Towards a neural network determination of Fragmentation Functions

4th Workshop on the QCD Structure of the Nucleon (QCD-N'16)

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Outline

1. Theory: the perturbative QCD framework
   or why we are interested in a determination of fragmentation functions à la NNPDF
   - Motivation and desiderata
   - The piece of theory we need
2. Practice: towards `NNFF1.0`
   or how we are dealing with a determination of fragmentation functions à la NNPDF
   - Observables, data sets
   - Methodological details of the fit
   - Results: fit quality, perturbative stability, comparison with other sets
3. Conclusions

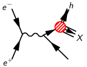
1. Theory: the perturbative QCD framework

Foreword [More in R. Sassot's talk]

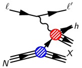
Fragmentation functions encode the information on how partons produced in hard-scattering processes are turned into an observed colorless hadronic bound final-state [PRD 15 (1977) 2590]

Starting point: (leading-twist) QCD factorization

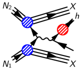
$$d\sigma^h(x, E_s^2) = \sum_{i=-n_f}^{n_f} \int_x^1 dz\, d\sigma^i \left(\frac{x}{z}, \frac{E_s^2}{\mu^2}, \frac{m_i^2}{E_s^2}, \alpha_s(\mu^2) \right) D_i^h(z, \mu^2)$$



$e^+ + e^- \to h + X$
single-inclusive annihilation (SIA)



$\ell + N \to \ell' + h + X$
semi-inclusive deep-inelastic scattering (SIDIS)



$N_1 + N_2 \to h + X$
high-p_T hadron production in pp collisions (PP)

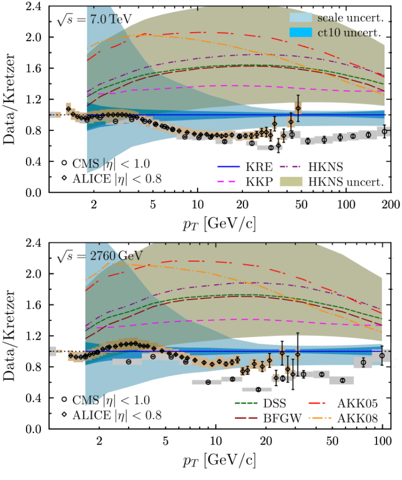
Process	DSS	HKNS	KRE	AKK08
SIA	☑	☑	☑	☑
SIDIS	☑	☒	☒	☒
PP	☑	☒	☒	☑
statistical treatment	Lagr. mult. $\Delta\chi^2/\chi^2 = 2\%$	Hessian $\Delta\chi^2 = 15.94$	no uncertainty determination	no uncertainty determination
hadron species	$\pi^\pm$, $K^\pm$, $p/\bar{p}$, $h^\pm$	$\pi^\pm$, $K^\pm$, $p/\bar{p}$	$\pi^\pm$, $K^\pm$, $h^\pm$	$\pi^\pm$, $K^\pm$, $p/\bar{p}$, K_S^0, $\Lambda/\bar{\Lambda}$
latest update	PRD 91 (2015) 014035	PRD 75 (2007) 094009	PR D62 (2000) 054001	NP B803 (2008) 42

+ some others: KKP [NP B582 (2000) 514], BFGW [EPJ C19 (2001) 89], AKK05 [NP B725 (2005) 181], . . .

some of them are publicly available at http://lapth.cnrs.fr/ffgenerator/

Fragmentation functions: why should we bother?

Example 1: Ratio of the inclusive charged-hadron spectra measured by CMS and ALICE



Figures taken from [NPB 883 (2014) 615]

Example 2: The strange polarized parton distribution at $Q^2 = 2.5$ GeV^2 ($\Delta s = \Delta\bar{s}$)

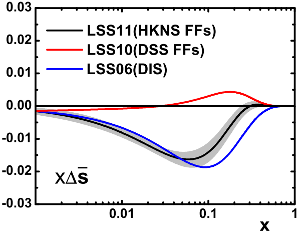


Figure taken from [PRD D84 (2011) 014002]

1 Predictions from all available FF sets are not compatible with CMS and ALICE data, not even within scale and PDF/FF uncertainties

2 If SIDIS data are used to determine Δs, $K^{\pm}$ FFs for different sets lead to different results. Such results may differ significantly among them and w.r.t. the results obtained from DIS

A determination of Fragmentation Functions à la NNPDF

List of desiderata (for the NNFF1.0 release)

