GMVFN scheme implementations with Subtraction and Residual PDFs for processes at hadron colliders

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Motivations 1

> We developed the theory framework to extend ACOT-like GMVFN schemes to PP collisions.

This effort is connected to many areas of investigations in global CTEQ analyses:

- HQ effects
- NNLO->N^3LO transition
- DGLAP evolution @N^3LO
- Intrinsic HQ in the proton
- Constrain HQ PDFs

Motivations 2

- Modern Parton Distribution Function (PDF) analyses: extend on wide range of collision energies. Sensitive to mass effects, e.g., phase space suppression, large radiative corrections to collinear $Q\bar{Q}$ production. Magnitude comparable to NNLO and N^3LO corrections.
- Natural to evaluate all fitted cross sections in a factorization (GMVFN) scheme, which assumes that the number of (nearly) massless quark flavors varies with energy, and at the same time includes dependence on heavy-quark masses in relevant kinematical regions.



Main idea behind ACOT/S-ACOT/S-ACOT-MPS

Inclusive production of a HQ as an example



Subtraction and Residual PDFs

Subtraction and Residual PDFs consist of convolutions between PDFs and universal operator matrix elements (OMEs). They are process independent.

Subtraction and Residual PDFs are provided in the form of LHAPDF6 grids for phenomenology applications: <u>https://sacotmps.hepforge.org/</u>

The new CTEQ fitting code will be equipped by a module specifically designed for this task

GMVFN Theory framework

The differential cross section for $p_A p_B \rightarrow F + X$ where F contains at least one HQ, can be written

$$\frac{\mathrm{d}\sigma(A+B\to F+X)}{\mathrm{d}\mathcal{X}} = \sum_{i,j} \int_{x_A}^1 \mathrm{d}\xi_A \int_{x_B}^1 \mathrm{d}\xi_B f_{i/A}(\xi_A,\mu) f_{j/B}(\xi_B,\mu) \frac{\mathrm{d}\widehat{\sigma}(i+j\to F+X)}{\mathrm{d}\mathcal{X}}$$

After UV renormalization on $d\sigma/d\chi$, we identify its infrared-safe part $d\hat{\sigma}/d\chi$ by factoring out parton-level PDFs

$$\begin{split} G_{ij} &\equiv \frac{\mathrm{d}\sigma(i+j\to F+X)}{\mathrm{d}\mathcal{X}} \text{ after UV renormalization,} \\ H_{km} &\equiv \frac{\mathrm{d}\widehat{\sigma}(k+m\to F+X)}{\mathrm{d}\mathcal{X}}, \end{split}$$

 $\widehat{x}_i \equiv x_i / \xi_i$

Convolution product with two variables

$$[f \rhd H](x_A, x_B) \equiv \int_{x_A}^1 \frac{\mathrm{d}\xi_A}{\xi_A} f(\xi_A) H(\widehat{x}_A, x_B),$$
$$[H \lhd f](x_A, x_B) \equiv \int_{x_B}^1 \frac{\mathrm{d}\xi_B}{\xi_B} H(x_A, \widehat{x}_B) f(\xi_B).$$

$$G_{ij}(x_A, x_B) = \sum_{k,m} \int_{x_A}^1 \mathrm{d}\xi_A \int_{x_B}^1 \mathrm{d}\xi_B f_{k/i}(\xi_A) f_{m/j}(\xi_B) H_{km}(\widehat{x}_A, \widehat{x}_B)$$
$$\equiv [f_{k/i} \triangleright H_{km} \triangleleft f_{m/j}](x_A, x_B).$$

Convolution product with one variable

$$\int_{x}^{1} \frac{\mathrm{d}\xi}{\xi} f(\xi) g\left(\frac{x}{\xi}\right) = \left[f \rhd g\right](x) = \left[g \lhd f\right](x)$$

GMVFN Theory framework

The perturbative expansion of terms leads to

 $G_{i,b}(x_A, x_B) = G_{i,b}^{(0)}(x_A, x_B) + a_s G_{i,b}^{(1)}(x_A, x_B) + a_s^2 G_{i,b}^{(2)}(x_A, x_B) + \dots,$ $H_{i,a}(\widehat{x}_A, \widehat{x}_B) = H_{i,a}^{(0)}(\widehat{x}_A, \widehat{x}_B) + a_s H_{i,a}^{(1)}(\widehat{x}_A, \widehat{x}_B) + a_s^2 H_{i,a}^{(2)}(\widehat{x}_A, \widehat{x}_B) + \dots,$ $f_{a/b}(\xi) = \delta_{ab}\delta(1-\xi) + a_s A_{ab}^{(1)}(\xi) + a_s^2 A_{ab}^{(2)}(\xi) + a_s^3 A_{ab}^{(3)}(\xi) + \dots,$

