Fragmentation Functions and their uncertainties

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Emanuele R. Nocera
in collaboration with V. Bertone, S. Carrazza and J. Rojo

Rudolf Peierls Centre for Theoretical Physics - University of Oxford

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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

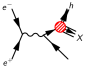
1. Theory: the perturbative QCD framework

Foreword

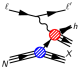
Fragmentation functions encode the information on how partons produced in hard-scattering processes are turned into an observed colorless hadronic bound final-state [PRD 15 (1977) 2590]

Starting point: (leading-twist) QCD factorization

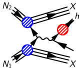
$$d\sigma^h(x, E_s^2) = \sum_{i=-n_f}^{n_f} \int_x^1 dz\, d\sigma^i \left(\frac{x}{z}, \frac{E_s^2}{\mu^2}, \frac{m_i^2}{E_s^2}, \alpha_s(\mu^2) \right) D_i^h(z, \mu^2)$$



$e^+ + e^- \to h + X$
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)

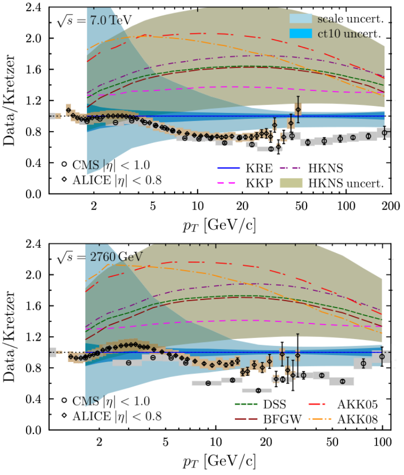
Process	DSS	HKNS	JAM	AKK08
SIA	☑	☑	☑	☑
SIDIS	☑	☒	☒	☒
PP	☑	☒	☒	☑
statistical treatment	Lagr. mult. $\Delta\chi^2/\chi^2 = 2\%$	Hessian $\Delta\chi^2 = 15.94$	Monte Carlo	no uncertainty determination
hadron species	$\pi^\pm$, $K^\pm$, $p/\bar{p}$, $h^\pm$	$\pi^\pm$, $K^\pm$, $p/\bar{p}$	$\pi^\pm$, $K^\pm$	$\pi^\pm$, $K^\pm$, $p/\bar{p}$, K_S^0, $\Lambda/\bar{\Lambda}$
latest update	PRD 91 (2015) 014035	arXiv:1608.04067	arXiv:1609.00899	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 ($\Delta s = \Delta\bar{s}$)

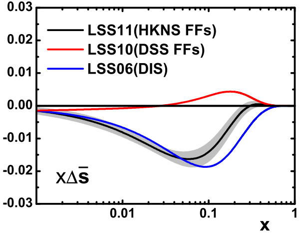


Figure taken from [PRD D84 (2011) 014002]

1 Predictions from all available FF sets are not compatible with CMS and ALICE data, not even within scale and PDF/FF uncertainties $\longrightarrow$ input for nuclear medium modifications

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 $\longrightarrow$ input for polarized PDFs and TMDs

A determination of Fragmentation Functions à la NNPDF

Possible limitations of current FF sets

1. Data: updated (global, consistent) data set?
2. Theory: higher orders? heavy quarks?
3. Methodology: parametrization? uncertainty determination?