1. Data:
   - all untagged and tagged SIA data for $\pi^{\pm}$, $K^{\pm}$, $p/\bar{p}$
2. Theory:
   - LO, NLO, NNLO (will be the only NNLO fit together with [PRD 92 (2015) 114017])
   - $\overline{\mathrm{MS}}$ scheme, ZM-VFNS
3. Fit methodology/technology:
   - à la NNPDF [more in J. Rojo's talk]

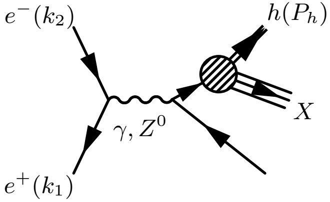
     Monte Carlo sampling of experimental data + neural network parametrization

     closure tests for a full characterization of procedural uncertainties
   - use of APFEL [CPC 185 (2014) 1647] for the calculation of SIA observables
   - keep mutual consistency with NNPDF unpolarized/polarized PDF sets

Results presented in this talk refer to $\pi^{\pm}$ fragmentation functions

work in progress for $K^{\pm}$ and $p/\bar{p}$

Factorization: single-inclusive annihilation cross section



$$e^+(k_1) + e^-(k_2) \xrightarrow{\gamma, Z^0} h(P_h) + X$$

$$q = k_1 + k_2 \qquad q^2 = Q^2 > 0 \qquad z = \frac{2P_h \cdot q}{Q^2}$$

$$\boxed{\frac{d\sigma^h}{dz} = \mathcal{F}_T^h(z, Q^2) + \mathcal{F}_L^h(z, Q^2) = \mathcal{F}_2^h(x, Q^2)}$$

$$\boxed{\mathcal{F}_{k=T,L,2}^h = \frac{4\pi\alpha_{\rm em}^2}{Q^2}\langle e^2\rangle \left\{ D_\Sigma^h \otimes \mathcal{C}_{k,q}^{\rm S} + n_f D_g^h \otimes \mathcal{C}_{k,g}^{\rm S} + D_{\rm NS}^h \otimes \mathcal{C}_{k,q}^{\rm NS} \right\}}$$

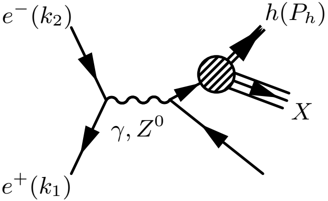
$$\langle e^2\rangle = \frac{1}{n_f}\sum_{p=1}^{n_f} \hat{e}_p^2 \qquad D_\Sigma^h = \sum_{p=1}^{n_f}\left(D_p^h + D_{\bar{p}}^h\right) \qquad D_{\rm NS}^h = \sum_{p=1}^{n_f}\left(\frac{\hat{e}_p^2}{\langle e^2\rangle} - 1\right)\left(D_p^h + D_{\bar{p}}^h\right)$$

$$\hat{e}_p^2 = e_p^2 - 2e_p\chi_1(Q^2)v_e v_p + \chi_2(Q^2)(1+v_e^2)(1+v_p^2)$$

$$\chi_1(s) = \frac{1}{16\sin^2\theta_W\cos^2\theta_W}\frac{s(s-M_Z^2)}{(s-M_Z^2)^2 + \Gamma_Z^2 M_Z^2}$$

$$\chi_2(s) = \frac{1}{256\sin^4\theta_W\cos^4\theta_W}\frac{s^2}{(s-M_Z^2)^2 + \Gamma_Z^2 M_Z^2}$$

Factorization: single-inclusive annihilation cross section



$$e^+(k_1) + e^-(k_2) \xrightarrow{\gamma, Z^0} h(P_h) + X$$

$$q = k_1 + k_2 \qquad q^2 = Q^2 > 0 \qquad z = \frac{2P_h \cdot q}{Q^2}$$

$$\boxed{\frac{d\sigma^h}{dz} = \mathcal{F}_T^h(z, Q^2) + \mathcal{F}_L^h(z, Q^2) = \mathcal{F}_2^h(x, Q^2)}$$

$$\boxed{\mathcal{F}^h_{k=T,L,2} = \frac{4\pi\alpha_{\rm em}^2}{Q^2}\langle e^2\rangle \left\{ D_\Sigma^h \otimes \mathcal{C}^{\rm S}_{k,q} + n_f D_g^h \otimes \mathcal{C}^{\rm S}_{k,g} + D^h_{\rm NS} \otimes \mathcal{C}^{\rm NS}_{k,q} \right\}}$$

$$\langle e^2 \rangle = \frac{1}{n_f}\sum_{p=1}^{n_f} \hat{e}_p^2 \qquad D_\Sigma^h = \sum_{p=1}^{n_f}\left(D_p^h + D_{\bar{p}}^h\right) \qquad D^h_{\rm NS} = \sum_{p=1}^{n_f}\left(\frac{\hat{e}_p^2}{\langle e^2\rangle} - 1\right)\left(D_p^h + D_{\bar{p}}^h\right)$$

