)$ and $rr(CC + SS) = rr(C \oplus C \oplus SS)$

 $\boldsymbol{K}_{q_1'\bar{q}_2'q_3}^{(3)} = \frac{(8\pi\alpha_s\mu^{2\epsilon})^2}{s_{123}^2} \left(K_{q_1'\bar{q}_2'q_3}^{CC} - K_{q_1'\bar{q}_2'q_3}^{C\oplus C} \right)$

where

$$K_{q_1'\bar{q}_2'q_3}^{CC} = \frac{1}{2} C_F T_R \frac{s_{123}}{s_{12}} \left[-\frac{t_{12,3}^2}{s_{12}s_{123}} + \frac{4z_3 + (z_1 - z_2)^2}{z_1 + z_2} + (1 - 2\epsilon) \left(z_1 + z_2 - \frac{s_{12}}{s_{123}} \right) \right]$$

is the function controlling the collinear limit of three partons and

$$K_{q_{1}'\bar{q}_{2}'q_{3}}^{C\oplus C} = \frac{1}{2} C_{F} T_{R} \frac{s_{123}}{s_{12}} \left[-\frac{t_{12,3}^{(S)^{2}}}{s_{12}s_{123}} + \frac{4z_{3} + (z_{1} - z_{2})^{2}}{z_{1} + z_{2}} + (1 - 2\epsilon)(z_{1} + z_{2}) \right]$$

is its form in the limit $s_{12} \ll s_{123}$

S. Catani, MG (1998)

$$t_{ij,k} \equiv 2 \ \frac{z_i s_{jk} - z_j s_{ik}}{z_i + z_j} + \frac{z_i - z_j}{z_i + z_j} s_{ij} \qquad \qquad t_{ij,k}^{(S)} \equiv 2 \ \frac{z_i s_{jk} - z_j s_{ik}}{z_i + z_j}$$

The kernel needed for \tilde{rr}_{-1} is just: $\langle \mu | \mathbf{K}_{q_1' \bar{q}_2'}^{(2)} | \nu \rangle = \frac{8\pi \alpha_s \mu^{2\epsilon}}{s_{12}} \hat{P}_{q\bar{q}}^{\mu\nu}$

where:
$$\hat{P}_{q\bar{q}}^{\mu\nu}(z,k_T) = T_R \left[-g^{\mu\nu} + 4z(1-z) \frac{k_T^{\mu}k_T^{\nu}}{k_T^2} \right]$$

Phase space

Express angles in terms of invariants using Gram determinants

$$\Delta_n(p_1, \dots, p_n) \equiv \begin{vmatrix} p_1^2 & p_1 \cdot p_2 & \dots & p_1 \cdot p_n \\ p_2 \cdot p_1 & p_2^2 & \dots & p_2 \cdot p_n \\ \dots & \dots & \dots & \dots \\ p_n \cdot p_1 & p_n \cdot p_2 & \dots & p_n^2 \end{vmatrix}$$

E. Byckling, K. Kajante (1972)

Introduce arbitrary lightlike vector n with $z_i = \frac{k_i \cdot n}{q \cdot n}$

$$d\Phi_2(q;k_1,k_2) = \frac{\Omega^{(d-2)}}{4(2\pi)^{d-2}} \left(-\frac{\Delta_3(n,k_1,k_2)}{\Delta_2(n,q)} \right)^{\frac{d-4}{2}} \times \delta\left(1-z_1-z_2\right) \delta\left(q^2-s_{12}-k_1^2-k_2^2\right) dz_1 dz_2 ds_{12}$$

with
$$-\frac{\Delta_3(n,k_1,k_2)}{\Delta_2(n,q)} = z_1 z_2 q^2 - z_1 k_2^2 - z_2 k_1^2$$

In the case of three massless partons we have:

$$d\Phi_3(q;k_1,k_2,k_3) = \frac{\Omega^{(d-2)}\Omega^{(d-3)}}{32(2\pi)^{2d-3}} \left(\frac{\Delta_4(n,k_1,k_2,k_3)}{\Delta_2(n,q)}\right)^{\frac{d-5}{2}}$$