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
3. Fit methodology/technology:
   - à la NNPDF

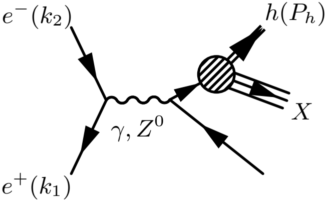
     Monte Carlo sampling of experimental data + neural network parametrization

     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 $\pi^\pm$ and $K^\pm$ fragmentation functions

π and K constitute the largest fraction in measured yields, work in progress for $p/\bar{p}$

Factorization: single-inclusive annihilation cross section



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

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

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

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

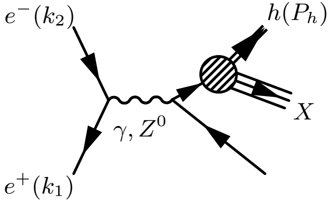
$$\langle e^2\rangle = \frac{1}{n_f}\sum_{p=1}^{n_f} \hat{e}_p^2 \qquad D_\Sigma^h = \sum_{p=1}^{n_f}\left(D_p^h + D_{\bar{p}}^h\right) \qquad D^h_{\rm NS} = \sum_{p=1}^{n_f}\left(\frac{\hat{e}_p^2}{\langle e^2\rangle} - 1\right)\left(D_p^h + D_{\bar{p}}^h\right)$$

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

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

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

Factorization: single-inclusive annihilation cross section



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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 $\hat{e}_i$ $\rightarrow$ handle on flavour decomposition of quark FFs

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

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 $z \to 0$

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 $m = 1, \ldots, 2k+1$: 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 $\log \frac{1}{z} \geq \mathcal{O}\left(a_s^{-1/2}\right)$

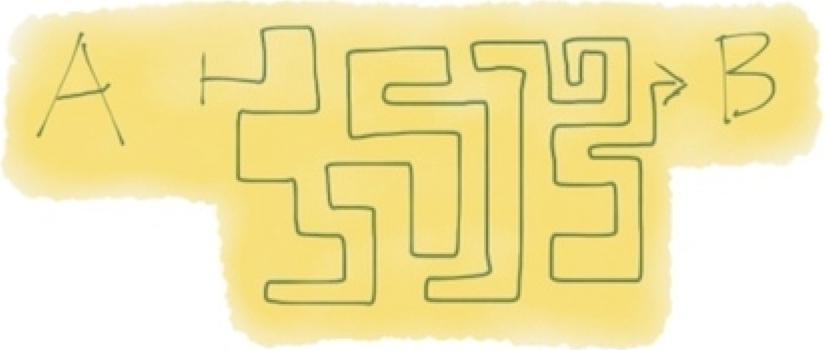
Note 3: numerical implementation of time-like evolution in `APFEL-MELA` [JHEP 1503 (2015) 046]

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

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

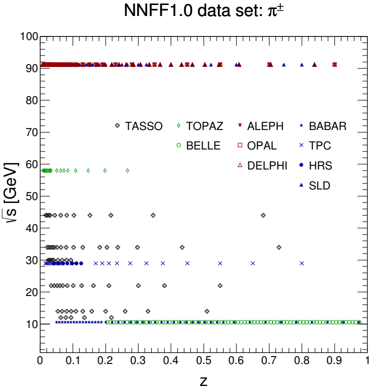
reliability and stability of time-like evolution in `APFEL` has been extensively studied [PRD 92 (2015) 114017]

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]

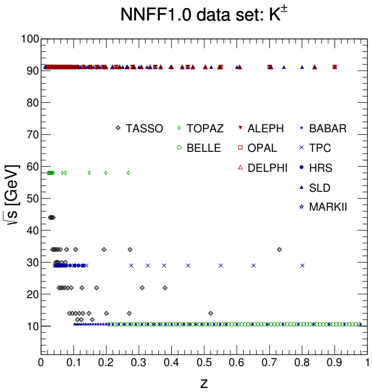
SLD

[PR D58 (1999) 052001]

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

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

Data sets



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

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: heavy-quark FFs are parametrized independently above their thresholds
ZM-VFNS w/ matching conditions between a n_f and a $n_f + 1$ schemes [JHEP 0510 (2005) 034]
GM-VFNS and FONLL may be required [PRD 94 (2016) 034037]

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

Parametrization basis: $\{D_\Sigma^{h^\pm}, D_g^{h^\pm}, D_{T_3+1/3\,T_8}^{h^\pm}, D_{T_{15}}^{h^\pm}, D_{24}^{h^\pm}\}$