Note 1: coefficient functions allow for a perturbative expansion

$\mathcal{C}^{i=\rm S,NS}_{k=T,L,2,f=q,g} = \sum_{l=0}\left(\frac{\alpha_s}{4\pi}\right)^l C^{i,(l)}_{k,f}$

with $C^{i,(l)}_{k,f}$ known up to NNLO ($l=2$) in $\overline{\rm MS}$ [NPB 751 (2006) 18, NPB 749 (2006) 1]

Note 2: only a subset of FFs can be determined from SIA

Note 3: different scaling with Q^2 of $\hat{e}_i$ → handle on flavour decomposition of quark FFs

$\hat{e}_u^2/\hat{e}_d^2(Q^2 = M_Z) \approx 0.78 \qquad \hat{e}_u^2/\hat{e}_d^2(Q^2 = 10\text{GeV}) \approx 4$

Evolution: time-like DGLAP

$$\frac{\partial}{\partial \ln \mu^2} D^h_{\rm NS}(z,\mu^2) = P^{\rm NS}(z,\mu^2) \otimes D^h_{\rm NS}(z,\mu^2)$$

$$\frac{\partial}{\partial \ln \mu^2} \begin{pmatrix} D^h_\Sigma(z,\mu^2) \\ D^h_g(z,\mu^2) \end{pmatrix} = \begin{pmatrix} P^{\rm qq} & 2n_f P^{\rm gq} \\ \frac{1}{2n_f} P^{\rm qg} & P^{\rm gg} \end{pmatrix} \otimes \begin{pmatrix} D^h_\Sigma(z,\mu^2) \\ D^h_g(z,\mu^2) \end{pmatrix}$$

Note 1: splitting functions allow for a perturbative expansion

$P_{ji} = \sum_{l=0} \left(\frac{\alpha_s}{4\pi}\right)^{l+1} P_{ji}^{(l)}$

with $P_{ji}^{(l)}$ known up to NNLO ($l=2$) in $\overline{\rm MS}$ [PLB 638 (2006) 61, NPB 845 (2012) 133]

an uncertainty still remains on the exact form of $P_{\rm qg}^{(2)}$ (it does not affect its logarithmic behavior)

Note 2: large perturbative corrections as $z \to 0$ [More in D. Anderle's talk]

SPACE-LIKE CASE

$$P_{ji} \propto \frac{a_s^{k+1}}{x} \log^{k+1-m} \frac{1}{x}$$

TIME-LIKE CASE

$$P_{ji} \propto \frac{a_s^{k+1}}{z} \log^{2(k+1)-m-1} z$$

with $m = 1, \dots, 2k+1$: soft gluon logarithms diverge more rapidly in the time-like case than in space-like case

as z decreases, the SGLs will spoil the convergence of the fixed-order series for P_{ji} once $\log \frac{1}{z} \geq \mathcal{O}\left(a_s^{-1/2}\right)$

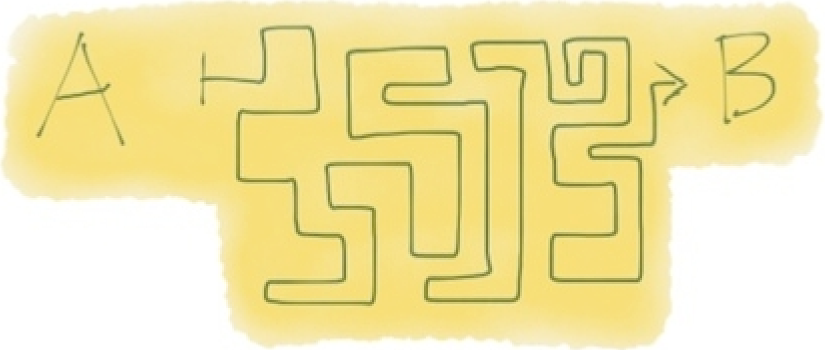
Note 3: numerical implementation of time-like evolution in `APFEL-MELA` [JHEP 1503 (2015) 046]

