

# News from NNPDF: collinear fragmentation functions from $e^+e^-$ and $pp$

Workshop on Novel Probes of the Nucleon Structure in SIDIS,  $e^+e^-$  and  $pp$

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Nikhef - Amsterdam

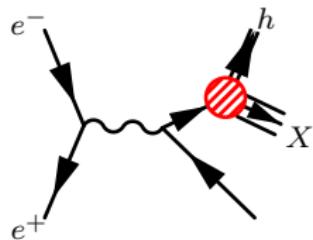
Duke University – 14<sup>th</sup> March 2019



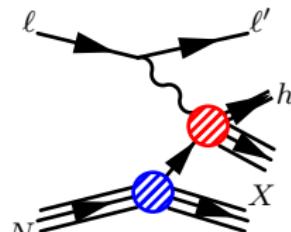
# Foreword

Underlying principle of a global fit: (collinear) factorisation of physical observables

$$\mathcal{O}_I = \sum_{i=q,\bar{q},g} C_{Ii}(y, \alpha_s(\mu^2)) \otimes D_i(y, \mu^2) + \text{p.s. corrections}$$

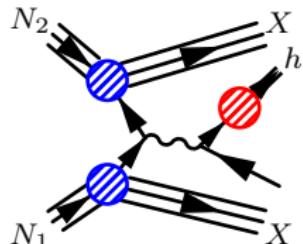


$e^+ + e^- \rightarrow h + X$   
single-inclusive  
annihilation (SIA)



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

$$f \otimes g = \int_x^1 \frac{dy}{y} f\left(\frac{x}{y}\right) g(y)$$



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

	DHESS	JAM	NNFF
SIA	✓	✓	✓
SIDIS	✓	✓	✗
PP	✓	✗	✓ ( $h^\pm$ )
statistical treatment	Iterative Hessian 68% - 90%	Monte Carlo	Monte Carlo
parametrisation	standard	standard	neural network
pert. order	(N)NLO	NLO	up to NNLO

DEHSS (see talk by Rodolfo)

$\pi^\pm$  [PRD 91 (2015) 014035]

$K^\pm$  [PRD 95 (2017) 094019]

JAM (see talk by Wally)

$\pi^\pm, K^\pm$  [PRD 94 (2016) 114004]

Simultaneous fit [PRL 119 (2017) 132001]

NNFF (this talk)

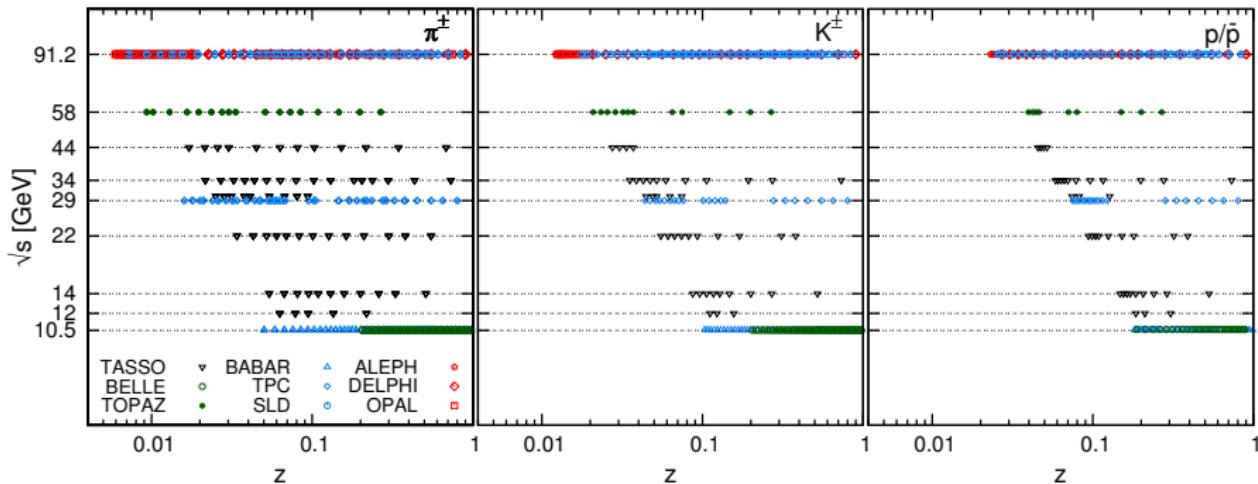
$\pi^\pm, K^\pm, p/\bar{p}$  [EPJ C77 (2017) 516]

$h^\pm$  [EPJ C78 (2018) 651]

# 1. Fragmentation Functions from lepton collisions

[EPJ C77 (2017) 516]

# The dataset



**CERN-LEP:** ALEPH [ZP C66 (1995) 353] DELPHI [EPJ C18 (2000) 203] OPAL [ZP C63 (1994) 181]

**KEK:** BELLE ( $n_f = 4$ ) [PRL 111 (2013) 062002] TOPAZ [PL B345 (1995) 335]

**DESY-PETRA:** TASSO [PL B94 (1980) 444, ZP C17 (1983) 5, ZP C42 (1989) 189]

**SLAC:** BABAR ( $n_f = 4$ ) [PR D88 (2013) 032011] SLD [PR D58 (1999) 052001] TPC [PRL 61 (1988) 1263]

$$\frac{d\sigma^h}{dz} = \frac{4\pi\alpha^2(Q^2)}{Q^2} \mathcal{F}_2^h(z, Q^2) \quad h = \pi^+ + \pi^-, K^+ + K^-, p + \bar{p} \quad \text{possibly normalised to } \sigma_{\text{tot}}$$

$$N_{\text{dat}}^{\pi^\pm} = 428$$

$$N_{\text{dat}}^{K^\pm} = 385$$

$$N_{\text{dat}}^{p/\bar{p}} = 360$$

# From observables to fragmentation functions

$$\mathcal{F}_2^h = \langle e^2 \rangle \left\{ C_{2,q}^S \otimes D_\Sigma^h + n_f C_{2,g}^S \otimes D_g^h + C_{2,q}^{NS} \otimes D_{NS}^h \right\}$$

$$\langle e^2 \rangle = \frac{1}{n_f} \sum_{q=1}^{n_f} \hat{e}_q^2 \quad D_\Sigma^h = \sum_{q=1}^{n_f} D_{q+}^h \quad D_{NS}^h = \sum_{q=1}^{n_f} \left( \frac{\hat{e}_q^2}{\langle e^2 \rangle} - 1 \right) D_{q+}^h \quad D_{q+}^h = D_q^h + D_{\bar{q}}^h$$

Coefficient functions and splitting functions known up to NNLO

[NPB 751 (2006) 18; NPB 749 (2006) 1; PLB 638 (2006) 61; NPB 845 (2012) 133]

$$\begin{aligned} F_2^{h, n_f=5} = & \frac{1}{5} \left[ (2\hat{e}_u^2 + 3\hat{e}_d^2) C_{2,q}^S + 3(\hat{e}_u^2 - \hat{e}_d^2) C_{2,q}^{NS} \right] \otimes \left( D_{u+}^h + D_{c+}^h \right) \\ & + \frac{1}{5} \left[ (2\hat{e}_u^2 + 3\hat{e}_d^2) C_{2,q}^S - 2(\hat{e}_u^2 - \hat{e}_d^2) C_{2,q}^{NS} \right] \otimes \left( D_{d+}^h + D_{s+}^h + D_{b+}^h \right) \\ & + (2\hat{e}_u^2 + 3\hat{e}_d^2) C_{2,g}^S \otimes D_g^h \end{aligned}$$

No sensitivity to individual quark and antiquark FFs

Limited sensitivity to flavour separation via the variation of  $\hat{e}_q$  with  $Q^2$   
 $\hat{e}_u^2/\hat{e}_d^2(Q^2 = 10 \text{ GeV}) \sim 4 \Rightarrow D_{u+}^h, D_{d+}^h + D_{s+}^h$ ;  $\hat{e}_u^2/\hat{e}_d^2(Q^2 = M_Z) \sim 0.8 \Rightarrow D_\Sigma^h$   
Flavor separation between  $uds$  and  $c, b$  quarks achieved thanks to tagged data

Direct sensitivity to  $D_g^h$  only beyond LO, as  $C_{2,g}^S$  is  $\mathcal{O}(\alpha_s^2)$ , and tenous  
Indirect sensitivity to  $D_g^h$  via scale violations in the time-like DGLAP evolution

# Fit settings

**Physical parameters:** consistent with the NNPDF3.1 PDF set [EPJC77 (2017) 663]

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

**Solution of DGLAP equations:** numerical solution in  $z$ -space as implemented in APFEL  
extensive benchmark performed up to NNLO [JHEP 1503 (2015) 046]

**Parametrisation:** each FF is parametrised with a feed-forward neural network (2-5-3-1)

$$D_i^h(Q_0, z) = \text{NN}(x) - \text{NN}(1), \quad Q_0 = 5 \text{ GeV}$$

$$h = \pi^+ + \pi^-, h = K^+ + K^-, h = p + \bar{p} \quad i = u^+, d^+ + s^+, c^+, b^+, g$$

we assume charge conjugation, from which  $D_{q^+}^{\pi^+} = D_{q^+}^{\pi^-}$

initial scale above  $m_b$ , but below the lowest c.m. energy of the data, avoid threshold crossing

**Heavy flavours:** heavy-quark FFs are parametrised independently at the initial scale  $Q_0$

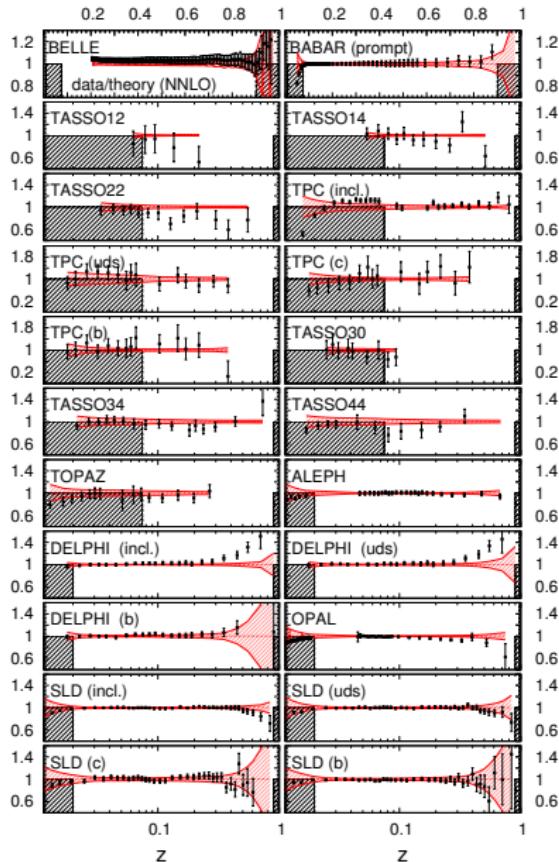
**Kinematic cuts:**  $z \rightarrow 0$ : contributions  $\propto \ln z$ ;  $z \rightarrow 1$ : contributions  $\propto \ln(1-z)$

$$z_{\min} = 0.075, z_{\max} = 0.02 (\sqrt{s} = M_Z); z_{\max} = 0.90$$

**Momentum sum rule:** check a posteriori that

$$\sum_{h=\pi^\pm, K^\pm, p/\bar{p}} \int_{z_{\min}}^1 dz z D_i^h(z, Q) < N \quad N \begin{cases} = 1 & \text{for } i = g \\ = 2 & \text{for } i = u^+, c^+, b^+ \\ = 4 & \text{for } i = d^+ + s^+ \end{cases}$$