Substituting these in the previous formula and solving for $H^{(k)}$ order by order in a_s

$$\begin{split} H_{ij}^{(0)}(x_A, x_B) &= G_{ij}^{(0)}(x_A, x_B), \\ H_{ij}^{(1)}(x_A, x_B) &= G_{ij}^{(1)}(x_A, x_B) - [A_{ki}^{(1)} \vartriangleright H_{kj}^{(0)}](x_A, x_B) - [H_{im}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B) \\ H_{ij}^{(2)}(x_A, x_B) &= G_{ij}^{(2)}(x_A, x_B) - [A_{ki}^{(1)} \vartriangleright H_{kj}^{(1)}](x_A, x_B) - [H_{im}^{(1)} \lhd A_{mj}^{(1)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \vartriangleright H_{kj}^{(0)}](x_A, x_B) - [H_{im}^{(0)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(1)} \bowtie H_{km}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B), \\ \\ H_{ij}^{(3)}(x_A, x_B) &= G_{ij}^{(3)}(x_A, x_B) - [A_{ki}^{(1)} \rhd H_{kj}^{(2)}](x_A, x_B) - [H_{im}^{(2)} \lhd A_{mj}^{(1)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{kj}^{(1)}](x_A, x_B) - [H_{im}^{(1)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(3)} \rhd H_{kj}^{(0)}](x_A, x_B) - [H_{im}^{(0)} \lhd A_{mj}^{(3)}](x_A, x_B) \\ &\quad - [A_{ki}^{(1)} \rhd H_{km}^{(1)} \lhd A_{mj}^{(1)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(1)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(1)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(1)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) \\ &\quad - [A_{ki}^{(2)} \rhd H_{km}^{(0)} \lhd A_{mj}^{(1)}](x_A, x_B) - [A_{ki}^{(1)} \rhd H_{km}^{(2)} \lhd A_{mj}^{(2)}](x_A, x_B) . \end{split}$$

$$\widehat{x} = x/\xi.$$

 $A^{(k)}_{ab} \ (k = 0, 1, 2, ...)$ OMEs
 $A^{(1)}_{hg}(\xi) = 2P^{(1)}_{hg}(\xi) \ln (\mu^2/m_h^2)$ For $g \to Q \overline{Q}$

Two forms for the OMEs

$$\begin{bmatrix}
A_{ij}^{(n)}(\xi,\mu^2) = \sum_{l=1}^n \left(\frac{1}{\epsilon}\right)^l P_{ij}^{(n,l)}(\xi) + \sum_{l=0}^n \ln^l \left(\frac{\mu^2}{\mu_{IR}^2}\right) P_{ij}^{\prime(n,l)}(\xi) \\
A_{Qj}^{(n)}\left(\xi,\frac{\mu^2}{m_Q^2}\right) = \sum_{l=0}^n \ln^l \left(\frac{\mu^2}{m_Q^2}\right) a_{Qj}^{(n,l)}(\xi)$$

Convention for the splitting functions $P_{ij}(x, a_s) = a_s P_{ij}^{(1)}(x) + a_s^2 P_{ij}^{(2)}(x) + a_s^3 P_{ij}^{(3)}(x) + \dots$ Let us apply this GMVN theory framework to a physical process of interest at the LHC: $pp \rightarrow Z + Q + X$ with Q = b-quark

Cancellation pattern at the lowest order ($pp \rightarrow Z+Q+X$)

(for $pp \rightarrow Z + Q + X$ this is $O(\alpha_s^2)$)

 $-\mathrm{d}\sigma_{\mathrm{sub}} = -a_s^2 \left[g \triangleright A_{Qg}^{(1)} \triangleright H_{Qg}^{(1)} \right] \triangleleft g + (\mathrm{exch.})$





Cancellation pattern at NLO ($pp \rightarrow Z+Q+X$)



Virtual diagrams are not shown here, but are included in the calculation.