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

$$D_{T_{15}}^{h^\pm} = D_{u+\bar{u}}^{h^\pm} + D_{d+\bar{d}}^{h^\pm} + D_{s+\bar{s}}^{h^\pm} - 3D_{c+\bar{c}}^{h^\pm} \qquad D_{T_{24}}^{h^\pm} = D_{u+\bar{u}}^{h^\pm} + D_{d+\bar{d}}^{h^\pm} + D_{s+\bar{s}}^{h^\pm} + D_{c+\bar{c}}^{h^\pm} - 4D_{b+\bar{b}}^{h^\pm}$$

equivalent to $\{D_{u+\bar{u}}^{h^\pm}, D_{d+\bar{d}}^{h^\pm} + D_{s+\bar{s}}^{h^\pm}, D_{c+\bar{c}}^{h^\pm}, D_{b+\bar{b}}^{h^\pm}, D_g^{h^\pm}\}$

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

$$D_i^{\pi^\pm}(Q_0, z) = \text{NN}(x) - \text{NN}(1),\ i = \Sigma,\ g,\ T_3 + 1/3\,T_8,\ Q_0 = 5\ \text{GeV}$$

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

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

Fit quality: $\pi^\pm$ $(K^\pm)$

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	(18)	0.69	(0.48)	0.55	(0.48)	0.54	(0.40)
DELPHI (untag)	91.2	16	(16)	2.64	(0.17)	2.55	(0.17)	2.53	(0.17)
DELPHI (uds)	91.2	16	(16)	2.03	(1.06)	1.97	(0.90)	1.94	(0.86)
DELPHI (b)	91.2	16	(16)	1.04	(0.31)	0.91	(0.29)	0.88	(0.28)
OPAL	91.2	22	(10)	1.79	(2.16)	1.78	(2.14)	1.76	(1.96)
SLD (untag)	91.2	29	(29)	0.85	(1.74)	0.85	(1.47)	0.66	(1.36)
SLD (uds)	91.2	29	(29)	0.76	(2.25)	0.72	(2.16)	0.61	(2.05)
SLD (c)	91.2	29	(29)	0.85	(1.74)	0.72	(0.72)	0.67	(0.61)
SLD (b)	91.2	29	(29)	0.57	(2.06)	0.55	(1.78)	0.52	(1.75)
TOPAZ	58	4	(3)	1.82	(0.52)	1.26	(0.51)	1.00	(0.35)
TPC	29	12	(12)	1.54	(0.48)	1.11	(0.41)	1.54	(0.38)
HRS	29	2	(3)	6.40	(0.38)	5.76	(0.20)	4.85	(0.19)
TASSO44	44	5	(–)	2.10	(—)	1.10	(—)	1.93	(—)
TASSO34	34	8	(4)	1.10	(0.06)	1.00	(0.06)	0.80	(0.04)
TASSO22	22	7	(4)	1.26	(0.23)	1.41	(0.21)	1.34	(0.16)
TASSO14	14	7	(7)	1.63	(3.52)	1.60	(2.79)	1.67	(2.68)
TASSO12	12	2	(3)	0.70	(2.01)	0.65	(1.79)	0.62	(1.75)
BABAR (promt)	10.54	37	(37)	1.17	(1.85)	0.99	(1.62)	0.88	(1.33)
BELLE	10.52	70	(70)	0.53	(0.28)	0.15	(0.26)	0.13	(0.18)
		362	(341)	1.03	(1.08)	0.93	(1.06)	0.91	(0.98)