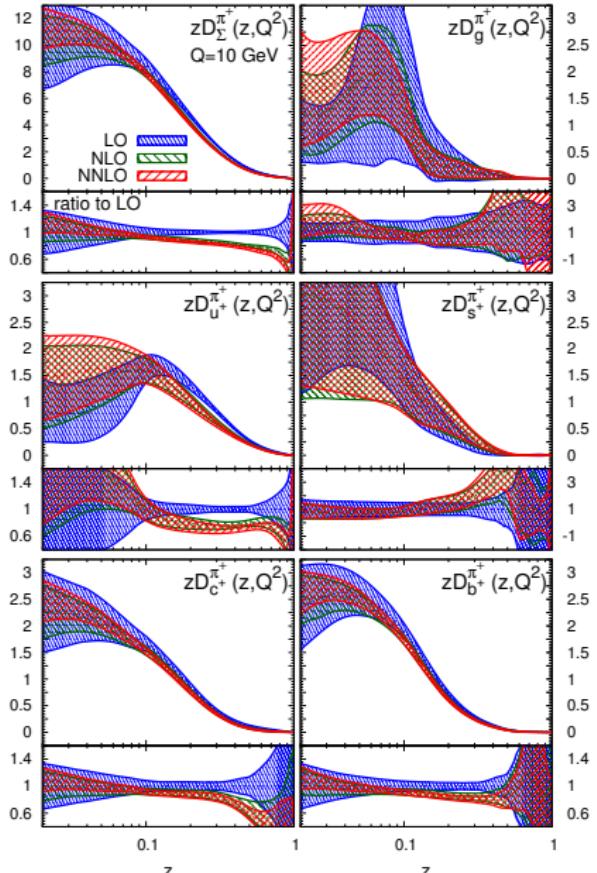
# Fit quality: $\pi^+$



Exp.	$N_{\text{dat}}$	NNLO theory	
		$\chi^2/N_{\text{dat}}$	remarks
BELLE	70	0.09	lack of correlations
BABAR	40	0.78	✓
TASSO12	4	0.87	small sample
TASSO14	9	1.70	
TASSO22	8	1.91	} data fluctuations
TPC	13	0.85	
TPC-UDS	6	0.49	✓
TPC-C	6	0.52	✓
TPC-B	6	1.43	✓
TASSO34	9	1.00	✓
TASSO44	6	2.34	data fluctuations
TOPAZ	5	0.80	
ALEPH	23	0.78	✓
DELPHI	21	1.86	tension with OPAL
DELPHI-UDS	21	1.54	
DELPHI-B	21	0.95	
OPAL	24	1.84	tension with DELPHI
SLD	34	0.83	
SLD-UDS	34	0.52	✓
SLD-C	34	1.06	✓
SLD-B	34	0.36	✓
<b>TOTAL</b>	<b>428</b>	<b>0.87</b>	✓

Overall good description of the dataset  
 Signs of tension OPAL vs DELPHI (inclusive)  
 Anomalously small  $\chi^2/N_{\text{dat}}$  for BELLE

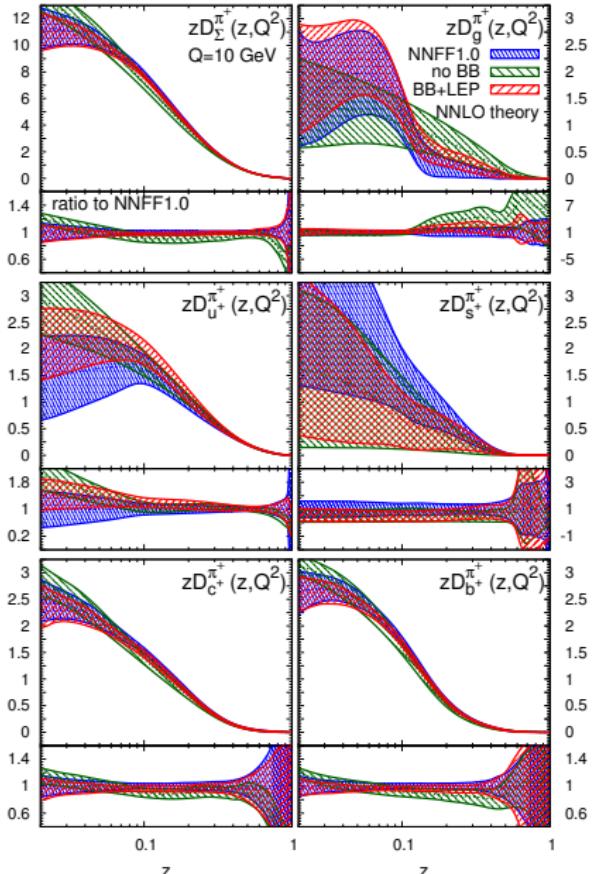
# Dependence upon perturbative order: $\pi^+$



Exp.	$N_{\text{dat}}$	LO $\chi^2/N_{\text{dat}}$	NLO $\chi^2/N_{\text{dat}}$	NNLO $\chi^2/N_{\text{dat}}$
BELLE	70	0.60	0.11	0.09
BABAR	40	1.91	1.77	0.78
TASSO12	4	0.70	0.85	0.87
TASSO14	9	1.55	1.67	1.70
TASSO22	8	1.64	1.91	1.91
TPC	13	0.46	0.65	0.85
TPC-UDS	6	0.78	0.55	0.49
TPC-C	6	0.55	0.53	0.52
TPC-B	6	1.44	1.43	1.43
TASSO34	9	1.16	0.98	1.00
TASSO44	6	2.01	2.24	2.34
TOPAZ	5	1.04	0.82	0.80
ALEPH	23	1.68	0.90	0.78
DELPHI	21	1.44	1.79	1.86
DELPHI-UDS	21	1.30	1.48	1.54
DELPHI-B	21	1.21	0.99	0.95
OPAL	24	2.29	1.88	1.84
SLD	34	2.33	1.14	0.83
SLD-UDS	34	0.95	0.65	0.52
SLD-C	34	3.33	1.33	1.06
SLD-B	34	0.45	0.38	0.36
<b>TOTAL</b>	428	1.44	1.02	0.87

Excellent perturbative convergence  
 FFs almost stable from NLO to NNLO  
 LO FF uncertainties larger than HO

# Dependence upon the dataset: $\pi^+$



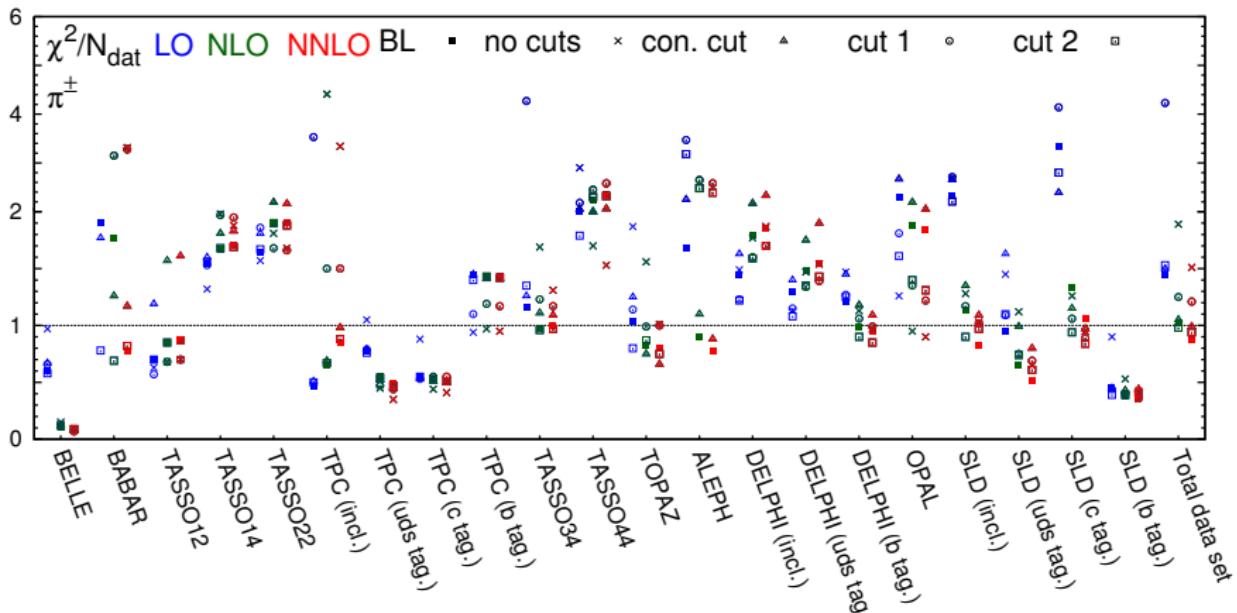
NNLO theory Exp.	$N_{\text{dat}}$	NNFF1.0 $\chi^2/N_{\text{dat}}$	no BB $\chi^2/N_{\text{dat}}$	BB+LEP $\chi^2/N_{\text{dat}}$
BELLE	70	0.09	[4.92]	0.09
BABAR	40	0.78	[144]	0.88
TASSO12	4	0.87	0.52	[0.87]
TASSO14	9	1.70	1.38	[1.71]
TASSO22	8	1.91	1.29	[2.15]
TPC	13	0.85	2.12	[2.15]
TPC-UDS	6	0.49	0.54	[0.77]
TPC-C	6	0.52	0.74	[0.58]
TPC-B	6	1.43	1.60	[1.48]
TASSO34	9	1.00	1.17	[1.38]
TASSO44	6	2.34	2.52	[1.97]
TOPAZ	5	0.80	0.92	[1.72]
ALEPH	23	0.78	0.57	0.74
DELPHI	21	1.86	1.97	1.82
DELPHI-UDS	21	1.54	1.56	1.42
DELPHI-B	21	0.95	1.01	0.95
OPAL	24	1.84	1.75	1.92
SLD	34	0.83	0.87	0.95
SLD-UDS	34	0.52	0.53	0.63
SLD-C	34	1.06	0.69	0.96
SLD-B	34	0.36	0.49	0.37
<b>TOTAL</b>		0.87	1.06	0.82

no BB: larger uncertainties; different gluon shape and different light flavour separation