 $\times \delta \left(1 - z_1 - z_2 - z_3 \right) \delta \left(q^2 - s_{12} - s_{13} - s_{23} \right) dz_1 dz_2 dz_3 ds_{12} ds_{13} ds_{23}$

with: $\frac{\Delta_4(n,k_1,k_2,k_3)}{\Delta_2(n,q)} = \frac{1}{4} \left(2z_1 z_2 s_{13} s_{23} + 2z_1 z_3 s_{12} s_{23} + 2z_2 z_3 s_{12} s_{13} - z_1^2 s_{23}^2 - z_2^2 s_{13}^2 - z_3^2 s_{12}^2 \right)$

This form is fully symmetric but suppose we want to study a strongly ordered double collinear limit

 k_3 k_1 k_2

The phase space can be written exactly in a 2 x 2 form

Defining the aximuthal variable x through

$$s_{13} = (s_{123} - s_{12})(1 - \zeta_2) + \frac{\sqrt{s_{12}}}{1 - z_3}\xi \qquad s_{23} = (s_{123} - s_{12})\zeta_2 - \frac{\sqrt{s_{12}}}{1 - z_3}\xi$$
$$\xi = 2\sqrt{z_2(2(1 - \zeta_2)(s_{122}(1 - z_3) - s_{12}))}x + z_2(2\zeta_2 - 1)\sqrt{s_{12}}$$

And the momentum fraction of the $12 \rightarrow 1+2$ splitting $\zeta_2 = z_2/(z_1+z_2)$

The three-parton phase space can be rewritten as

$$d\Phi_{3} = \frac{\Omega^{(d-2)}\Omega^{(d-3)}}{16(2\pi)^{2d-3}} (s_{123})^{\frac{d-4}{2}} (s_{12})^{\frac{d-4}{2}} \left(1 - \frac{s_{12}}{s_{123}(1-z_{3})}\right)^{\frac{d-4}{2}} (s_{12}-z_{3})^{\frac{d-4}{2}} (s_{12}-z_{3})^{\frac$$

We now use these results to properly define the phase spaces needed to implement our master subtraction formula

Exploit phase space factorization

$$d\Phi_{n+2} = \frac{ds_{123}}{2\pi} d\Phi_n(123) d\Phi_3(1,2,3)$$

$$d\tilde{\Phi}_{n+2}^{-2} = \frac{ds_{123}}{2\pi} d\Phi_n(\widetilde{123}) d\Phi_3(1,2,3)$$
on shell

We could define analogously: $d\widetilde{\Phi}_{n+2}^{-1} = \frac{ds_{12}}{2\pi} d\Phi_n(\widetilde{12}) d\Phi_2(1,2)$

But this definition would induce a mismatch with $d\Phi_3(1,2,3)$

we define:
$$d\widetilde{\Phi}_{n+2}^{-1} = d\Phi_n(\widetilde{12}) \frac{ds_{12}}{2\pi} \left(1 - \frac{s_{12}}{s_{12}^{\max}}\right)^{-\epsilon} d\Phi_2(1,2)$$

The integral of the three-parton kernel is:

$$\int \frac{ds_{123}}{2\pi} K_{q_1' \bar{q}_2' q_3}^{(3)} d\Phi_3(1,2,3) = \left(\frac{\alpha_s}{2\pi}\right)^2 C_F T_R \left(\frac{s_{123}^{\max}}{\mu^2}\right)^{-2\epsilon} \frac{1}{6\epsilon} \left(1 + \frac{31}{6}\epsilon\right) + \mathcal{O}(\epsilon)$$

where s_{123}^{\max} is an arbitrary parameter
Combining the integral of \tilde{rr}_{-1} with rv we find

$$rv^{(s)}d\Phi_3 \equiv rv|_{T_R}d\Phi_3 + \sum_f \int \tilde{rr}_{-1}d\tilde{\Phi}_4^{-1} = \frac{\alpha_s}{2\pi} \frac{T_R n_F}{\epsilon} \left| \mathcal{M}_{gq\bar{q}}^{(0)} \right|^2 d\Phi_3$$

$$\left\{ \frac{2}{3} - \left(\frac{\mu^2}{s_{12}^{\max}}\right)^{\epsilon} \frac{e^{\epsilon\gamma}}{\Gamma(1-\epsilon)} \left[\frac{2}{3} + \frac{10}{9}\epsilon + \left(\frac{56}{27} - \frac{\pi^2}{9}\right)\epsilon^2 + \left(\frac{328}{81} - \frac{5}{27}\pi^2 - \frac{4}{3}\zeta_3\right)\epsilon^3 \right] \left(1 - \frac{\pi^2}{6}\epsilon^2 - 2\epsilon^3\zeta_3\right) \right\} + \mathcal{O}(\epsilon^3)$$

which is finite as it must be as $\epsilon \to 0$ but still has to be integrated over the phase space of the gluon