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

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

Fit quality: $\pi^\pm$ $(K^\pm)$

Data set	$\sqrt{s}$ [GeV]	$N_{\rm dat}$		$\chi^2_{\rm LO}/N_{\rm dat}$		$\chi^2_{\rm NLO}/N_{\rm dat}$		$\chi^2_{\rm NNLO}/N_{\rm dat}$	
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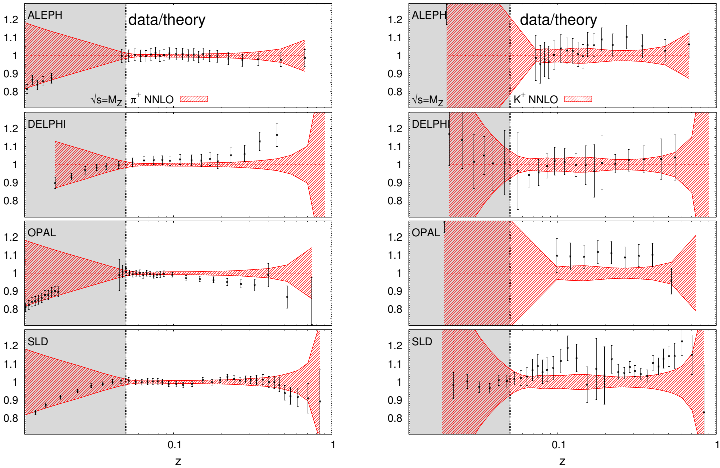
BELLE	10.52	70	(70)	0.53	(0.28)	0.15	(0.26)	0.13	(0.18)
		362	(341)	1.03	(1.08)	0.93	(1.06)	0.91	(0.98)

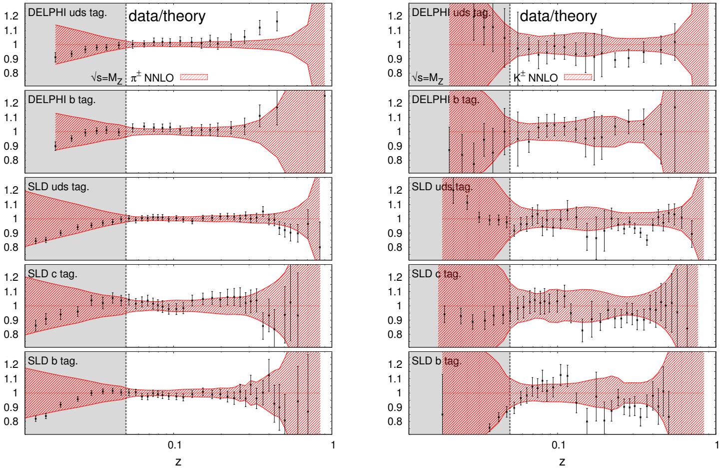
Note 1: overall good description of SIA cross sections/multiplicities $\chi^2_{\rm tot}/N_{\rm dat} \sim 1$
Note 2: the quality of the fit increases as higher order QCD corrections are included
Note 3: good consistency of data sets at different energy scales
Note 4: fair description of old data sets with limited information on systematics
Note 5: poor description of DELPHI $\pi^\pm$ (untag) and OPAL and SLD $K^\pm$

Data/theory comparison



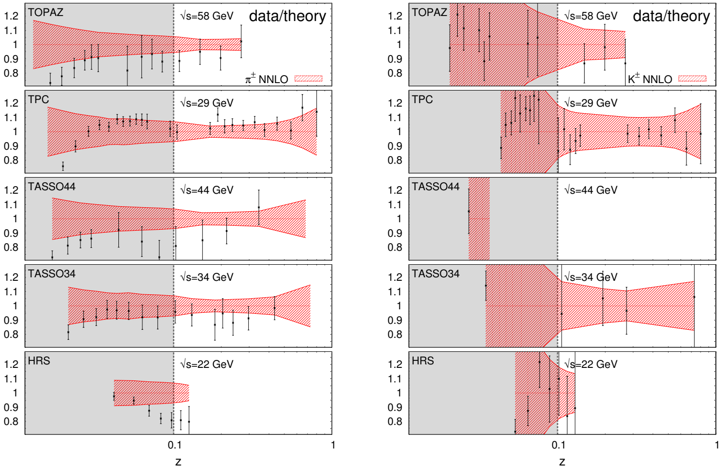
Quick deterioration of the description of the data in the small-z extrapolation region
Slight deterioration of the description of the data as z increases
Apparent tension of DELPHI ($\pi^{\pm}$) and SLD ($K^{\pm}$) with all other data sets at M_Z