$$\begin{aligned} H_{Qi}^{(2)}(x_A, x_B) &= \left. \widehat{G}_{Qi}^{(2)}(x_A, x_B) \right|_{\text{FE}} & \text{for } i = g, q, \bar{q}; \\ H_{ij}^{(3)}(x_A, x_B) &= \left. \widehat{G}_{ij}^{(3)}(x_A, x_B) \right|_{\text{FC}} - \left[A_{Qi}^{(1)} \triangleright H_{Qj}^{(2)} \right] (x_A, x_B) - \left[H_{iQ}^{(2)} \triangleleft A_{Qj}^{(1)} \right] (x_A, x_B) \\ &- \left[A_{Qi}^{(2)} \triangleright H_{Qj}^{(1)} \right] (x_A, x_B) - \left[H_{iQ}^{(1)} \triangleleft A_{Qj}^{(2)} \right] (x_A, x_B) & \text{for } i, j = g, q, \bar{q}; \\ H_{q\bar{q}}^{(3)}(x_A, x_B) &= \left. \widehat{G}_{q\bar{q}}^{(3)}(x_A, x_B) \right|_{\text{FC}}. \end{aligned}$$

$$a_{s}H^{(1)} + a_{s}^{2}H^{(2)} + a_{s}^{3}H^{(3)} = a_{s}H^{(1)}_{Qg}(x_{A}, x_{B}) + a_{s}^{2}H^{(2)}_{gg}(x_{A}, x_{B}) + a_{s}^{2}H^{(2)}_{q\bar{q}}(x_{A}, x_{B}) + a_{s}^{2}H^{(2)}_{Qg}(x_{A}, x_{B}) + a_{s}^{2}H^{(2)}_{Qq}(x_{A}, x_{B}) + a_{s}^{3}H^{(3)}_{gg}(x_{A}, x_{B}) + a_{s}^{3}H^{(3)}_{qg}(x_{A}, x_{B}) + a_{s}^{3}H^{(3)}_{q\bar{q}}(x_{A}, x_{B})$$

Subtraction PDFs

Once the $H_{ii}^{(k)}$ functions are determined, the hadronic cross section can be written as

$$d\sigma = \sum_{i,j} f_{i/A} \triangleright \left[a_s H^{(1)} + a_s^2 H^{(2)} + a_s^3 H^{(3)} + \dots \right]_{ij} \triangleleft f_{j/B}$$

Then, the various subtraction ("sub") terms can be collected as follows:

$$\begin{split} -\mathrm{d}\sigma_{\mathrm{sub}} &= -a_s^2 \left[g \rhd A_{Qg}^{(1)} \bowtie H_{Qg}^{(1)} \right] \lhd g - a_s^3 \left[\sum_{i,j=g,q,\bar{q}} f_i \rhd A_{Qi}^{(2)} \triangleright H_{Qj}^{(1)} \right] \lhd f_j \\ &- a_s^3 \left[\sum_{i,j=g,q,\bar{q}} f_i \rhd A_{Qi}^{(1)} \rhd H_{Qj}^{(2)} \right] \lhd f_j + (\mathrm{exch.}) \,, \end{split}$$

At this point we can define subtraction HQ PDFs $\tilde{f}_Q^{(1)} = a_s [A_{Qg}^{(1)} \lhd g], \tilde{f}_Q^{(2)} = a_s^2 \sum_{i=g,q,\bar{q}} [A_{Qi}^{(2)} \lhd f_i]$ $\tilde{f}_Q^{(\text{NLO})}(x,\mu) \equiv \tilde{f}_Q^{(1)} + \tilde{f}_Q^{(2)}$

$$(x,\mu) = J_Q + J_Q$$
$$-d\sigma_{\rm sub} = -a_s \,\tilde{f}_Q^{(\rm NLO)} \triangleright H_{Qg}^{(1)} \triangleleft g - a_s^2 \sum_{i=g,q,\bar{q}} \tilde{f}_Q^{(1)} \triangleright H_{Qi}^{(2)} \triangleleft f_i$$

Residual PDFs

$$\delta f_Q^{(1)} = f_Q - \tilde{f}_Q^{(1)}, \quad \delta f_Q^{(\text{NLO})} = f_Q - \tilde{f}_Q^{(\text{NLO})}$$

FE and SUB share the same matrix elements and can be combined in one piece in terms of residual PDFs!