BB+LEP: comparable uncertainties; slightly different size of gluon and light flavoured quarks

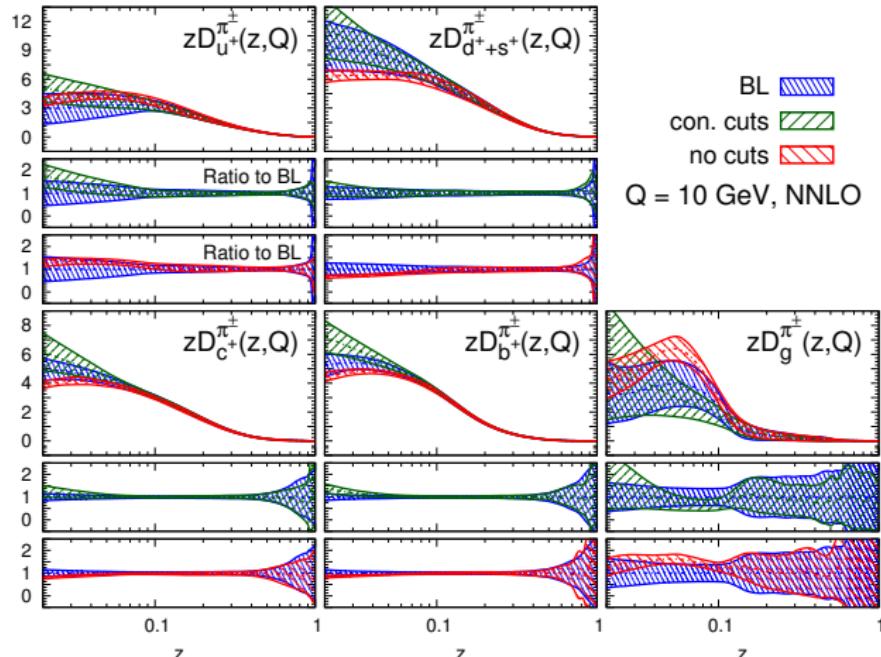
# Dependence upon kinematic cuts: $\pi^+$

BL $z_{\min}^{(m_Z)}$	$z_{\min}$	no cuts $z_{\min}^{(m_Z)}$	$z_{\min}$	con. cut $z_{\min}^{(m_Z)}$	$z_{\min}$	cut1 $z_{\min}^{(m_Z)}$	$z_{\min}$	cut2 $z_{\min}^{(m_Z)}$	$z_{\min}$
0.02	0.075	0.00	0.00	0.05	0.10	0.01	0.05	0.01	0.075

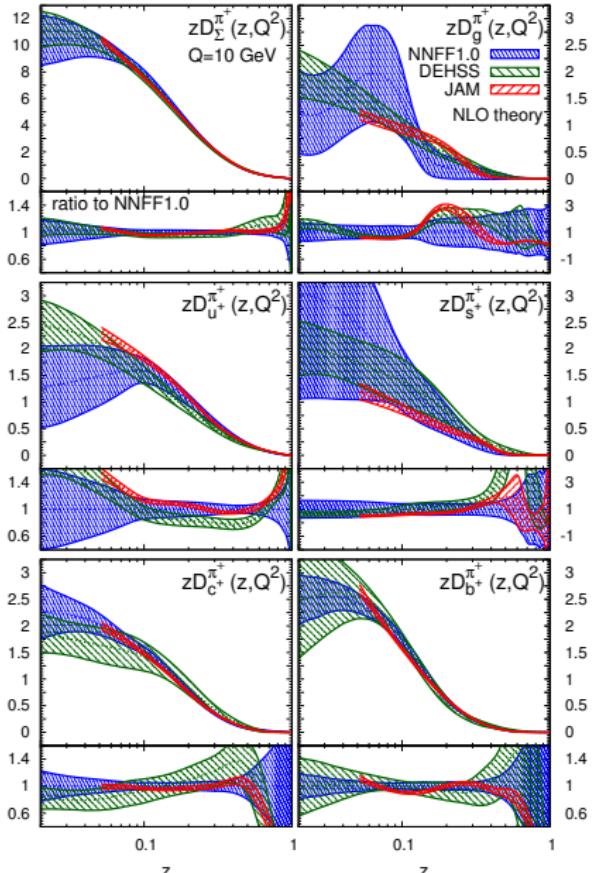


# Dependence upon kinematic cuts: $\pi^+$

BL	no cuts		con. cut		cut1		cut2		
$z_{\min}^{(m_Z)}$	$z_{\min}$								
0.02	0.075	0.00	0.00	0.05	0.10	0.01	0.05	0.01	0.075



# Comparison with other FF determinations: $\pi^+$



DEHSS [PRD 91 (2015) 014035]  
(+SIDIS +PP)

JAM [PRD 94 (2016) 114004]  
(almost same dataset as NNFF1.0)

different cuts at small  $z$

$D_{\Sigma}^{\pi^+}$ : excellent mutual agreement  
both c.v. and unc. (bulk of the dataset)

$D_g^{\pi^+}$ : slight disagreement  
different shapes, larger uncertainties  
DEHSS: data; JAM: parametrisation

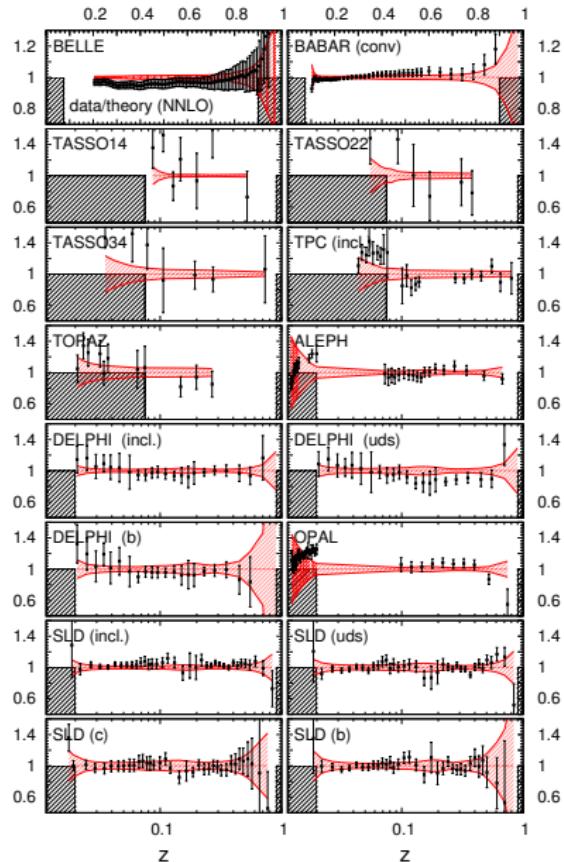
$D_{u^+}^{\pi^+}$ ,  $D_{s^+}^{\pi^+}$ : good overall agreement  
excellent with JAM, though larger uncertainties  
slightly different shape w.r.t. DHESS (dataset)

$D_{c^+}^{\pi^+}$ ,  $D_{b^+}^{\pi^+}$ : good overall agreement  
excellent with JAM, same uncertainties  
slightly different shape w.r.t. DHESS (dataset)

# Fit quality: $K^+$

Exp.	$N_{\text{dat}}$	$\chi^2/N_{\text{dat}}$	NNLO theory remarks
BELLE	70	0.32	lack of correlations
BABAR	43	0.95	✓
TASSO12	3	1.02	
TASSO14	9	2.07	} small sample
TASSO22	6	2.62	
TPC	13	1.01	✓
TASSO34	5	0.36	} small sample
TOPAZ	3	0.99	
ALEPH	18	0.56	✓
DELPHI	22	0.34	✓
DELPHI-UDS	22	1.32	✓
DELPHI-B	22	0.52	✓
OPAL	10	1.66	tension with other $M_Z$ data
SLD	35	0.57	✓
SLD-UDS	35	0.93	✓
SLD-C	34	0.38	✓
SLD-B	35	0.62	✓
<b>TOTAL</b>	<b>385</b>	<b>0.73</b>	✓

Overall good description of the dataset  
 Excellent BELLE/BABAR consistency  
 Signs of tension OPAL vs DELPHI (inclusive)  
 Anomalously small  $\chi^2/N_{\text{dat}}$  for BELLE  
 Dependence upon the data set and kin cuts  
 similar to pions

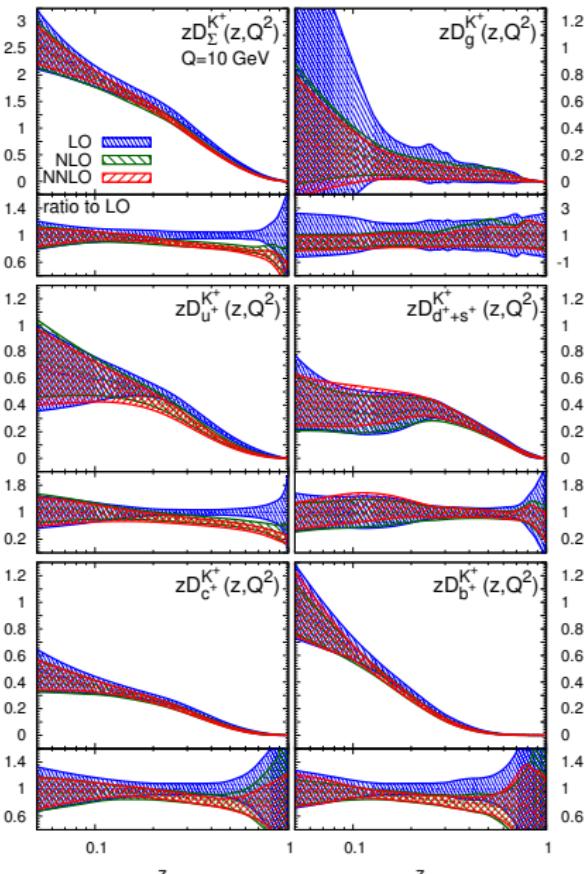


# Dependence upon perturbative order: $K^+$

Exp.	$N_{\text{dat}}$	LO $\chi^2/N_{\text{dat}}$	NLO $\chi^2/N_{\text{dat}}$	NNLO $\chi^2/N_{\text{dat}}$
BELLE	70	0.21	0.32	0.32
BABAR	43	2.86	1.11	0.95
TASSO12	3	1.10	1.03	1.02
TASSO14	9	2.17	2.13	2.07
TASSO22	6	2.14	2.77	2.62
TPC	13	0.94	1.09	1.01
TASSO34	5	0.27	0.44	0.36
TOPAZ	3	0.61	1.19	0.99
ALEPH	18	0.47	0.55	0.56
DELPHI	22	0.28	0.33	0.34
DELPHI-UDS	22	1.38	1.49	1.32
DELPHI-B	22	0.58	0.49	0.52
OPAL	10	1.67	1.57	1.66
SLD	35	0.86	0.62	0.57
SLD-UDS	35	1.31	1.02	0.93
SLD-C	34	0.92	0.47	0.38
SLD-B	35	0.59	0.67	0.62
<b>TOTAL</b>	<b>385</b>	<b>1.02</b>	<b>0.78</b>	<b>0.73</b>