Data/theory comparison



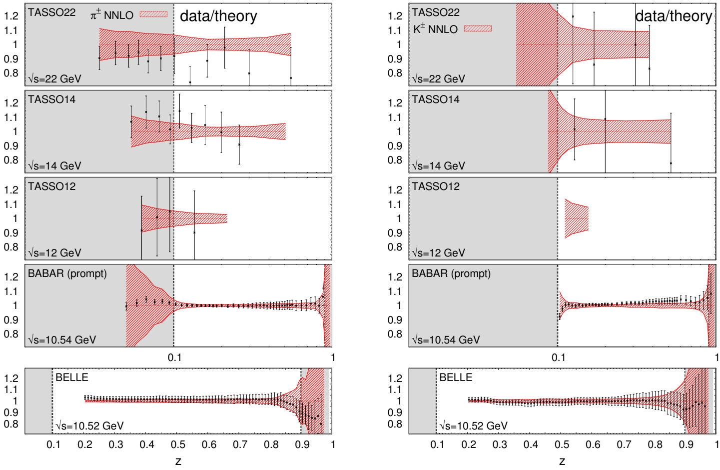
Overall good description of all tagged data sets at $\sqrt{s} = M_Z$
Again, deterioration of the description of the data at small and very large values of z
Accuracy of $K^\pm$ data (and of the corresponding fit) worse than $\pi^\pm$

Data/theory comparison



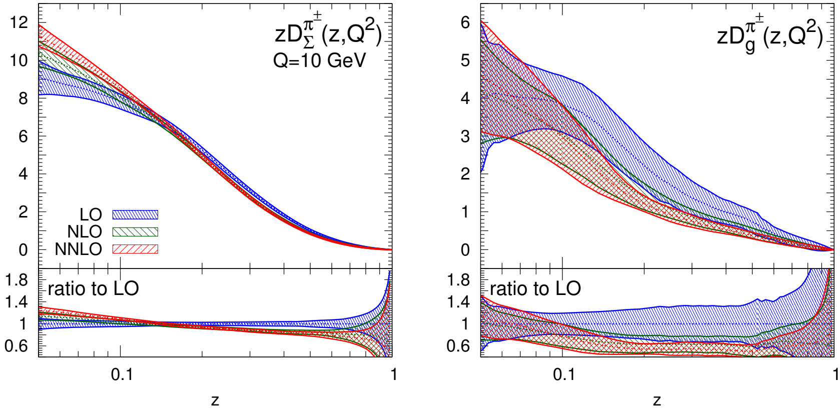
Fair description of old data sets (TOPAZ, TPC, TASSO44, TASSO34, HRS)
(limited number of data points, limited information on systematics/modelling, . . .)
Again, the accuracy of $K^{\pm}$ data (and of the corresponding fit) is worse than $\pi^{\pm}$

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:

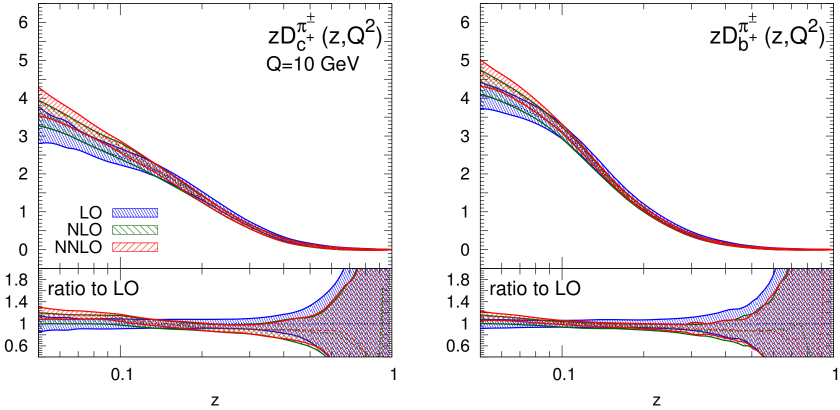
sizable for LO $\rightarrow$ NLO, moderate for NLO $\rightarrow$ NNLO

both at the level of CV and 1σ error bands

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

LO uncertainties larger than higher orders (missing perturbative accuracy)

Fragmentation functions: perturbative stability



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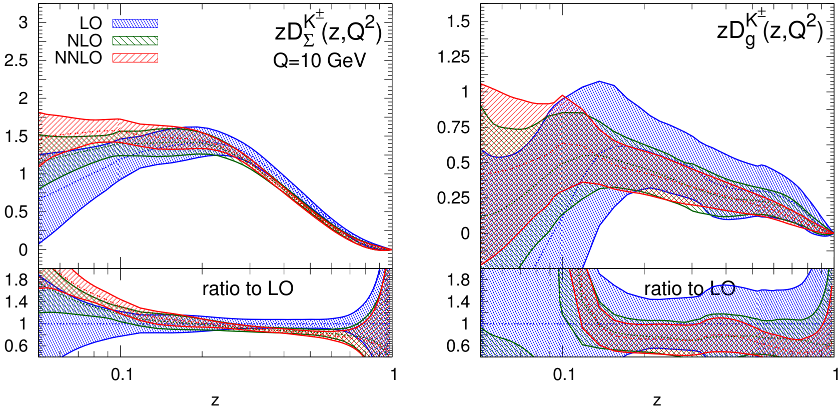

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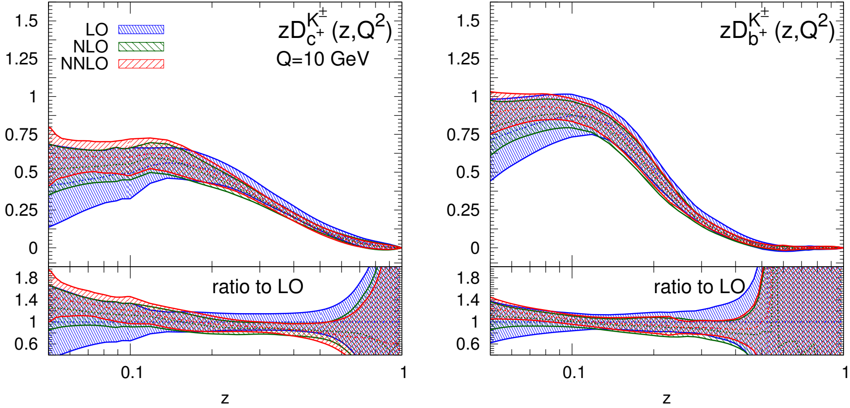

Impact of higher-order QCD corrections:

sizable for LO → NLO, moderate for NLO → NNLO

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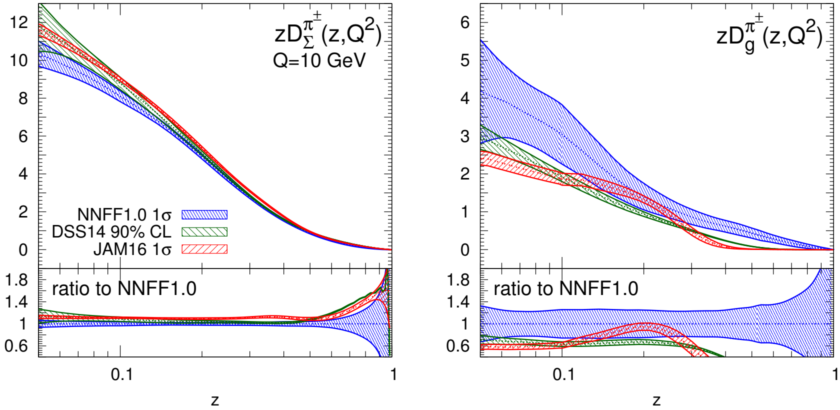
Fragmentation functions: comparison with other FF sets