$$d\sigma_{\rm FE} - d\sigma_{\rm sub} = a_s (f_Q - \tilde{f}_Q^{(\rm NLO)}) \triangleright H_{Qg}^{(1)} \triangleleft g$$

$$+ a_s^2 (f_Q - \tilde{f}_Q^{(1)}) \triangleright \left[H_{Qg}^{(2)} \triangleleft g + \sum_{i=q,\bar{q}} H_{Qq}^{(2)} \triangleleft f_i \right] + (\text{exch.})$$

$$= a_s \,\delta f_Q^{(\rm NLO)} \triangleright H_{Qg}^{(1)} \triangleleft g + a_s^2 \,\delta f_Q^{(1)} \triangleright \left[H_{Qg}^{(2)} \triangleleft g + \sum_{i=q,\bar{q}} H_{Qq}^{(2)} \triangleleft f_i \right]$$



GMVFN scheme hadronic cross section

Equivalently, with the $d\sigma_{FE} - d\sigma_{sub}$ reorganized in terms of HQ PDF residuals we obtain a very simple form

$$d\sigma_{\rm GMVFN}^{\rm NLO} = d\sigma_{\rm FC}^{\rm NLO} + a_s \ f_g \rhd \left[d\widehat{\sigma}_{gQ \to ZQ}^{(1)} \right] \lhd \delta f_Q^{(\rm NLO)} + a_s^2 \ f_g \rhd \left[d\widehat{\sigma}_{gQ \to ZQ(g)}^{(2)} \right] \lhd \delta f_Q^{(1)} + a_s^2 \ \sum_{i=q,\bar{q}} f_i \rhd \left[d\widehat{\sigma}_{qQ \to ZQ(q)}^{(2)} \right] \lhd \delta f_Q^{(1)} + (\text{exch.})$$

Lowest mandatory order" (LMO) representation at NLO in that it retains only the unambiguous terms up to order a_s^3 required by order-by-order factorization and scale invariance. Any ACOT-like scheme must contain such terms.

Z+b differential distributions (gg channel)



Z+b differential distributions (qg channel)



Z+b: ACOT vs S-ACOT



Further simplifications in ACOT-type schemes

$$d\sigma_{\rm GMVFN}^{\rm NLO} = d\sigma_{\rm FC}^{\rm NLO} + a_s \ f_g \triangleright \left[d\widehat{\sigma}_{gQ \to ZQ}^{(1)} \right] \lhd \delta f_Q^{(\rm NLO)} + a_s^2 \ f_g \triangleright \left[d\widehat{\sigma}_{gQ \to ZQ(g)}^{(2)} \right] \lhd \delta f_Q^{(1)} + a_s^2 \ \sum_{i=q,\bar{q}} f_i \triangleright \left[d\widehat{\sigma}_{qQ \to ZQ(q)}^{(2)} \right] \triangleleft \delta f_Q^{(1)} + (\text{exch.})$$

Lowest mandatory order" (LMO) representation at NLO in that it retains only the unambiguous terms up to order a_s^3 required by order-by-order factorization and scale invariance. Any ACOT-like scheme must contain such terms.

Further simplifications in ACOT-type schemes

One generally can augment $d\sigma_{GMVFN}^{NLO}$ with extra radiative contributions from higher orders with the goal to improve consistency with the specific GMVFN scheme adopted in the fit of the used PDFs. The GMVFN scheme assumed for determination of CTEQ-TEA PDFs with up to 5 active flavors is closely matched with the following additional choices:

1. Evolve $\alpha s(\mu)$ and PDFs fi(ξ,μ) with Nf = 5 at $\mu \ge mb$. The hard cross sections are also evaluated with Nf = 5 in virtual loops both for massive and massless channels. If the virtual contributions are obtained in the Nf = 4 scheme, they should be converted to the Nf = 5 scheme by adding known terms to the hard cross sections

2. The sums over initial-state light quarks and antiquarks in $d\sigma_{\text{GMVFN}}^{\text{NLO}}$ are extended to also include the b-quark PDF via the introduction of the singlet PDF $\Sigma \equiv \sum_{i=1}^{5} (f_i + \bar{f}_i)$

3. replace $\tilde{f}_Q^{(1)}$ in $d\sigma_{\text{sub}}^{\text{NLO}}$ and $\delta f_Q^{(1)}$ in $d\sigma_{\text{GMVFN}}^{\text{NLO}}$ by f^(NLO) and δ f^(NLO), respectively.