Excellent perturbative convergence  
 FFs almost stable from NLO to NNLO  
 LO FF uncertainties larger than HO

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



# Comparison with other FF determinations: $K^+$

DEHSS [PRD 95 (2017) 094019]  
(+SIDIS +PP)

JAM [PRD 94 (2016) 114004]  
(almost same dataset as NNFF1.0)

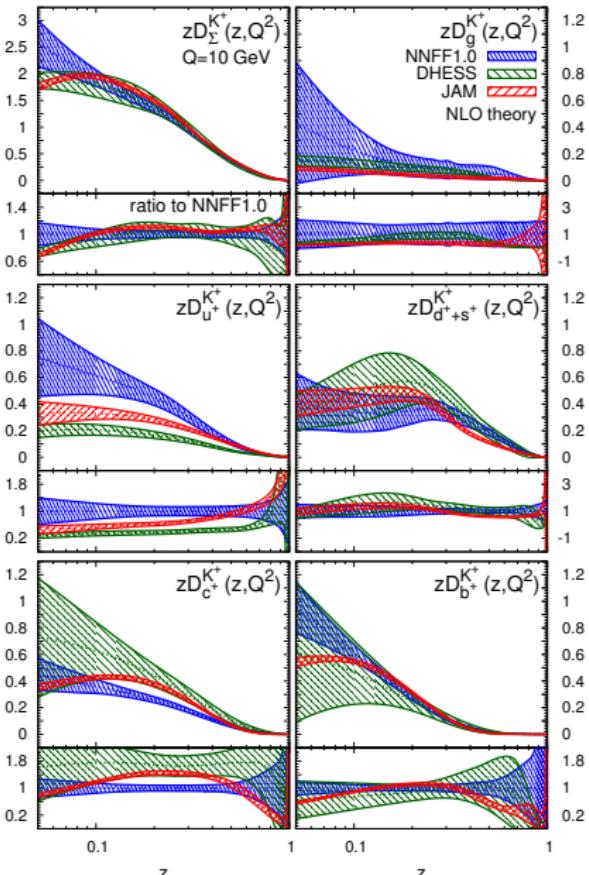
$D_{\Sigma}^{\pi^+}$ : excellent agreement (both c.v. and unc.)  
bulk of the dataset

$D_g^{\pi^+}$ : good mutual agreement  
similar shapes, larger uncertainties  
DEHSS: data; JAM: parametrisation

$D_{u^+}^{\pi^+}$ : mutual sizable disagreement  
differences in dataset and parametrisation  
comparable uncertainties in the data region

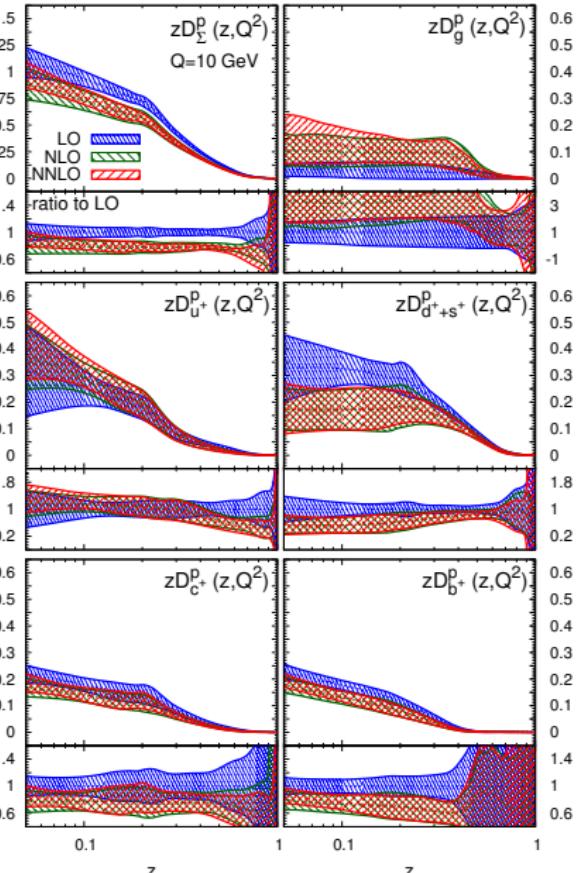
$D_{d^+}^{\pi^+} + D_{s^+}^{\pi^+}$ : fair mutual agreement  
differences in dataset and parametrisation  
comparable uncertainties in the data region

$D_{c^+}^{\pi^+}, D_{b^+}^{\pi^+}$ : excellent mutual agreement  
uncertainties similar to JAM  
DHESS shows inflated uncertainties



# Dependence upon perturbative order: $p/\bar{p}$

Exp.	$N_{\text{dat}}$	LO	NLO	NNLO
		$\chi^2/N_{\text{dat}}$	$\chi^2/N_{\text{dat}}$	$\chi^2/N_{\text{dat}}$
BABAR	43	0.10	0.31	0.50
BELLE	29	4.74	2.75	1.25
TASSO12	3	0.69	0.70	0.72
TASSO14	9	1.32	1.25	1.22
TASSO22	9	0.98	0.92	0.93
TPC	20	1.04	1.10	1.08
TASSO30	2	0.25	0.19	0.18
TASSO34	6	0.82	0.81	0.78
TOPAZ	4	0.79	1.21	0.19
ALEPH	26	1.36	1.43	1.28
DELPHI	22	0.48	0.49	0.49
DELPHI-UDS	22	0.47	0.46	0.45
DELPHI-B	22	0.89	0.89	0.91
SLD	36	0.66	0.65	0.64
SLD-UDS	36	0.77	0.76	0.78
SLD-C	36	1.22	1.22	1.21
SLD-B	35	1.12	1.29	1.33
<b>TOTAL</b>	<b>360</b>	<b>1.31</b>	<b>1.13</b>	<b>0.98</b>



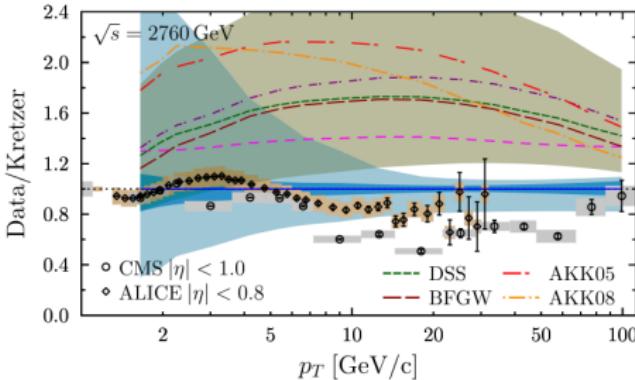
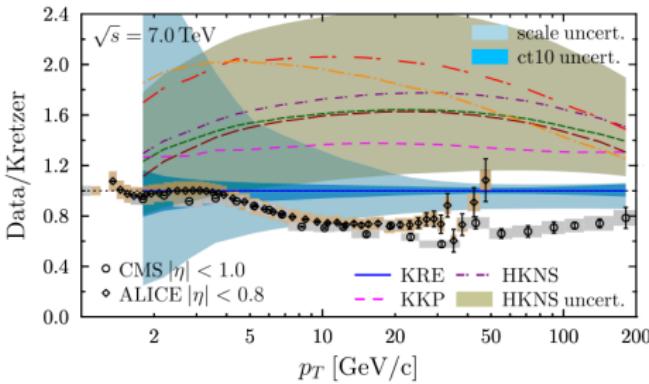
Excellent perturbative convergence  
 FFs almost stable from NLO to NNLO  
 LO FF uncertainties larger than HO  
 Dependence upon data set and kin cuts  
 similar to pions and kaons

## 2. Fragmentation Functions from hadron collisions

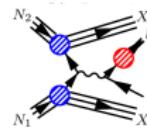
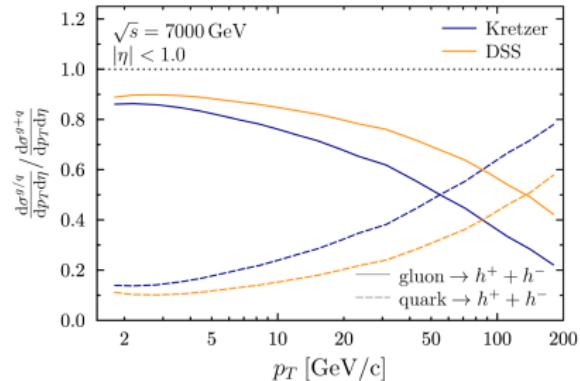
[EPJ C78 (2018) 651]

# Motivation

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



Figures taken from [NPB 883 (2014) 615]



$$E_h \frac{d^3 \sigma^{h\pm}}{d^3 p^h} = \sum_{a,b,c} \hat{\sigma}_{ab}^c \otimes f_a \otimes f_b \otimes D_c^h$$

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

→ Can this discrepancy be reconciled?

