A Numerical Implementation of the LASS Subtraction Scheme

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in collaboration with

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Motivation

Motivation

LASS : Local Analytic Sector Subtraction scheme arXiv:2212.11190, 2010.14493, 1806.09570

- Massless partons
- For final state radiation (i.e. $e^+ e^-$ collisions)

Subtraction and slicing methods at NNLO QCD:

- Several methods for final/initial state both for massless and massive partons
- Several processes already calculated with several different methods
- Methods already started to be extended to N^3LO

What is the point creating yet another?

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Motivation

Motto:

Zoltán Nagy: "We solve a math problem"

- Can have multiple solutions
- Can reach the same answer on a multitude of paths
- Physics and math is also about elegance
- Life will not stop at NNLO:
  - Can an $N^{n}LO$ scheme extended to $N^{n+1}LO$?
  - Can a scheme for $e^{+}e^{-}$ extended to pp collisions?
  - At what cost?

What about carbon-friendly computing?

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LASS, a practitioner's intro

LASS, a practitioner's intro

Key ingredients of the subtraction scheme:

- Grouping of the subtraction terms
- Phase space mappings used to get underlying Born and real configurations
- Phase space partitioning

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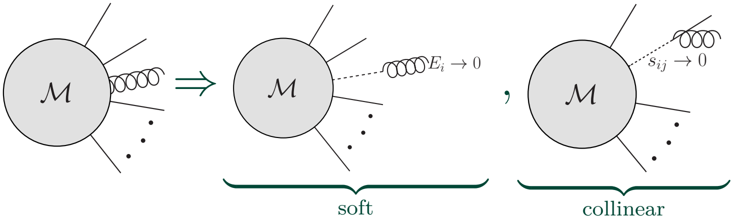
LASS, a practitioner's intro – grouping of terms

Kinematic singularity structure is easy at NLO (up to one unresolved emission):



$$d\sigma^{R} : \left|\mathcal{M}^{R}\right|^{2} - K^{(1)}$$

$$K^{(1)} = \sum_{i} \mathcal{S}_{i} + \sum_{i,j<i} \left(\mathcal{C}_{ij} - \mathcal{S}_{i}\mathcal{C}_{ij} - \mathcal{S}_{j}\mathcal{C}_{ij} \right)$$

$\Rightarrow$ Removal of overlapping results in proliferation of terms!

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LASS, a practitioner's intro – grouping of terms

$\Rightarrow$ Removal of overlapping results in proliferation of terms!

$$K^{(1)} = \sum_{i} \mathcal{S}_i + \sum_{i,j<i} \underbrace{\left(\mathcal{C}_{ij} - \mathcal{S}_i\mathcal{C}_{ij} - \mathcal{S}_j\mathcal{C}_{ij}\right)}_{\mathcal{C}_{ij}^{\mathrm{hc}}} = \sum_{i} \mathcal{S}_i + \sum_{i,j<i} \mathcal{C}_{ij}^{\mathrm{hc}}$$

Simple replacement of AP kernels with their hard-collinear variants:

$$\langle P_{q\bar{q}} \rangle = T_R \left[1 - \frac{2x_q x_{\bar{q}}}{1-\epsilon}\right], \langle P_{qg} \rangle = C_F \left[2\frac{x_q}{x_g} + (1-\epsilon)x_g\right], \langle P_{gg} \rangle = 2C_A \left[\frac{x_1}{x_2} + \frac{x_2}{x_1} + x_1 x_2\right],$$

$$\langle P_{q\bar{q}} \rangle = \left\langle P_{q\bar{q}}^{\mathrm{hc}} \right\rangle, \qquad \left\langle P_{qg}^{\mathrm{hc}} \right\rangle = C_F(1-\epsilon)x_g, \qquad \left\langle P_{gg}^{\mathrm{hc}} \right\rangle = 2C_A x_1 x_2$$

$$\mathcal{C}_{ij} \to \mathcal{C}_{ij}^{\mathrm{hc}} \quad : \quad P_{ij(r)}^{\mu\nu} \to P_{ij(r)}^{\mu\nu,\mathrm{hc}} \quad , \quad \mathcal{S}_i\mathcal{C}_{ij} \to \emptyset$$