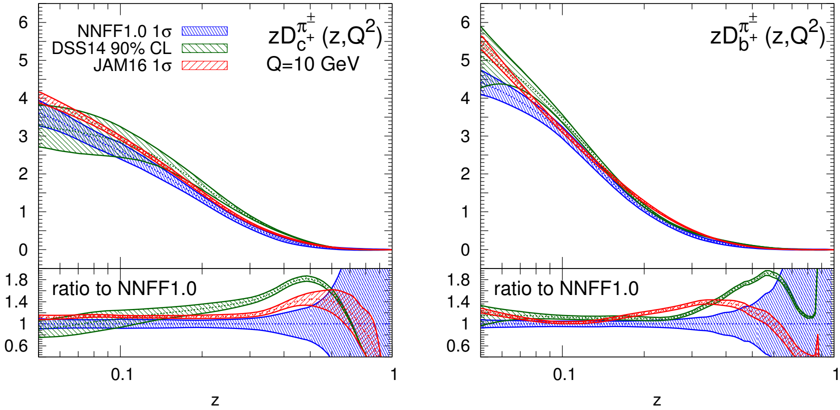


$\pi^\pm$: Compare NNFF1.0, DSS14 [PRD 91 (2015) 014035] and JAM16 [arXiv:1609.00899] at NLO
caveat: different data sets, different treatment of uncertainties

Shape: good agreement for $D_\Sigma^{\pi^\pm}$; sizable difference for $D_g^{\pi^\pm}$

Uncertainties: comparable uncertainties for $D_\Sigma^{\pi^\pm}$; larger NNFF1.0 uncertainties for $D_g^{\pi^\pm}$

Fragmentation functions: comparison with other FF sets

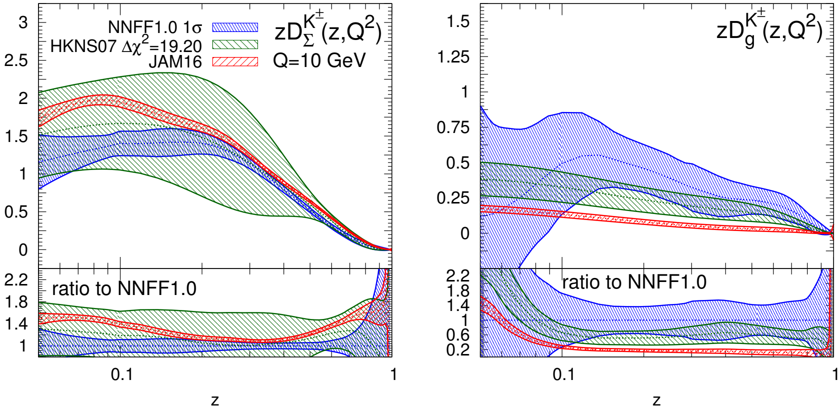


$\pi^\pm$: Compare NNFF1.0, DSS14 [PRD 91 (2015) 014035] and JAM16 [arXiv:1609.00899] at NLO
caveat: different data sets, different treatment of uncertainties

Shape: sizable discrepancy among all the three sets, especially in the large-z region

Uncertainties: comparable uncertainties for $D_{c^+}^{\pi^\pm}$ and $D_{b^+}^{\pi^\pm}$