# A strategy to determine FFs from hadronic data

Construct a prior set of Monte Carlo replicas from  $e^+e^-$  data: NNFF1.0h

Reweight NNFF1.0h with the hadronic data to obtain a posterior set of FFs: NNFF1.1h

## Construction of the prior: fit quality

Repeat the NNFF1.0 analysis, but for unidentified charged hadron FFs  
(measurements are also available for the longitudinal structure function  $F_L$ )

**CERN-LEP:** ALEPH [PLB 357 (1995) 487] DELPHI [EPJC5 (1998) 585; C6 (1999) 19] OPAL [EPJC7 (1999) 369]

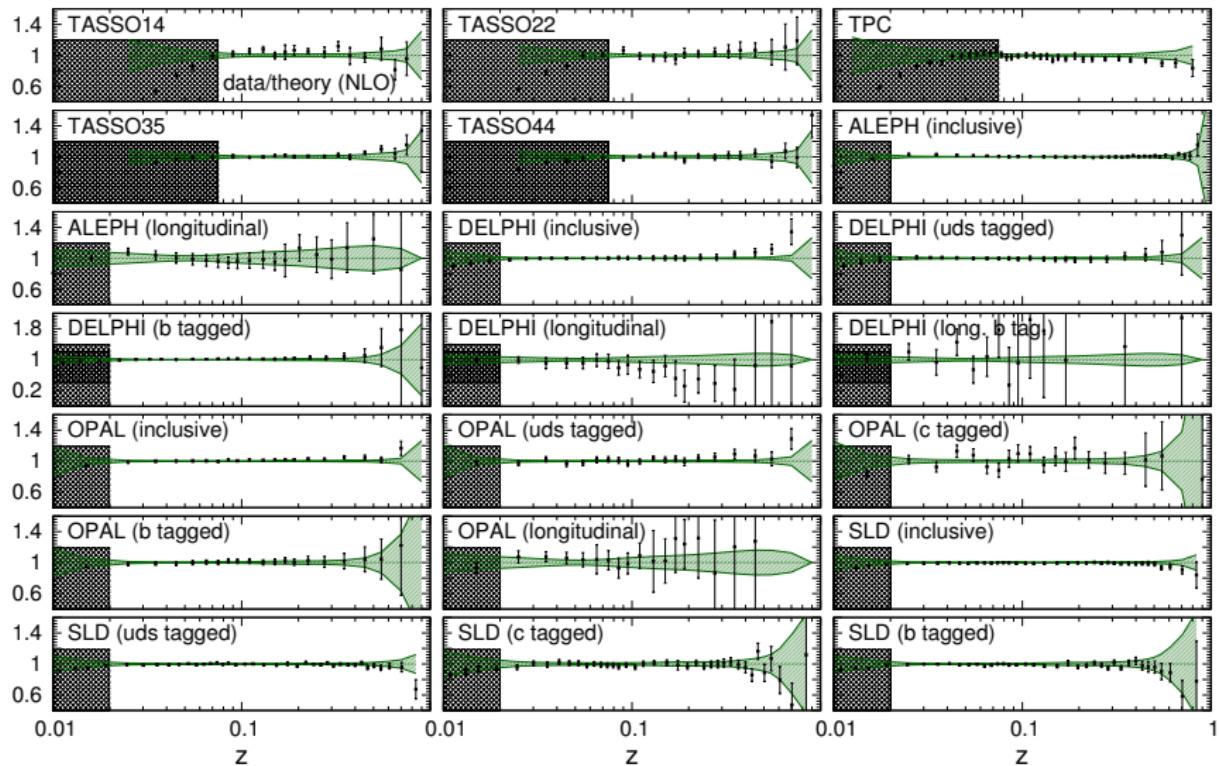
**DESY-PETRA:** TASSO [ZPC47 (1990) 187]

**SLAC:** SLD [PRD 69 (2004) 072003] TPC [PRL 61 (1988) 1263]

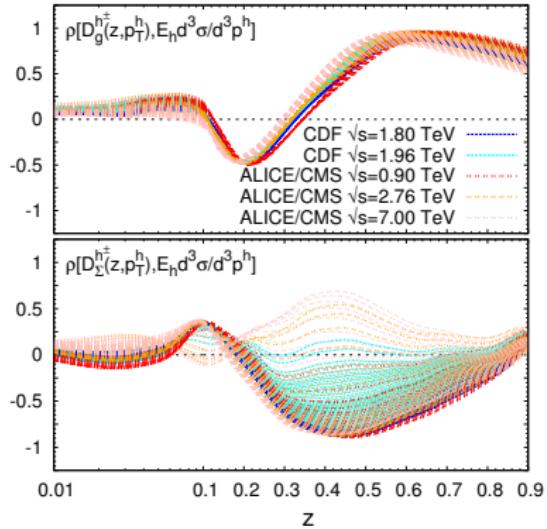
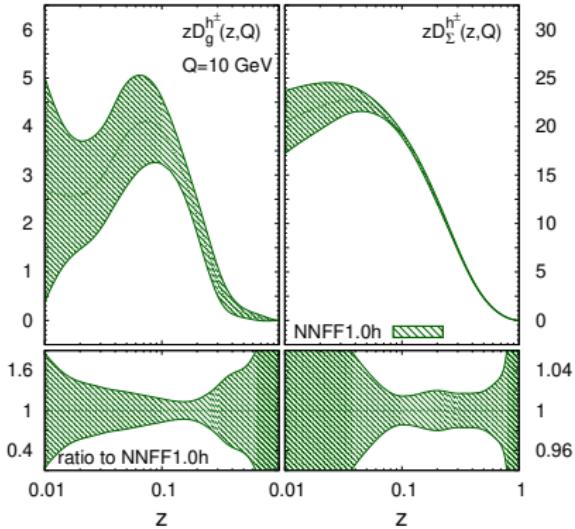
Experiment	$\sqrt{s}$	$N_{\text{dat}}$	$\chi^2_{\text{dat}}$	Experiment	$\sqrt{s}$	$N_{\text{dat}}$	$\chi^2_{\text{dat}}$	Experiment	$\sqrt{s}$	$N_{\text{dat}}$	$\chi^2_{\text{dat}}$
TASSO14	14.00	15	<b>1.23</b>	TASSO22	22.00	15	<b>0.51</b>	TPC	29.00	21	<b>1.65</b>
TASSO35	35.00	15	<b>1.14</b>	TASSO44	44.00	15	<b>0.68</b>	ALEPH	91.20	32	<b>1.04</b>
ALEPH (L)	91.20	19	<b>0.36</b>	DELPHI	91.20	21	<b>0.65</b>	DELPHI (uds)	91.20	21	<b>0.17</b>
DELPHI (b)	91.20	20	<b>0.82</b>	DELPHI (L)	91.20	20	<b>0.72</b>	DELPHI (Lb)	91.20	20	<b>0.44</b>
OPAL	91.20	20	<b>2.41</b>	OPAL (uds)	91.20	20	<b>0.90</b>	OPAL (c)	91.20	20	<b>0.61</b>
OPAL (b)	91.20	20	<b>0.21</b>	OPAL (L)	91.20	20	<b>0.31</b>	SLD	91.28	34	<b>0.75</b>
SLD (uds)	91.28	34	<b>1.03</b>	SLD (c)	91.28	34	<b>0.62</b>	SLD (b)	91.28	34	<b>0.97</b>

$\sqrt{s}$  in GeV

# Construction of the prior: data/theory agreement



# Construction of the prior: fragmentation functions



Consider all the available data from the Tevatron and the LHC

CDF [[PRD 79 \(2009\) 112005](#)] CMS [[JHEP 08 \(2011\) 086; EPJ C72 \(2012\) 1945](#)] ALICE [[EPJ C73 \(2013\) 2662](#)]

What is the expected sensitivity of these measurements to the fragmentation functions?

$$\rho[A, B] = \frac{\langle AB \rangle_{\text{rep}} - \langle A \rangle_{\text{rep}} \langle B \rangle_{\text{rep}}}{\sigma_A \sigma_B}$$

$$D_g^{h\pm}: z \gtrsim 0.4$$

$$D_\Sigma^{h\pm}: 0.2 \lesssim z \lesssim 0.7$$

# Reweighting: fit quality

Apply  $p_T^h > p_{T,\text{cut}}^h = 7 \text{ GeV}$  (to ensure accuracy of fixed-order theory)

Most of SppS and PHENIX data (low  $p_T$ , low  $\sqrt{s}$ ) are excluded by this cut

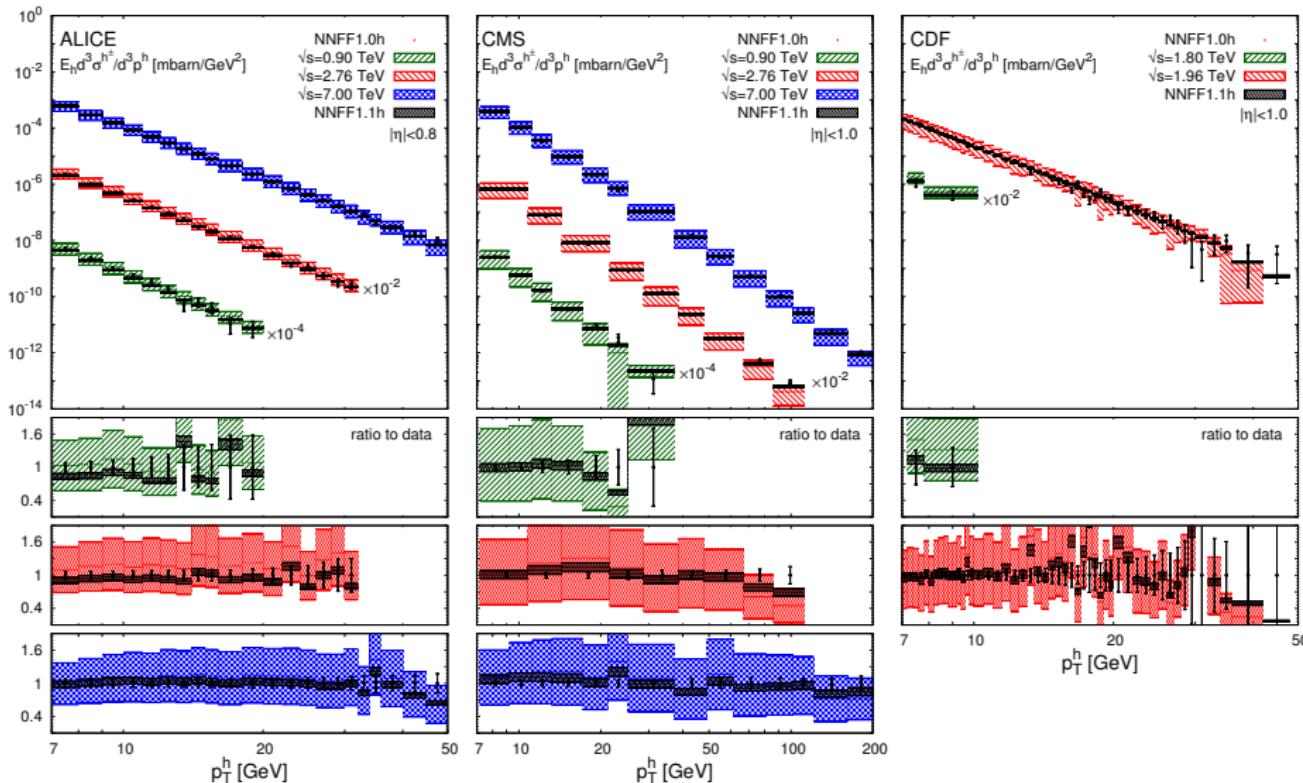
Reweight NNFF1.0h with the remaining collider data