`https://apfel.hepforge.org/mela.html`

at LO, NLO, NNLO, allow for $\mu_F \neq \mu_R$, relative accuracy below 10^{-4}

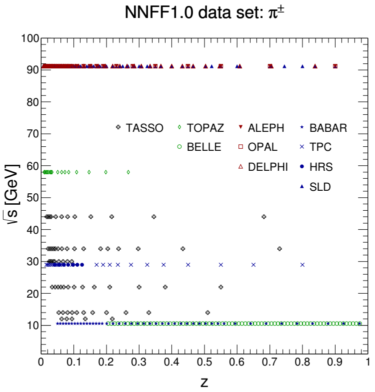
reliability and stability of time-like evolution in `APFEL` has been extensively studied [PRD 92 (2015) 114017]

after bug corrections, found perfect agreement with time-like evolution in `QCDNUM` [arXiv:1602.08383]



2. Practice: towards `NNFF1.0`

Data sets



CERN-LEP

ALEPH

[ZP C66 (1995) 353]

OPAL

[ZP C63 (1994) 181]

DELPHI

[EPJ C18 (2000) 203]

KEK

TOPAZ

[PL B345 (1995) 335]

BELLE ($n_f = 4$)

[PRL 111 (2013) 062002]

DESY-PETRA

TASSO

[PL B94 (1980) 444, ZP C17 (1983) 5, ZP C42 (1989) 189]

SLAC

BABAR ($n_f = 4$)

[PR D88 (2013) 032011]

TPC

[PRL 61 (1988) 1263]

HRS

[PR D35 (1987) 2639]

SLD

[PR D58 (1999) 052001]

OBSERVABLE	EXPERIMENT	OBSERVABLE	EXPERIMENT	OBSERVABLE	EXPERIMENT
$\frac{d\sigma}{dz}$	BELLE	$\frac{1}{\sigma \text{tot}}\frac{d\sigma}{dx_p}$	SLD, ALEPH, TASSO34/44	$\frac{1}{\sigma_{\text{tot}}}\frac{d\sigma}{dp_h}$	BABAR, OPAL, DELPHI
$\frac{1}{\beta\sigma_{\text{tot}}}\frac{d\sigma}{dz}$	TPC	$\frac{s}{\beta}\frac{d\sigma}{dz}$	TASSO12/14/22/30, HRS	$\frac{1}{\sigma_{\text{tot}}}\frac{d\sigma}{d\xi}$	TOPAZ

$$z = \frac{E_h}{E_b} = \frac{2|\mathbf{p}_h|}{\sqrt{s}} \qquad x_p = \frac{|\mathbf{p}_h|}{\mathbf{p}_b} = \frac{2|\mathbf{p}_h|}{\sqrt{s}} \qquad \xi = \ln(1/x_p) \qquad \beta = \frac{|\mathbf{p}_h|}{E_h}$$

Some methodological details

Physical parameters: consistent with the upcoming `NNPDF3.1` PDF set

$$\alpha_s(M_Z) = 0.118,\ \alpha_{\rm em}(M_Z) = 1/127,\ m_c = 1.51 \text{ GeV},\ m_b = 4.92 \text{ GeV}$$

Running couplings: we include the effects of the running of both α_s and $\alpha_{\rm em}$
in the case of QCD the RGE is solved exactly using a fourth-order Runge-Kutta algorithm

Heavy flavors: we use the ZM-VFN scheme with a maximum of $n_f = 5$ active flavors
heavy-quark FFs are generated dynamically above the threshold neglecting HQ mass effects
matching conditions for the transition between a n_f and a $n_f + 1$ schemes in the evolution:
included at NLO [JHEP 0510 (2005) 034]; set to zero at NNLO (they are not known)

Solution of DGLAP equations: numerical solution in z-space as implemented in `APFEL`

Parametrization basis: $\{D_\Sigma^{\pi^\pm}, D_g^{\pi^\pm}, D_{T_3+1/3\,T_8}^{\pi^\pm}\}$ $(\{D_{u+\bar{u}}^{\pi^\pm}, D_{d+\bar{d}}^{\pi^\pm} + D_{s+\bar{s}}^{\pi^\pm}, D_g^{\pi^\pm}\})$

$$D_{T_3+1/3\,T_8}^{\pi^\pm} = D_{T_3}^{\pi^\pm} + 1/3 D_{T_8}^{\pi^\pm} = 2\,D_{u+\bar{u}}^{\pi^\pm} - D_{d+\bar{d}}^{\pi^\pm} - D_{s+\bar{s}}^{\pi^\pm}$$