4. The α s and PDFs must be evolved at least at NLO, although evolution at NNLO is acceptable or even desirable in some contexts.

5. In the hard cross sections inside doFE – dosub, dependence on the HQ mass can be eliminated altogether or simplified, producing a difference only in higher-order terms.

Further simplifications in ACOT-type schemes

With the simplifications discussed above, we obtain

$$\begin{split} \tilde{f}_Q^{(1)} &= a_s \left[A_{Qg}^{S,(1)} \lhd g \right], \quad \tilde{f}_Q^{(2)} = a_s^2 \left[A_{Qq}^{\text{PS},(2)} \lhd \Sigma + A_{Qg}^{S,(2)} \lhd g \right] \\ \tilde{f}_Q^{(\text{NLO})}(x,\mu) &\equiv \tilde{f}_Q^{(1)} + \tilde{f}_Q^{(2)} \qquad \delta f_Q^{(\text{NLO})} = f_Q - \tilde{f}_Q^{(\text{NLO})} \end{split}$$

$$\begin{split} \mathrm{d}\sigma_{\mathrm{ACOT}}^{\mathrm{NLO}} &= \mathrm{d}\sigma_{\mathrm{FC}}^{\mathrm{NLO}} + \left(a_s \ f_g \rhd \mathrm{d}\widehat{\sigma}_{gQ \to ZQ}^{(1)} \right. \\ &+ a_s^2 f_g \rhd \mathrm{d}\widehat{\sigma}_{gQ \to ZQ(g)}^{(2)} + a_s^2 \Sigma \rhd \mathrm{d}\widehat{\sigma}_{qQ \to ZQ(q)}^{(2)} \right) \lhd \delta f_Q^{(\mathrm{NLO})} + (\mathrm{exch.}) \,. \end{split}$$

Other Results which used S-ACOT-MPS

- Prompt charm production at central and forward rapidity
- inclusive b-production

ACOT-MPS Results

Prompt charm production at central and forward rapidity





Transverse momentum at central rapidity at LHCb 13TeV. Error bands are scale uncertainties.



Rapidity distributions of prompt charm at the LHC 13 TeV in the very forward region (yc > 8). Error band represents the CT18NLO induced PDF uncertainty at 68% C.L.

Charm hadroproduction and Z + c production at the LHC can constrain the IC contributions. In CT14IC, we looked at Z+c at LHC 8 and 13 TeV. LHCb Z+c data deserve attention as they can potentially discriminate gluon functional forms at $x \ge 0.2$ and improve gluon accuracy.

For small x below 10^{-4} , higher-order QCD terms with $\ln(1/x)$ dependence grow quickly at factorization scales of order 1 GeV. FPF facilities like FASERv will access a novel kinematic regime where both large-x and small-x QCD effects contribute to charm hadroproduction rate.

NNLO gluon PDF in CT18/CT18X with IC. Error PDFs at 90% C.L. FPF paper 2109.10905

Applications and Results: inclusive b-production



Strong sensitivity to the gluon and the b-quark PDFs. Corresponding PDF uncertainties obtained with the asymmetric Hessian approach at the 90% CL, with positive (negative) direction denoted as black solid (blue dashed) lines [arXiv:2203.06207]

NLO theory predictions for the pT and y distributions obtained with CT18NLO and CT18XNLO PDFs compared to B^{\pm} production data from LHCb 13 TeV [arXiv:2203.06207]

Theoretical uncertainties at NLO are large (O(50%)) and mainly ascribed to scale variation. This can be improved by including higher-order corrections which imply an extension of the S-ACOT-MPS scheme to NNLO

Concluding remarks

- We applied ACOT-like schemes at NLO to Z+Q production in pp collisions at the LHC
- ACOT/S-ACOT developed at NLO: used to describe Z+Q production differentially
- Technically possible to generate predictions within the ACOT-type schemes at NNLO
- Direct access to c/b-PDF: Important to constrain heavy-flavor PDFs.
- Subtracted PDFs are provided in the form of LHAPDF grids to allow users for multiple pheno applications
- Work toward simplifying implementation of GMVFN schemes in (N)NLO QCD calculations using the formalism of subtracted PDFs