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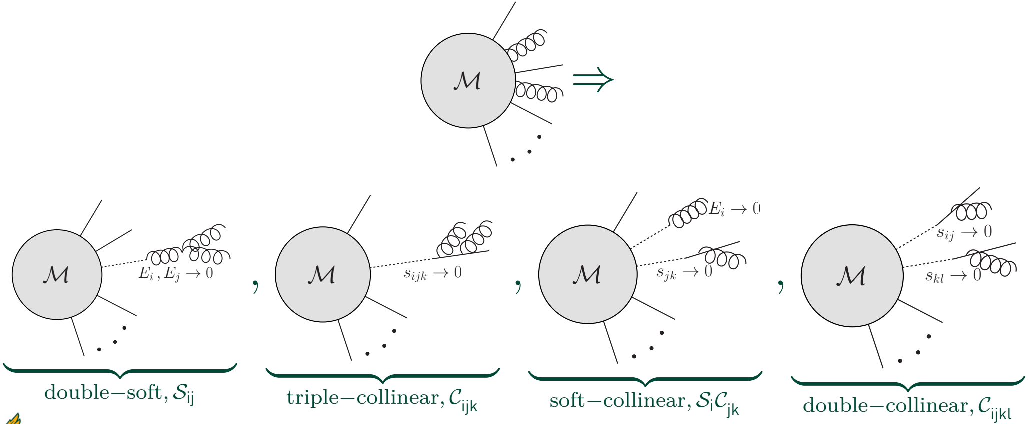
LASS, a practitioner's intro – grouping of terms

At NNLO we have many more kinematic singularities:



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LASS, a practitioner's intro – grouping of terms

With a much richer overlap between various terms:

$$K^{(2)} = \sum_{i,j<i} \mathcal{S}_{ij} + \sum_{j,k<j} \sum_{i\neq j,k} \left(\mathcal{S}_i \mathcal{C}_{jk} - \mathcal{S}_i \mathcal{C}_{jk} \mathcal{S}_{ij} - \mathcal{S}_i \mathcal{C}_{jk} \mathcal{S}_{ik} \right) +$$

$$+ \sum_{i,j<i,k<j} \left(\mathcal{C}_{ijk} - \mathcal{C}_{ijk}\mathcal{S}_{ij} - \mathcal{C}_{ijk}\mathcal{S}_{ik} - \mathcal{C}_{ijk}\mathcal{S}_{jk} - \mathcal{C}_{ijk}\mathcal{S}_i\mathcal{C}_{jk} - \mathcal{C}_{ijk}\mathcal{S}_j\mathcal{C}_{ik} - \mathcal{C}_{ijk}\mathcal{S}_k\mathcal{C}_{ij} + \right.$$

$$\left. + \mathcal{C}_{ijk}\mathcal{S}_{ij}\mathcal{S}_i\mathcal{C}_{jk} + \mathcal{C}_{ijk}\mathcal{S}_{ij}\mathcal{S}_j\mathcal{C}_{ik} + \mathcal{C}_{ijk}\mathcal{S}_{ik}\mathcal{S}_i\mathcal{C}_{jk} + \mathcal{C}_{ijk}\mathcal{S}_{ik}\mathcal{S}_k\mathcal{C}_{ij} + \mathcal{C}_{ijk}\mathcal{S}_{jk}\mathcal{S}_j\mathcal{C}_{ik} + \mathcal{C}_{ijk}\mathcal{S}_{jk}\mathcal{S}_k\mathcal{C}_{ij} \right) +$$

$$+ \sum_{i,j<i} \sum_{\substack{k,l<k \\ k<i,j\neq l}} \left(\mathcal{C}_{ijkl} - \mathcal{C}_{ijkl}\mathcal{S}_i\mathcal{C}_{kl} - \mathcal{C}_{ijkl}\mathcal{S}_j\mathcal{C}_{kl} - \mathcal{C}_{ijkl}\mathcal{S}_k\mathcal{C}_{ij} - \mathcal{C}_{ijkl}\mathcal{S}_l\mathcal{C}_{ij} + \right.$$

$$\left. + \mathcal{C}_{ijkl}\mathcal{S}_{ik} + \mathcal{C}_{ijkl}\mathcal{S}_{il} + \mathcal{C}_{ijkl}\mathcal{S}_{jk} + \mathcal{C}_{ijkl}\mathcal{S}_{jl} \right)$$