Fragmentation functions: comparison with other FF sets

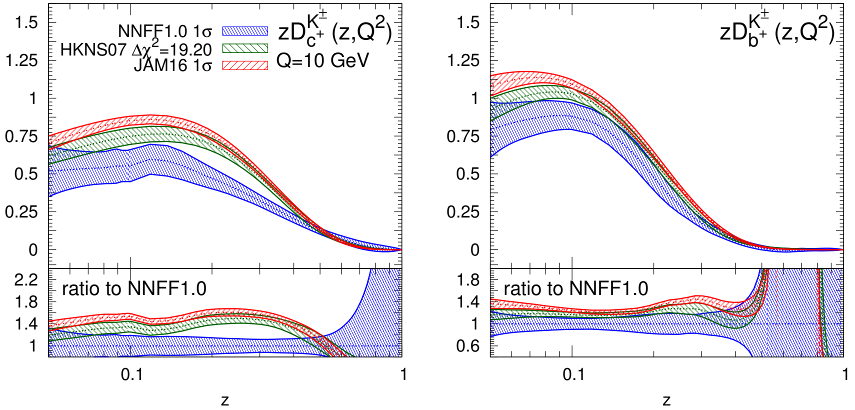


$K^{\pm}$: Compare NNFF1.0, HKNS07 [PRD 75 (2007) 094009] and JAM16 [arXiv:1609.00899] at NLO
caveat: different data sets, different treatment of uncertainties

Shape: similar trend of $D_{\Sigma}^{K^{\pm}}$ in all FF sets; NNPDF1.0 $D_{g}^{K^{\pm}}$ harder than the other FF sets

Uncertainties: HKNS07 uncertainties on $D_{\Sigma}^{K^{\pm}}$ significantly larger (no BELLE and BABAR data)

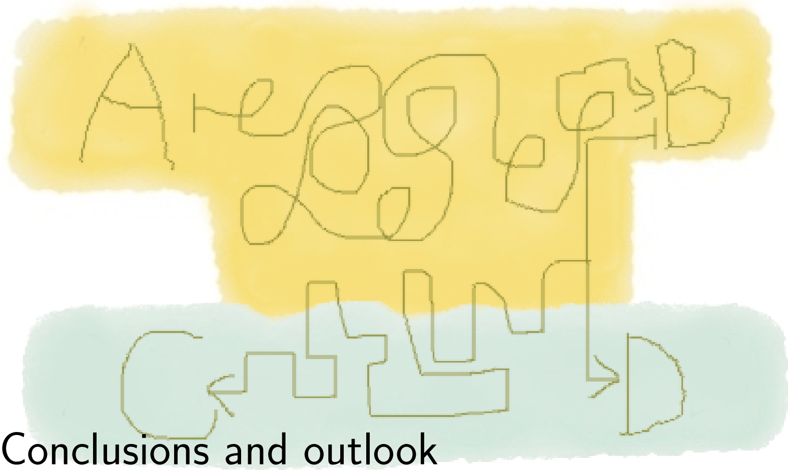
Fragmentation functions: comparison with other FF sets



$K^{\pm}$: Compare NNFF1.0, HKNS07 [PRD 75 (2007) 094009] and JAM16 [arXiv:1609.00899] at NLO
caveat: different data sets, different treatment of uncertainties

Shape: sizable discrepancy among all the three sets, over all the range of z

Uncertainties: NNFF1.0 uncertainties are larger than those of other FF sets



3. Conclusions and outlook

Summary and final remarks

1. NNFF1.0 is 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 $\pi^{\pm}$ and $K^{\pm}$ fragmentation functions were presented
   - good description of all inclusive untagged and tagged SIA data
   - inclusion of higher-order corrections up to NNLO
   - shape and size of the uncertainties of D_{Σ} comparable to other sets
   - uncertainties larger than other sets for D_{c^+} and D_{b^+}
   - uncertainties larger than other sets for D_g (with different shapes)
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