Process	Experiment	$\sqrt{s} [\text{TeV}]$	$N_{\text{dat}}$	$\chi^2_{\text{in}}/N_{\text{dat}}$	$\chi^2_{\text{rw}}/N_{\text{dat}}$	$N_{\text{eff}}$
SIA			471 (527)	0.83	0.83	—
$pp$	ALICE	0.90	11 (54)	4.94	1.88	1012
		2.76	27 (60)	13.3	0.82	574
		7.00	22 (65)	6.03	0.53	779
	CMS	0.90	7 (20)	4.20	0.70	1206
		2.76	9 (22)	10.6	1.24	579
		7.00	14 (27)	12.4	1.64	396
	CDF	1.80	2 (49)	3.32	0.20	1420
		1.96	50 (230)	2.93	1.23	735
			603 (1054)	6.54	1.11	407

The description of the data set in the prior is almost unaffected

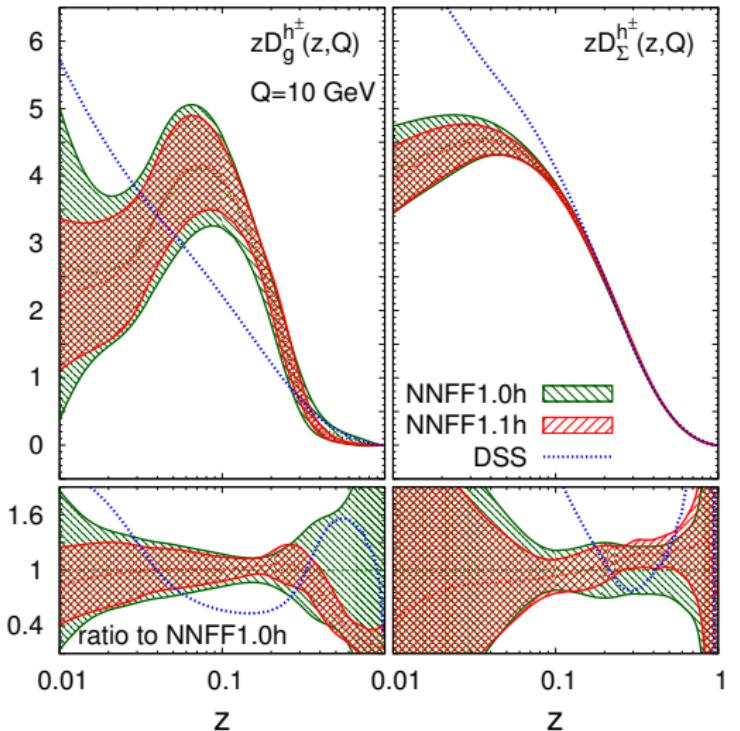
Excellent description/consistency of  $e^+e^-$  and  $pp$  data

# Reweighting: observables



Significant reduction of the uncertainties for all data sets

# Reweighting: fragmentation functions



Modifications in shape

$D_g^{h^\pm}$  slightly harder  
for  $0.1 \lesssim z \lesssim 0.3$

$D_g^{h^\pm}$  significantly softer  
for  $0.3 \lesssim z \lesssim 0.9$

$D_\Sigma^{h^\pm}$  almost stable  
slightly reduced for  $0.1 \lesssim z \lesssim 0.4$

Reduction of uncertainties

$D_g^{h^\pm}$  reduced  
from 20%-60% to 10%-15%  
for  $z \gtrsim 0.1$

$D_\Sigma^{h^\pm}$  reduced  
from 2% to  $\simeq 1\%$   
for  $0.1 \lesssim z \lesssim 0.4$

The NNFF1.1h shape is significantly different from the DSS [PRD 76 (2007) 074033] shape

# Dependence on the value of $p_{T,\text{cut}}^h$

Examine the dependence of the results upon the value of  $p_{T,\text{cut}}^h$

Vary  $p_{T,\text{cut}}^h$  by incremental steps of 1 GeV in the range  $5 \text{ GeV} \leq p_{T,\text{cut}}^h \leq 10 \text{ GeV}$

Experiment	5 GeV		6 GeV		7 GeV		8 GeV		9 GeV		10 GeV	
	$\frac{\chi^2_{\text{rw}}}{N_{\text{dat}}}$	$N_{\text{dat}}$										
CDF	1.30	7	0.28	4	0.10	2	0.04	1	—	—	—	—
	1.32	60	1.26	55	1.23	50	1.20	45	1.15	40	1.15	35
CMS	0.93	10	0.67	8	0.70	7	0.71	7	0.80	6	0.80	6
	1.38	11	1.27	10	1.24	9	1.17	9	1.22	8	1.16	8
ALICE	2.01	17	1.80	15	1.64	14	1.52	14	1.47	13	1.40	13
	2.56	15	2.05	13	1.88	11	1.71	10	1.51	9	1.52	8
	0.61	21	0.72	19	0.82	17	0.89	16	0.98	15	1.08	14
Total	0.56	26	0.52	24	0.53	22	0.55	21	0.57	20	0.60	19
	1.27	167	1.14	148	1.11	132	1.09	123	1.08	111	1.08	103

The overall fit quality turns out to be very similar for  $p_{T,\text{cut}}^h \geq 6 \text{ GeV}$

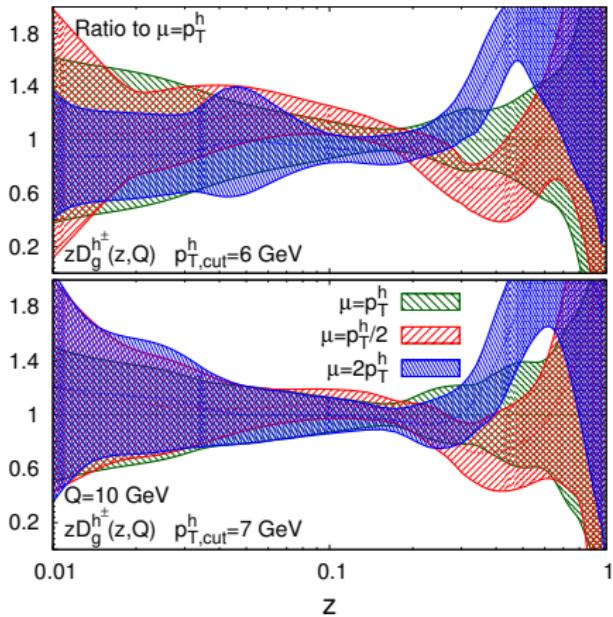
What is the best cut in the restricted range  $6 \text{ GeV} \leq p_{T,\text{cut}}^h \leq 10 \text{ GeV}$ ?

# Dependence on the value of $p_{T,\text{cut}}^h$

What is the size of missing higher order uncertainties?  
Repeat the reweighting exercise with different values of the scale  $\mu$

How are FFs affected by varying  $p_{T,\text{cut}}^h$ ?

Repeat the reweighting exercise with different values of  $p_{T,\text{cut}}^h$



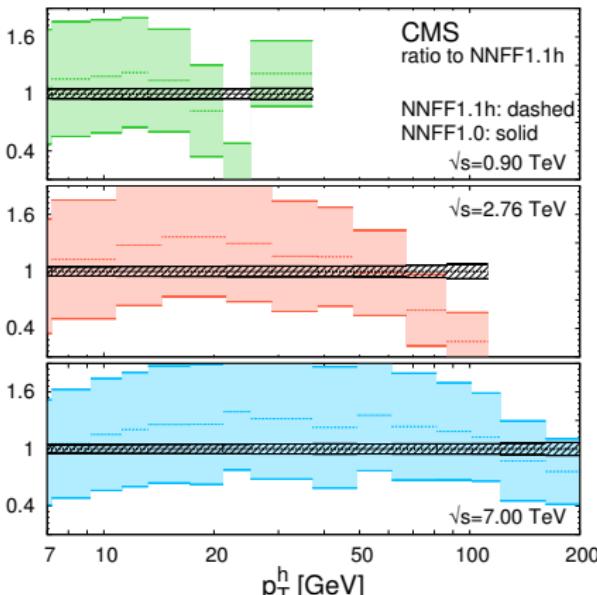
# Compatibility with NNFF1.0

Fragmentation functions should satisfy “conservation of hadrons“

$$D_i^{h^\pm} = D_i^{\mathcal{H}} + D_i^{\text{res}^\pm} \quad D_i^{\mathcal{H}} = D_i^{\pi^\pm} + D_i^{K^\pm} + D_i^{p/\bar{p}} \quad \forall i = q, \bar{q}, g$$

Are the FFs for  $h^\pm$  (NNFF1.1h) and the FFs for  $\pi^\pm$ ,  $K^\pm$  and  $p/\bar{p}$  (NNFF1.0) compatible?

$$E_h \frac{d^3\sigma^{h^\pm}}{d^3p^h} > \sum_{\mathcal{H}=\pi^\pm, K^\pm, p/\bar{p}} E_h \frac{d^3\sigma^{\mathcal{H}}}{d^3p^h} \quad M_i^{h^\pm}(Q) \gtrsim M_i^{\text{light}}(Q)$$



$Q = 5 \text{ GeV}$	NNFF1.1h	NNFF1.0
$i$	$M_i^{h^\pm}(Q)$	$M_i^{\text{light}}(Q)$
$g$	$0.86 \pm 0.06$	$0.80 \pm 0.18$
$u^+$	$1.24 \pm 0.07$	$1.42 \pm 0.12$
$d^+ + s^+$	$2.05 \pm 0.08$	$2.07 \pm 0.27$
$c^+$	$1.09 \pm 0.03$	$1.01 \pm 0.08$
$b^+$	$1.06 \pm 0.02$	$0.98 \pm 0.08$

$$M_i^{h^\pm}(Q) \equiv \int_{z_{\min}}^1 dz z D_i^{h^\pm}(z, Q)$$

$$M_i^{\text{light}}(Q) \equiv \sum_{\mathcal{H}=\pi^\pm, K^\pm, p/\bar{p}} \int_{z_{\min}}^1 dz z D_i^{\mathcal{H}}(z, Q)$$