The singularity in $rv^{(s)}$ can be subtracted using the NLO kernel

$$\boldsymbol{K}_{qg}^{(2)} = -\frac{8\pi\mu^{2\epsilon}\alpha_s}{s_{qg}}\sum_{k\neq q} \mathcal{V}_{qg,k}^{(2)} \boldsymbol{T}_q \cdot \boldsymbol{T}_k$$

with

$$\mathcal{V}_{qg,k}^{(2)} = \frac{2p_q \cdot p_k}{(p_q + p_k) \cdot p_g} + (1 - z)(1 - \epsilon)$$



The corresponding integrals over $d\Phi_2(q,g)$ can be performed to the required accuracy and depend on the upper limit of s_{qg}

We set: $s_{qg} \le y_{\max} Q^2$ and also $s_{123}^{\max} = y_{\max} Q^2$

In general the construction of the counterterm $\tilde{rv}^{(s)}$ will require the knowledge of the soft and collinear limits of one-loop amplitudes

Z.Bern, V. Del Duca, W. Kilgore, C. Schmidt (1999), D. Kosower, P. Uwer (1999), S. Catani, MG (2000)

Results

We combine the results with the well known double virtual contribution T. Matsuura, S.C. Van der Marck, W.L. van Neerven (1989)

The poles correctly cancel out leaving a finite result We implemented the subtracted contributions in a numerical code We first checked that the total rate is correctly recovered

 $R = \sigma(e^+e^- \rightarrow \text{hadrons}) / \sigma(e^+e^- \rightarrow \mu^+\mu^-)$

 $R = \sum_{q} e_{q}^{2} \left\{ 1 + \left(\frac{\alpha_{s}}{2\pi}\right) \frac{3}{2} C_{F} + \left(\frac{\alpha_{s}}{2\pi}\right)^{2} \left[-\frac{3}{8} C_{F}^{2} + C_{F} C_{A} \left(\frac{123}{8} - 11\zeta_{3}\right) + C_{F} T_{R} n_{F} \left(-\frac{11}{2} + 4\zeta_{3}\right) \right] + \mathcal{O}(\alpha_{s}^{3}) \right\}$ -0.69177 K.G.Chetyrkin, A.L.Kataev, F.V. Tkachov (1979), M.Dine, J.R.Sapirstein (1979), W.Celmaster, R.J.Gonsalves (1980)

y_{\max}	4-parton	3-parton	analytic	total	pull
0.2	-0.692 ± 0.002	1.4241 ± 0.0004	-1.4236	-0.692 ± 0.002	0.11
0.4	-0.229 ± 0.004	9.8001 ± 0.0003	-10.2610	-0.690 ± 0.004	0.44
0.6	0.074 ± 0.02	12.3440 ± 0.0003	-13.0753	-0.657 ± 0.02	1.74
0.8	0.235 ± 0.005	13.3759 ± 0.0003	-14.2989	-0.688 ± 0.005	0.75
1.0	0.383 ± 0.004	13.8284 ± 0.0003	-14.9005	-0.689 ± 0.004	0.69

The various terms in the subtraction formula separately depend on the arbitrary parameter y_{max} but their sum is independent on it and in good agreement with the known analytic result

We also implemented a measurement function corresponding to the JADE algorithm with $y_{cut} = 0.1$

We find for the term proportional to n_F

 $1.7998 \pm 0.0016 \qquad y_{\rm max} = 0.6$

 1.7992 ± 0.0015 $y_{\rm max} = 0.4$

In nice agreement with results of Anastasiou et al.

Conclusions

- We have proposed a framework to extend the subtraction method to NNLO
- The method combines some of the aspects of the dipole and FKS approaches:
 - Explicit Lorentz invariance
 - No exact phase-space factorization
 - IR singularities are combined in universal kernels factorizing the same reduced matrix element
- We have shown that it works in a simple case: the calculation of the $C_F T_R$ contribution to $e^+e^- \rightarrow 2$ jets
- Although very simple, this example shows some of the complications of more involved processes

- To my knowledge, it is the first application where process independent subtraction counterterms have been constructed and integrated over the corresponding phase spaces to achieve the explicit cancellation of IR singularities
- A lot of work remains to be done before our proposal can give a complete subtraction formalism: further tests are in progress in more complicated processes