Parametrization form: each FF is parametrized with a feed-forward neural network

$$D_i^{\pi^\pm}(Q_0, z) = \text{NN}(x) - \text{NN}(1),\ i = \Sigma,\ g,\ T_3 + 1/3\,T_8,\ Q_0 = 1 \text{ GeV}$$

Kinematic cuts: $z_{\min} \leq z \leq z_{\max}$, $z_{\min} = 0.1$, $z_{\min} = 0.05$ $(\sqrt{s} = M_Z)$; $z_{\max} = 0.90$

$z \to 0$: corrections $\propto M_\pi/(sz^2)$ + contributions $\propto \ln z$; $z \to 1$: contributions $\propto \ln(1-z)$

Fit quality

Data set	$\sqrt{s}$ [GeV]	$N_{\rm dat}$	$\chi^2_{\rm LO}/N_{\rm dat}$	$\chi^2_{\rm NLO}/N_{\rm dat}$	$\chi^2_{\rm NNLO}/N_{\rm dat}$
ALEPH	91.2	22	0.60	0.57	0.55
DELPHI	91.2	16	3.04	3.12	2.98
OPAL	91.2	22	1.26	1.25	1.32
SLD	91.2	29	0.73	0.66	0.65
TOPAZ	58	4	1.81	1.49	0.85
TPC	29	12	1.78	0.94	0.90
HRS	29	2	4.26	4.26	2.93
TASSO44	44	5	2.04	1.81	1.53
TASSO34	34	8	1.65	1.38	0.63
TASSO22	22	7	2.04	2.10	1.46
TASSO14	14	7	2.00	2.37	2.30
TASSO12	12	2	1.06	0.89	0.59
BABAR (promt)	10.54	37	1.17	0.99	0.88
BELLE	10.52	70	0.46	0.11	0.10
		243	1.14	0.96	0.91

$$\chi^2\left\{\mathcal{T}[D],\mathcal{E}\right\} = \sum_{i,j}^{N_{\rm dat}} \left(T_i[D]-E_i\right) c_{ij}^{-1} \left(T_j[D]-E_j\right)$$

$$c_{ij}^{t_0} = \delta_{ij} s_i^2 + \sum_{\alpha=1}^{N_c} \sigma_{i,\alpha}^{(c)} \sigma_{j,\alpha}^{(c)} E_i E_j + \sum_{\alpha=1}^{N_{\mathcal{L}}} \sigma_{i,\alpha}^{(\mathcal{L})} \sigma_{j,\alpha}^{(\mathcal{L})} T_i^{(0)} T_j^{(0)}$$

s_i: uncorrelated unc.; $\sigma_{i,\alpha}^{(\mathcal{L})}$: $N_{\mathcal{L}}$ multiplicative norm. unc.; $\sigma_{i,\alpha}^{(c)}$ all other N_c correlated unc.

a fixed theory prediction $T_i^{(0)}$ is used to define the normalization contribution to the χ^2
this prescription allows for the proper inclusion of multiplicative systematic uncertainties in c_{ij}

Fit quality

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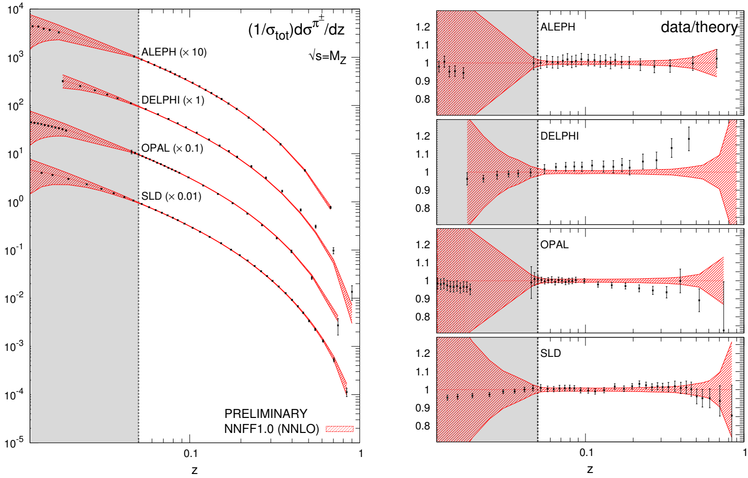
Note 1: overall good description of SIA cross sections/multiplicities $\chi^2_{\rm tot}/N_{\rm dat} \sim 1$
Note 2: the quality of the fit increases as higher order QCD corrections are included
Note 3: good consistency of data sets at different energy scales
good consistency between BELLE and BABAR (prompt) data sets
good consistency among BELLE, BABAR (prompt) and LEP/SLAC data sets
fair description of old data sets (TASSO, HRS) with limited information on systematics
poor description of DELPHI (though χ^2 consistent with HKNS07 [PRD 75 (2007) 094009])