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LASS, a practitioner's intro – grouping of terms

Subterms can be grouped into hard-collinear groups:

$$K^{(2)} = \sum_{i,j<i} \mathcal{S}_{ij} + \sum_{j,k<j} \sum_{i\neq j,k} \underbrace{\left(\mathcal{S}_i\mathcal{C}_{jk} - \mathcal{S}_i\mathcal{C}_{jk}\mathcal{S}_{ij} - \mathcal{S}_i\mathcal{C}_{jk}\mathcal{S}_{ik}\right)}_{\mathcal{S}_i\mathcal{C}^{\mathrm{hc}}_{jk}} +$$

$$+ \sum_{\substack{i,j<i\\k<j}} \Big(\underbrace{\mathcal{C}_{ijk} - \mathcal{C}_{ijk}\mathcal{S}_{ij} - \mathcal{C}_{ijk}\mathcal{S}_{ik} - \mathcal{C}_{ijk}\mathcal{S}_{jk}}_{\mathcal{C}^{\mathrm{hc}}_{ijk}} - \underbrace{\mathcal{C}_{ijk}\mathcal{S}_i\mathcal{C}_{jk} + \mathcal{C}_{ijk}\mathcal{S}_{ij}\mathcal{S}_i\mathcal{C}_{jk} + \mathcal{C}_{ijk}\mathcal{S}_{ik}\mathcal{S}_i\mathcal{C}_{jk}}_{\mathcal{S}_i\mathcal{C}^{\mathrm{hc}}_{jk}\mathcal{C}_{ijk}} - \ldots\Big) +$$

$$+ \sum_{i,j<i} \sum_{\substack{k,l<k\\k<i\\j\neq l}} \underbrace{\left(\mathcal{C}_{ijkl} - \mathcal{C}_{ijkl}\mathcal{S}_i\mathcal{C}_{kl} - \cdots - \mathcal{C}_{ijkl}\mathcal{S}_l\mathcal{C}_{ij} + \mathcal{C}_{ijkl}\mathcal{S}_{ik} + \cdots + \mathcal{C}_{ijkl}\mathcal{S}_{jl}\right)}_{\mathcal{C}^{\mathrm{hc}}_{ijkl}}$$

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LASS, a practitioner's intro – grouping of terms

Using the hard-collinear formalism the structure becomes very compact:

$$\begin{aligned} K^{(2)} = &\sum_{i,j<i} \mathcal{S}_{ij} + \\ &+ \sum_{j,k<j} \sum_{i\neq j,k} \mathcal{S}_i \mathcal{C}^{\mathrm{hc}}_{jk} + \\ &+ \sum_{\substack{i,j<i \\ k<j}} \left(\mathcal{C}^{\mathrm{hc}}_{ijk} - \mathcal{S}_i \mathcal{C}^{\mathrm{hc}}_{jk} \mathcal{C}_{ijk} - \mathcal{S}_j \mathcal{C}^{\mathrm{hc}}_{ik} \mathcal{C}_{ijk} - \mathcal{S}_k \mathcal{C}^{\mathrm{hc}}_{ij} \mathcal{C}_{ijk} \right) + \\ &+ \sum_{i,j<i} \sum_{\substack{k,l<k \\ k<i \\ j\neq l}} \mathcal{C}^{\mathrm{hc}}_{ijkl} \end{aligned}$$

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LASS, a practitioner's intro – mappings

- The method heavily relies on single and iterated Catani-Seymour mappings
  - $K^{(1)}$ in the $n+2$ parton cont.:

$$\{k\}_{(n+2)} \xrightarrow{i,j,r\to\bar{j},\bar{r}} \{\bar{k}\}^{(ijr)}_{(n+1)}\,, \qquad \{k\}_{(n+2)} \xrightarrow{i,c,d\to\bar{c},\bar{d}} \{\bar{k}\}^{(icd)}_{(n+1)}$$