### 3. To conclude

# Summary

- ① A number of hard-scattering processes require an appropriate knowledge of FFs
  - ▶ probing nucleon momentum, spin and flavour
  - ▶ underlying spatial distributions and the dynamics of nuclear matter
- ② FFs are poorly known in comparison to PDFs
  - ▶ limited set of available data, observables often require PDFs and FFs simultaneously
  - ▶ troubles in describing some observables in  $pp$  and SIDIS from current FF sets
- ③ New analyses based on the NNPDF methodology
  - ▶ NNFF1.0 at LO, NLO and NNLO, based on SIA data for  $\pi^\pm$ ,  $K^\pm$  and  $p/\bar{p}$   
detailed study of the stability of the results upon variations of the data set/kin cuts  
FF uncertainties (gluon) seem to be underestimated in previous determinations  
differences in shapes, to be further investigated  
applicability limited by insensitivity to complete flavour decomposition
  - ▶ NNFF1.1h at NLO, based on SIA and  $pp$  data for  $h^\pm$   
significant impact of  $pp$  data on FF shape and uncertainty  
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**Thank you**

# Parametrisation: two alternative choices

$$zD_i^h(z, Q_0^2) = z^{a_i^h} (1-z)^{b_i^h} \mathcal{F}_i^h(z, \{\mathbf{c}\})$$

- ① Standard parametrisation, e.g.

$$\mathcal{F}_i^h(z, \{\mathbf{c}\}) = \frac{1 + \gamma_i^h (1-z)^{\delta_i^h}}{B[2 + a_i^h, b_i^h + 1] + \gamma_i^h B[2 + a_i^h, b_i^h + \delta_i^h + 1]}$$

in terms of a (relatively) small set of parameters ( $\mathcal{O}(30)$  per PDF set)

$$\{\mathbf{a}\} = \{a_i^h, b_i^h\} \cup \{\mathbf{c}\} = \{a_i^h, b_i^h, \gamma_i^h, \delta_i^h\}$$

- ⇒ smooth behavior (a desirable feature for a PDF)
- ⇒ potential source of bias if the parametrisation is too rigid

- ② Redundant parametrisation, e.g.

$\mathcal{F}_i^h(z, \{\mathbf{c}\})$  is a neural network

in terms of a huge set of parameters ( $\mathcal{O}(200)$  per PDF set)

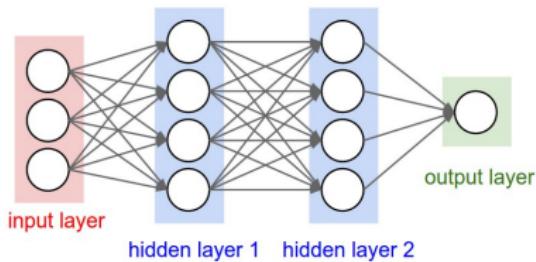
$$\{\mathbf{a}\} = \{\omega_{ij}^{(L-1), f_i^h}, \theta_i^{(L), f_i^h}\}$$

- ⇒ potentially non-smooth
- ⇒ bias due to the parametrisation reduced as much as possible

# Parametrisation: what a neural network exactly is?

A convenient **functional form** providing a **flexible** parametrization used as a generator of random functions in the FF space

## EXAMPLE: MULTI-LAYER FEED-FORWARD PERCEPTRON



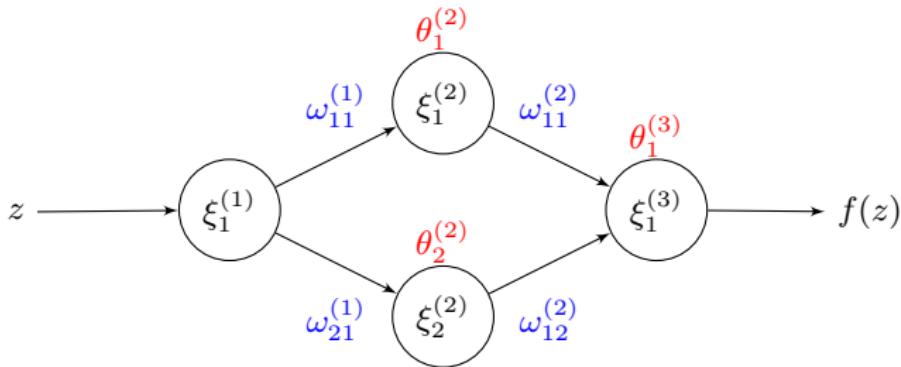
$$\xi_i^{(l)} = g \left( \sum_j^{n_l-1} \omega_{ij}^{(l-1)} \xi_j^{(l-1)} - \theta_i^{(l)} \right)$$

$$g(y) = \frac{1}{1 + e^{-y}}$$

- made of neurons grouped into layers (define the architecture)
- each neuron receives input from neurons in the preceding layer (feed-forward NN)
- activation  $\xi_i^{(l)}$  determined by a set of parameters (**weights** and **thresholds**)
- activation determined according to a **non-linear function** (except the last layer)

# Parametrisation: what a neural network exactly is?

EXAMPLE: THE SIMPLEST 1-2-1 MULTI-LAYER FEED-FORWARD PERCEPTRON



$$f(z) \equiv \xi_1^{(3)} = \left\{ 1 + \exp \left[ \theta_1^{(3)} - \frac{\omega_{11}^{(2)}}{1 + e^{\theta_1^{(2)} - x\omega_{11}^{(1)}}} - \frac{\omega_{12}^{(2)}}{1 + e^{\theta_2^{(2)} - x\omega_{21}^{(1)}}} \right] \right\}^{-1}$$

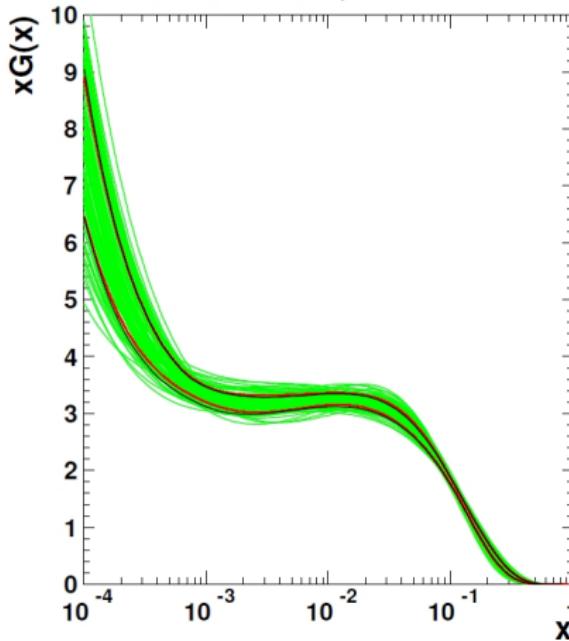
Recall:

$$\xi_i^{(l)} = g \left( \sum_j^{n_l-1} \omega_{ij}^{(l-1)} \xi_j^{(l-1)} - \theta_i^{(l)} \right) ; \quad g(z) = \frac{1}{1 + e^{-z}}$$

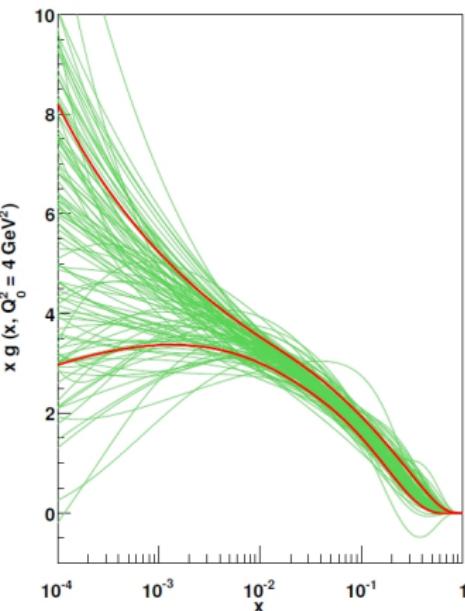
# Parametrisation: standard vs redundant

HERA-LHC 2009 PDF benchmark

Fit vs H1PDF2000,  $Q^2 = 4.$  GeV $^2$



simple parametrization



redundant parametrization (NN)

# Parameter optimisation

Optimisation usually performed by means of simple gradient descent:  
compute and minimise the gradient of the fit quality with respect to the fit parameters

$$\frac{\partial \chi^2}{\partial a_i}, \quad \text{for } i = 1, \dots, N_{\text{par}} \quad \chi^2 = \sum_{i,j}^{N_{\text{dat}}} (T_i[\{\mathbf{a}\}] - D_i) (\text{cov}^{-1})_{ij} (T_j[\{\mathbf{a}\}] - D_j)$$

$$(\text{cov})_{ij} = \delta_{ij} s_i^2 + \left( \sum_{\alpha}^{N_c} \sigma_{i,\alpha}^{(c)} \sigma_{j,\alpha}^{(c)} + \sum_{\alpha}^{N_{\mathcal{L}}} \sigma_{i,\alpha}^{(\mathcal{L})} \sigma_{j,\alpha}^{(\mathcal{L})} \right) D_i D_j$$

Optimisation should minimise the noise in the  $\chi^2$  driven by noisy experimental data

Additional complications in case of a redundant parametrisation (huge parameter space)

- ① need to explore the parameter space as uniformly as possible  
(in order to avoid stopping the fit in a local minimum)  
→ genetic algorithms
- ② need for a computationally efficient minimisation  
(non-trivial relationship between FFs and observables via convolution)  
→ adaptive algorithms
- ③ need to define a criterion for minimisation stopping  
(avoid learning statistical fluctuations of the data)  
→ cross-validation

# The Hessian method: general strategy

- ① Expand the  $\chi^2$  about its global minimum at first (nontrivial) order

$$\chi^2\{\mathbf{a}\} \approx \chi^2\{\mathbf{a}_0\} + \delta a^i H_{ij} \delta a^j, \quad H_{ij} = \frac{1}{2} \left. \frac{\partial^2 \chi^2\{\mathbf{a}\}}{\partial a_i \partial a_j} \right|_{\{\mathbf{a}\}=\{\mathbf{a}_0\}}$$

- ② Assume linear error propagation for any observable  $\mathcal{O}$  depending on  $\{\mathbf{a}\}$

$$\langle \mathcal{O}\{\mathbf{a}\} \rangle \approx \mathcal{O}\{\mathbf{a}_0\} + a_i \left. \frac{\partial \mathcal{O}\{\mathbf{a}\}}{\partial a_i} \right|_{\{\mathbf{a}\}=\{\mathbf{a}_0\}} \quad \sigma_{\mathcal{O}\{\mathbf{a}\}} \approx \sigma_{ij} \left. \frac{\partial \mathcal{O}\{\mathbf{a}\}}{\partial a_i} \right. \left. \frac{\partial \mathcal{O}\{\mathbf{a}\}}{\partial a_j} \right|_{\{\mathbf{a}\}=\{\mathbf{a}_0\}}$$

- ③ Determine  $\sigma_{ij}$  from  $H_{ij}$  from maximum likelihood (under Gaussian hypothesis)

$$\sigma_{ij}^{-1} = \left. \frac{\partial^2 \chi^2\{\mathbf{a}\}}{\partial a_i \partial a_j} \right|_{\{\mathbf{a}\}=\{\mathbf{a}_0\}} = H_{ij}$$