Data/theory comparison

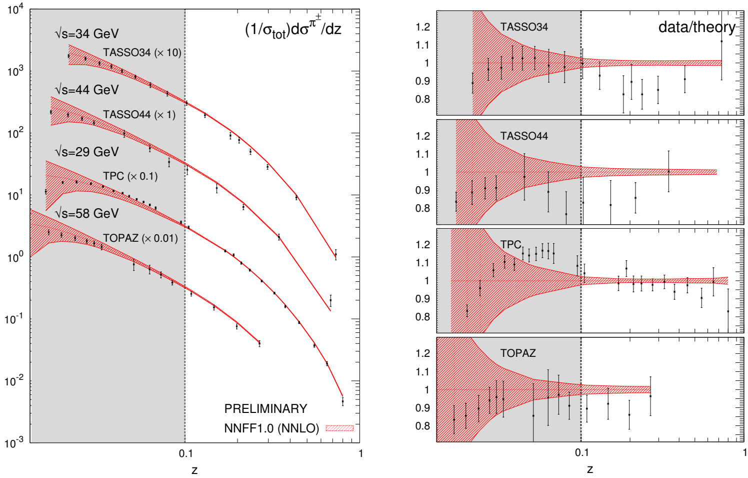


Fair description of the data in the small-z extrapolation region excluded by kinematic cuts

Slight deterioration of the data description as z increases

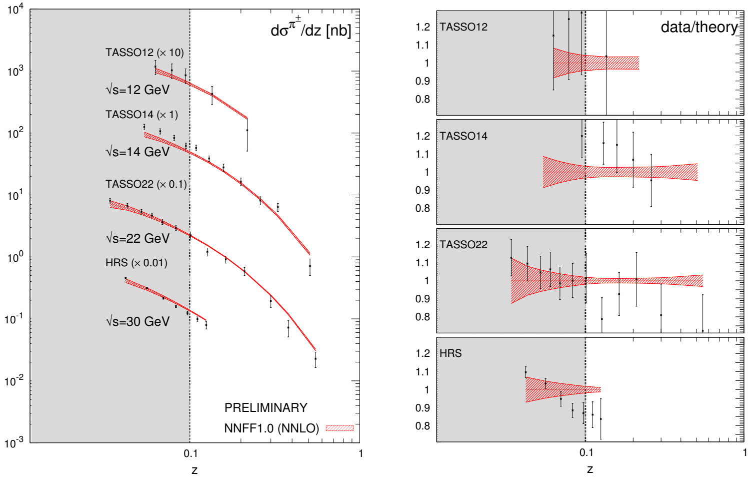
Apparent inconsistency of DELPHI with all other data sets at M_Z, especially for $z \geq 0.3$

Data/theory comparison



Good description of TPC data set, which deteriorates in the small-z region excluded by cuts
Fair/poor description of TASSO/HRS data sets, including the small-z extrapolation region
(limited number of data points + limited information on systematics)