  - Also in $K^{(2)}$ and in $K^{(12)}$ in all possible ways:

$$\{k\}_{(n+2)} \xrightarrow{i,c,d\to\bar{c},\bar{d}} \{\bar{k}\}^{(icd)}_{(n+1)} \xrightarrow{j,e,f\to\tilde{e},\tilde{f}} \left\{\tilde{k}\right\}^{(icd,jef)}_{(n)}\,,$$

$$\vdots$$

$$\{k\}_{(n+2)} \xrightarrow{k,r,j\to\bar{r},\bar{j}} \{\bar{k}\}^{(krj)}_{(n+1)} \xrightarrow{i,\bar{r},\bar{j}\to\tilde{r},\tilde{j}} \left\{\tilde{k}\right\}^{(krj,i\bar{r}\bar{j})}_{(n)}$$

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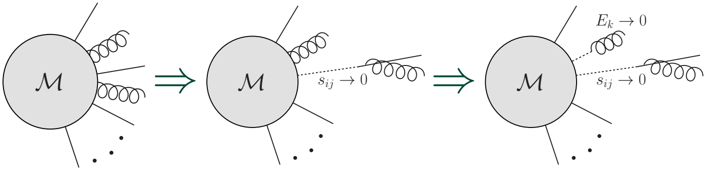
LASS, a practitioner's intro – phase space partitioning

- $\mathsf{K}^{(1)}$ can also diverge in doubly unresolved limits:



- $\mathsf{K}^{(2)}$ can also diverge in singly unresolved limits!

$\Rightarrow$ These double-countings (spurious singularities) should also be removed:

$$\left|\mathcal{M}^{\mathrm{RR}}\right|^2 - \mathsf{K}^{(1)} - \mathsf{K}^{(2)} - \mathsf{K}^{(12)}$$

- Careful synchronization is needed in mappings and parametrizations!

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LASS, a practitioner's intro – phase space partitioning

- Careful synchronization is needed in mappings and parametrizations!

$\Rightarrow$ Introduction of sector functions can simplify the procedure:

$$1 = \sum_{i<j<k} \mathcal{Z}_{ijk} + \sum_{i<j} \sum_{\substack{k<l \\ i<k\,,j\neq l}} \mathcal{Z}_{ijkl}$$

- Certain sectors only allow certain limits/subterms (and overlaps):

$$\mathcal{Z}_{ijk} \left\{ \begin{array}{c} \mathcal{S}_i\,,\mathcal{S}_j\,,\mathcal{S}_k\,,\mathcal{C}_{ij}\,,\mathcal{C}_{ik}\,,\mathcal{C}_{jk}\,, \\ \mathcal{S}_{ij}\,,\mathcal{S}_{ik}\,,\mathcal{S}_{jk}\,, \\ \mathcal{S}_i\mathcal{C}_{jk}\,,\mathcal{S}_j\mathcal{C}_{ik}\,,\mathcal{S}_k\mathcal{C}_{ij}\,, \\ \mathcal{C}_{ijk} \end{array} \right. \qquad \mathcal{Z}_{ijkl} \left\{ \begin{array}{c} \mathcal{S}_i\,,\mathcal{S}_j\,,\mathcal{S}_k\,,\mathcal{S}_l\,,\mathcal{C}_{ij}\,,\mathcal{C}_{kl}\,, \\ \mathcal{S}_{ik}\,,\mathcal{S}_{il}\,,\mathcal{S}_{jk}\,,\mathcal{S}_{jl}\,, \\ \mathcal{S}_i\mathcal{C}_{kl}\,,\mathcal{S}_j\mathcal{C}_{kl}\,,\mathcal{S}_k\mathcal{C}_{ij}\,,\mathcal{S}_l\mathcal{C}_{ij}\,, \\ \mathcal{C}_{ijkl} \end{array} \right.$$

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LASS, a practitioner's intro – phase space partitioning

- Subterms have operator-like effect on sector functions
- To ensure analytic integrability sum-rules should be fullfiled:

$$\sum_{k\neq i,j}\Big[\mathcal{Z}_{ijk} + \sum_{l\neq i,j,k}\mathcal{Z}_{ikjl}\Big]\mathcal{S}_{ij} = \mathcal{S}_{ij}\,, \quad \Big[\mathcal{Z}_{ikl} + \sum_{j\neq i,k,l}\mathcal{Z}_{ijkl}\Big]\mathcal{S}_{i}\mathcal{C}_{kl} = \mathcal{S}_{i}\mathcal{C}_{kl}\,,$$

$$\mathcal{Z}_{ijk}\mathcal{C}_{ijk} = \mathcal{C}_{ijk}\,, \quad \mathcal{Z}_{ijkl}\mathcal{C}_{ijkl} = \mathcal{C}_{ijkl}$$

- Note: this is not the case in $K^{(1)}$ and $K^{(12)}$!

$$\sum_{j<k}\mathcal{Z}_{ijk}\mathcal{S}_{i} = \mathcal{S}_{i}\,, \quad \sum_{k}\mathcal{Z}_{ijk}\mathcal{C}_{ij} = \mathcal{C}_{ij}\overline{\mathcal{Z}}_{jk}\left(\{\overline{k}\}^{(ijr)}\right)\,,$$

$$\ldots$$

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A way to check subtractions

A way to check subtractions

- Numerical checks are essential for validating both individual subterms and whole contributions:
  - Individual subterms:
    - Proper usage of mappings
    - Parameters are calculated correctly
    - Normalizations are correct
  - Full ensemble:
    - Parametrizations are synchronized (where need be)
    - Spurious cancellations are happening:

$$\mathsf{K}^{(1)} \text{ limits}: \quad \mathsf{K}^{(2)} \leftrightarrow \mathsf{K}^{(12)}\,, \quad \mathsf{K}^{(2)} \text{ limits}: \quad \mathsf{K}^{(1)} \leftrightarrow \mathsf{K}^{(12)}$$

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A way to check subtractions

Idea: check everything numerically, but with arbitrary precision!

- `Fortran90` and `MPFUN20` by David Bailey to have arbitrary precision floating numbers
- 50-60 digits suffice for most checks (only for checks, MC in double precision)
- Starting with an $\mathsf{n}+2$ or $\mathsf{n}+1$ parton PS point we create a sequence of PS points bringing partons to specific limits
- Ratio is monitored between SME and subterm/full contribution:

$$\mathsf{n}+2\,\text{parton line}: \quad \lim_{5||6||7} \frac{\left|\mathcal{M}^{\mathrm{RR}}\right|^2}{\mathcal{C}_{765}}, \quad \lim_{5\,,6\to 0} \frac{\mathcal{S}_{65}\mathcal{C}_{765}}{\mathcal{C}_{765}}, \quad \frac{\left|\mathcal{M}^{\mathrm{RR}}\right|^2}{\mathsf{K}^{(1)}+\mathsf{K}^{(2)}+\mathsf{K}^{(12)}}$$

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A way to check subtractions – example

- LASS currently is for final state radiation only (e^+e^- collisions)
- Three-jet production is the obvious choice
- Most complicated subprocess: $e^+e^- \to q\bar{q}\,ggg$
  - 187 subtraction terms
  - 49 singular regions

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A way to check subtractions – example

Ratio sequence for a single soft subtraction term and the RR SME:

$$\lim_{5\to 0} \frac{\left|\mathcal{M}^{\mathrm{RR}}\right|^2}{\mathcal{S}_5}$$

Ratio sequence for the complete $\mathsf{K}^{(1)} + \mathsf{K}^{(2)} + \mathsf{K}^{(12)}$ and the RR SME in a collinear limit:

$$\lim_{7||3} \frac{\left|\mathcal{M}^{\mathrm{RR}}\right|^2}{\mathsf{K}^{(1)} + \mathsf{K}^{(2)} + \mathsf{K}^{(12)}}$$