Data/theory comparison



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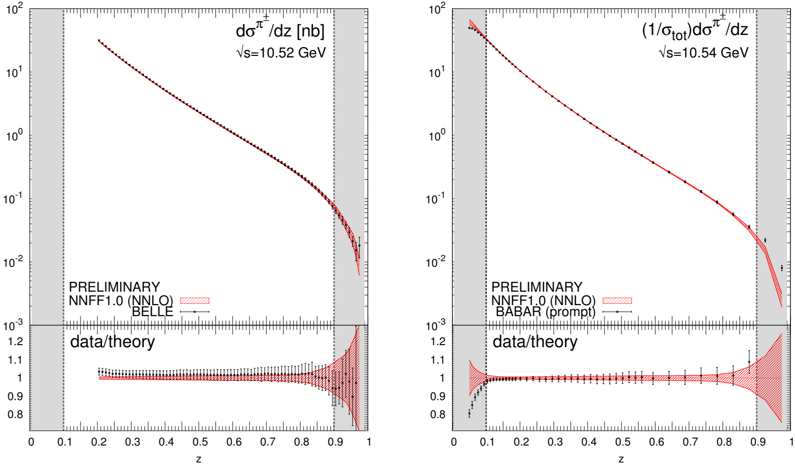
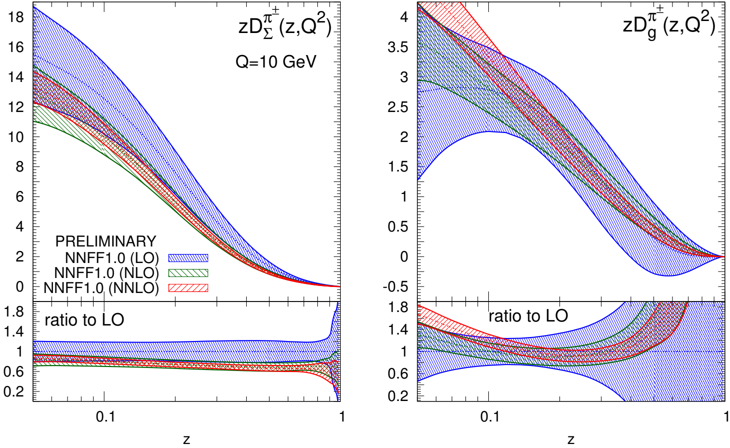
Data/theory comparison



BELLE: good description of the data in the large-z region excluded by kinematic cuts
BABAR: the description of the data in the excluded small- and large-z regions deteriorates
Overall good consistency between BELLE and BABAR data sets within kinematic cuts

Fragmentation functions: perturbative stability



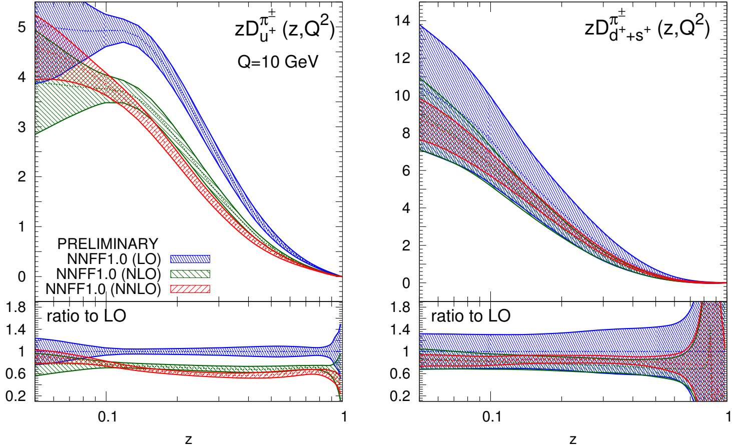
Impact of higher-order QCD corrections:

sizable for LO $\rightarrow$ NLO, moderate for NLO $\rightarrow$ NNLO

both at the level of CV and 1σ error bands

i	N^{i+1}LO/N^{i}LO	D_g	D_Σ	D_{u^+}	$D_{d^+ + s^+}$
0	NLO/LO [%]	95-300	70-80	65-80	70-85
1	NNLO/NLO [%]	70-130	90-100	90-110	95-115

Fragmentation functions: perturbative stability



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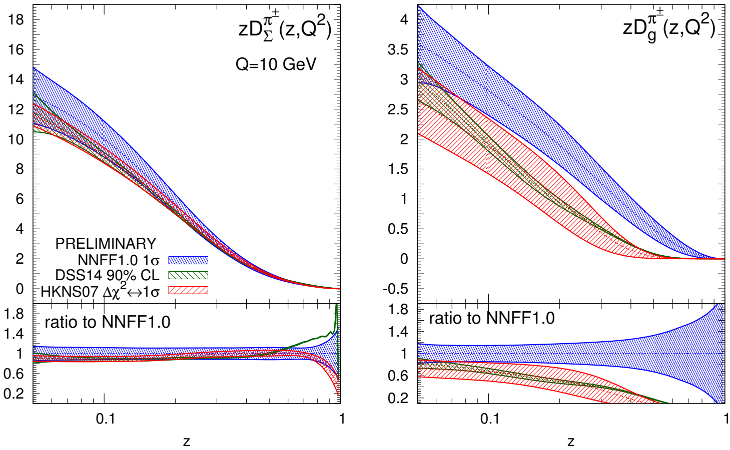
i	$N^{i+1}LO/N^iLO$	D_g	D_Σ	D_{u^+}	$D_{d^++s^+}$
0	NLO/LO [%]	95-300	70-80	65-80	70-85
1	NNLO/NLO [%]	70-130	90-100	90-110	95-115