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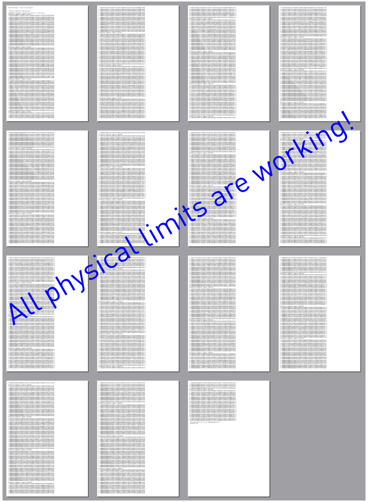
A way to check subtractions – example

```
Checking subtractions for ep em > d db g g g
Checking individual subterm (1/187)
1.3615262894238763826759820725791757465583666344146e1
1.0694493566690845438842431546992987055507713973236e0
1.0007162821758278182424090928223132563018751174295e0
1.0000071987341108237419042328666792441638763318880e0
1.0000000720247434870412374459056904352354450789094e0
1.000000007202849869842647183822196539254192619824e0
```

```
Checking singular region (12/49)
9.6594481743241900295619875419238279005187022510109e-1
1.0058615538802959144867884196860137973711485348134e0
9.9231059807099869356172685061099655988514093224880e-1
9.9583088426373405730413153367459343558862822235912e-1
9.9849562883100781816326951516801463419402897054026e-1
9.9950556967204941845739013900159932542190523615067e-1
9.9984177766130266861510092596371921504512639386555e-1
9.9994977880695929580926317624625089086796062180328e-1
9.9998409997765460232995100855871423405820977458026e-1
9.9999497010288688320443743161728335546792151263641e-1
9.9999840922001909000444820286260247019193046061875e-1
9.9999949693251516037014963280570874098054795389092e-1
9.9999984091422459144755648094664046742776493134045e-1
9.9999994969247378539788299063072534264967525981580e-1
9.9999998409134468611615545698564930910050993985655e-1
9.9999999496923960123804514553411354665657800543057e-1
9.9999999840913369088147655043925236337199932696573e-1
9.9999999949692388235079173196393701217379754206853e-1
9.9999999984091336131084641210578013734477707761172e-1
9.9999999994969238745734905001952273575863643999079e-1
```

A way to check subtractions – example



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A first glimpse at numerical integrations

A first glimpse at numerical integrations

- Checking subterms and complete subtractions are important but thorough numerical checks are also needed
  - A sequence does not cover whole phase space
  - A sequence is too artificial
  - What happens close to two-jet limit?
  - ...
- One possible check is the saturation of cross section:

$$\min_{i,j} y_{ij} = \min_{i,j} \frac{s_{ij}}{s} \geq y_{\min}$$

- Cut at edge of phase space, than decrease the cut
- In case all singularities are regularized contribution should stabilize (saturate)

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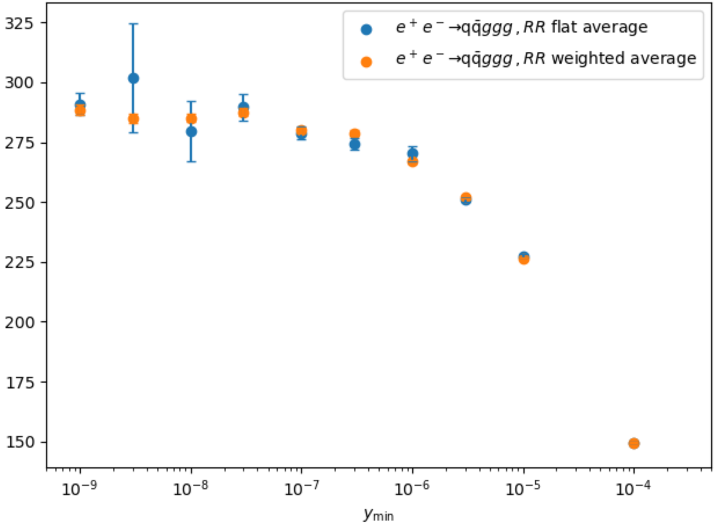
A first glimpse at numerical integrations

$n+2$ parton contribution (double-real):

Saturation plot for $e^+e^- \to q\bar{q}ggg$



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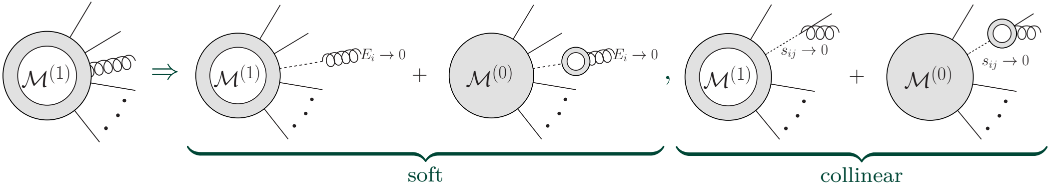
A first glimpse at numerical integrations

Contributions at NNLO:

$$\mathrm{d}\sigma = \mathrm{d}\sigma^{\mathrm{RR}} + \mathrm{d}\sigma^{\mathrm{RV}} + \mathrm{d}\sigma^{\mathrm{VV}}$$

- $\mathrm{d}\sigma^{\mathrm{RR}}$ is the most difficult, double-unresolved radiation
- $\mathrm{d}\sigma^{\mathrm{RV}}$ only has single-unresolved radiation but with one-loop amplitudes!