Fragmentation functions: comparison with other FF sets



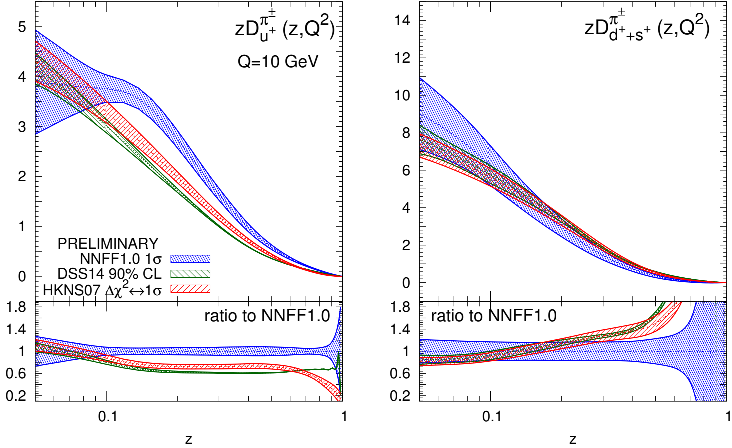
Compare only the FF sets provided with an estimate of the uncertainties at NLO

Caveat: different data sets, dfferent theory (heavy quarks), different treatment of uncertainties

Shape: good agreement for $D_\Sigma^{\pi^\pm}$ (and $D_{d^++s^+}^{\pi^\pm}$); sizable difference for $D_g^{\pi^\pm}$ (and $D_{u^+}^{\pi^\pm}$)

Uncertainties: `NNFF1.0` significantly larger than `DSS14` and slightly larger than `HKNS07`

Fragmentation functions: comparison with other FF sets



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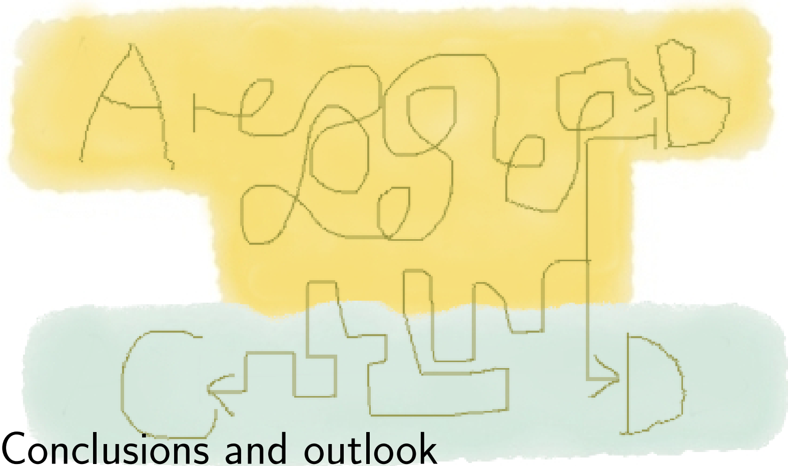
Uncertainties: NNFF1.0 significantly larger than DSS14 and slightly larger than HKNS07



3. Conclusions and outlook

Summary and final remarks

1. NNFF1.0 will be the first determination of fragmentation functions à la NNPDF
   - based on inclusive data in SIA
   - provided at LO, NLO and NNLO
   - with a faithful uncertainty estimate
2. Preliminary results for $\pi^{\pm}$ fragmentation functions from NNFF1.0 were presented
   - good description of all inclusive untagged SIA data
   - inclusion of higher-order corrections up to NNLO
   - larger uncertainties than in other available sets (caveat applies)
3. The NNFF1.0 release will include fragmentation functions of $\pi^{\pm}$, $K^{\pm}$ and $p/\bar{p}$
   - they will be made available for each hadron species through the LHAPDF interface

     https://lhapdf.hepforge.org/
4. Beyond NNFF1.0: inclusion of SIDIS and PP data, GM-VFNS, resummation(s), ...

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Thank you