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A first glimpse at numerical integrations

- The $n+1$ parton contribution is NLO in nature
- Subterms are more complicated (and have more)
  - Kernels from one-loop factorization
  - Integrated subterms ($I^{(1)}$, from $n+2$ parton cont.) also diverge

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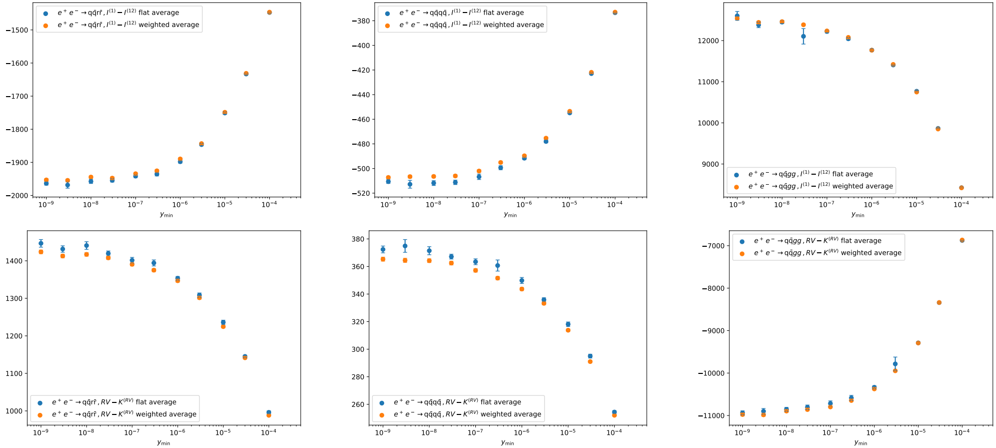
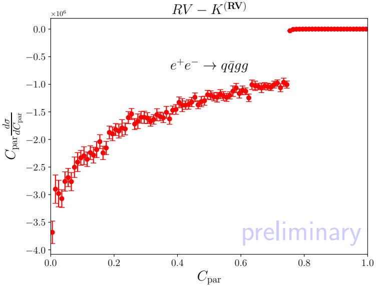
A first glimpse at numerical integrations

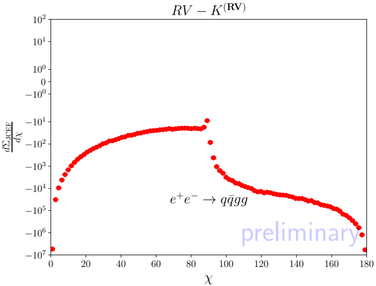


Saturation works for all contributions!

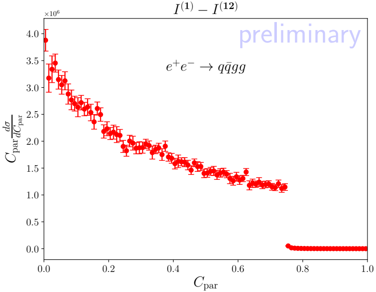
A first glimpse at numerical integrations

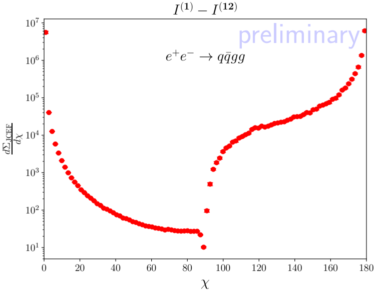
One-loop part:





Integrated subterms:





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Summary

Summary

- First numerical implementation of LASS (at NNLO) in the making
- Numerically proved: subterms regularize kinematic singularities
- Framework is created: generate subtractions automatically to arbitrary processes
- Applied to three-jet production in $e^+ e^-$
- Cross section contributions saturate in the $n+2$ and $n+1$ parton contributions
- Histograms can already be produced for the $n+1$ parton contribution

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Thank you for your attention!