- ④ A C.L. about the best fit is obtained as the volume (in parameter space) about  $\chi^2\{\mathbf{a}_0\}$  that corresponds to a fixed increase of the  $\chi^2$ ; for Gaussian uncertainties:

$$68\% \text{ C.L.} \iff \Delta \chi^2 = \chi^2\{\mathbf{a}\} - \chi^2\{\mathbf{a}_0\} = 1$$

# The Hessian method: some remarks

- ① Parameters can always be adjusted so that all eigenvalues of  $H_{ij}$  are equal to one (diagonalise  $H_{ij}$  and rescale the eigenvectors by their eigenvalues)

$$\delta a_i H_{ij} \delta a_j = \sum_{i=1}^{N_{\text{par}}} [a'_i(a_i)]^2 \iff \sigma_{\mathcal{O}\{\mathbf{a}'\}} = |\nabla' \mathcal{O}\{\mathbf{a}'\}|$$

- ② Compact representation and computation of observables and their uncertainties

$$\langle \mathcal{O}[D(x, Q^2)] \rangle = \mathcal{O}[D_0(x, Q^2)]$$

$$\sigma_{\mathcal{O}}[D(x, Q^2)] = \left[ \sum_{i=1}^{N_{\text{par}}} (\mathcal{O}[D_i(x, Q^2)] - \mathcal{O}[D_0(x, Q^2)])^2 \right]^{1/2}$$

- ③ Uncertainties obtained with  $\Delta\chi^2 = 1$  might be unrealistically small (inadequacy of the linear approximation)
- ④ Rescale to the  $\Delta\chi^2 = T$  interval such that correct C.L.s are reproduced (no statistically rigorous interpretation of  $T$  (tolerance))
- ⑤ Unmanageable Hessian matrix if the number of parameters is huge

# The Monte Carlo method: general strategy

- ① Generate (*art*) replicas of (*exp*) data according to the distribution

$$\mathcal{O}_i^{(art)(k)} = \mathcal{O}_i^{(exp)} + r_i^{(k)} \sigma_{\mathcal{O}_i}, \quad i = 1, \dots, N_{\text{dat}}, \quad k = 1, \dots, N_{\text{rep}}$$

where  $r_i^{(k)}$  are (Gaussianly distributed) random numbers for each  $k$ -th replica  
( $r_i^{(k)}$  can be generated with any distribution, not necessarily Gaussian)

- ② Validate the Monte Carlo sample size against experimental data
- ③ Perform a fit for each replica  $k = 1, \dots, N_{\text{rep}}$
- ④ Compact computation of observables and their uncertainties  
(PDF replicas are equally probable members of a statistical ensemble)

$$\langle \mathcal{O}[D(x, Q^2)] \rangle = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \mathcal{O}[D^{(k)}(x, Q^2)]$$

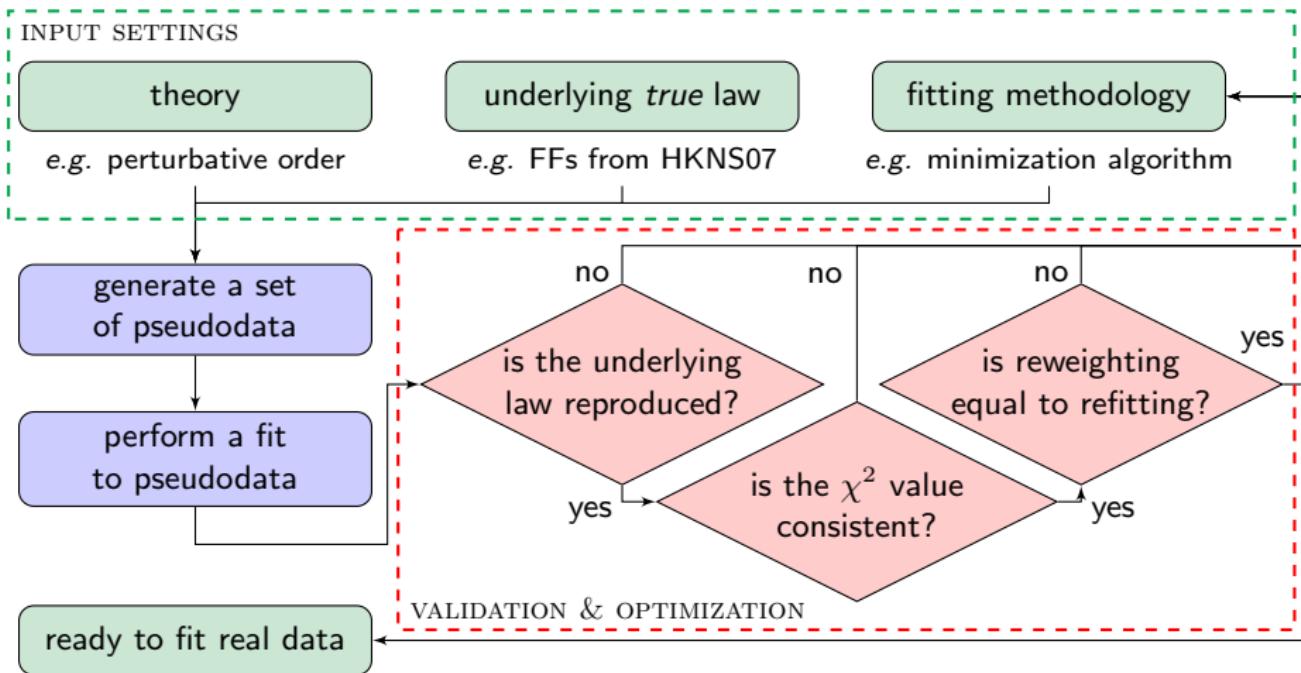
$$\sigma_{\mathcal{O}}[D(x, Q^2)] = \left[ \frac{1}{N_{\text{rep}} - 1} \sum_{k=1}^{N_{\text{rep}}} \left( \mathcal{O}[D^{(k)}(x, Q^2)] - \langle \mathcal{O}[D(x, Q^2)] \rangle \right)^2 \right]^{1/2}$$

- ⇒ no need to rely on linear approximation  
⇒ computational expensive: need to perform  $N_{\text{rep}}$  fits instead of one

# Methodology validation: closure tests

[JHEP 1504 (2015) 040]

Validation and optimization of the fitting strategy with known underlying physical law



Full control of procedural uncertainties

# Methodology validation: closure tests [JHEP 1504 (2015) 040]

- ① Level 0: generate pseudodata  $D_i^0$  with zero uncertainty  
(but  $(\text{cov})_{ij}$  in the  $\chi^2$  is the data covariance matrix)
  - fit quality can be arbitrarily good, if the fitting methodology is efficient:  $\chi^2/N_{\text{dat}} \sim 0$
  - validate fitting methodology (parametrisation, minimisation)
  - interpolation and extrapolation uncertainty
- ② Level 1: generate pseudodata  $D_i^1$  with stochastic fluctuations (no replicas)

$$D_i^1 = (1 + r_i^{\text{nor}} \sigma_i^{\text{nor}}) \left( D_i^0 + \sum_p^{N_{\text{sys}}} r_{i,p}^{\text{sys}} \sigma_{i,p}^{\text{sys}} + r_i^{\text{stat}} \sigma_i^{\text{stat}} \right)$$

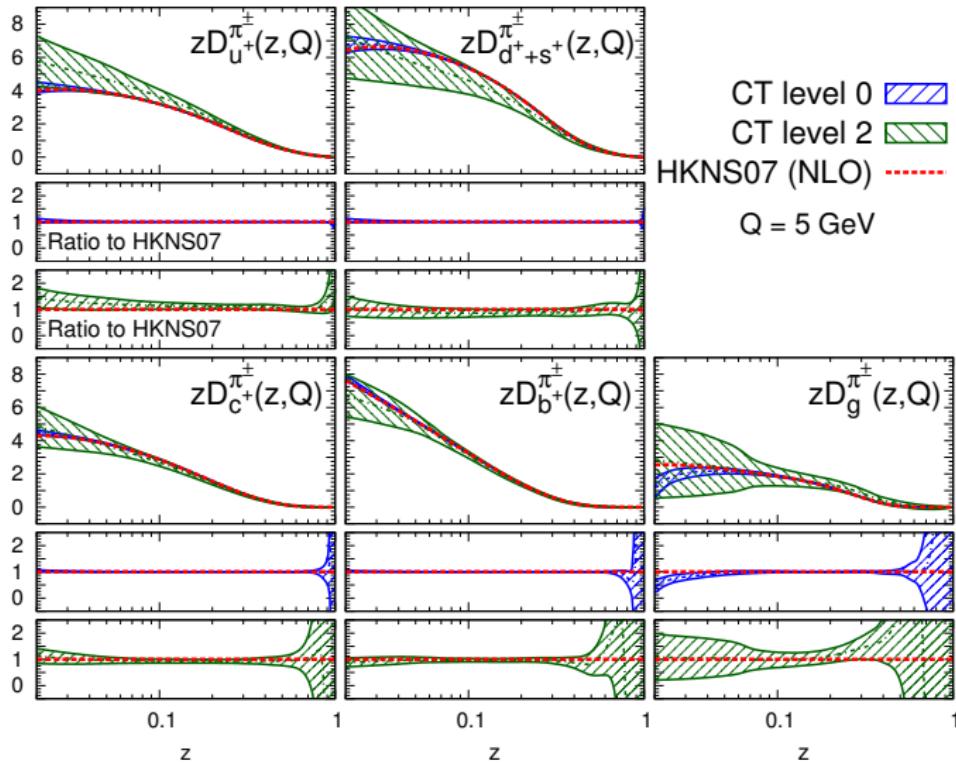
- experimental uncertainties are not propagated into FFs:  $\chi^2/N_{\text{dat}} \sim 1$
- functional uncertainty (a large number of functional forms with equally good  $\chi^2$ )

- ③ Level 2: generate  $N_{\text{rep}}$  Monte Carlo pseudodata replicas  $D_i^{2,k}$  on top of Level 1

$$D_i^{2,k} = (1 + r_i^{\text{nor},k} \sigma_i^{\text{nor}}) \left( D_i^1 + \sum_p^{N_{\text{sys}}} r_{i,p}^{\text{sys},k} \sigma_{i,p}^{\text{sys}} + r_i^{\text{stat},k} \sigma_i^{\text{stat}} \right)$$

- propagate the fluctuations due to experimental uncertainties into FFs:  $\chi^2/N_{\text{dat}} \sim 1$
- input FFs lie within the one-sigma band of the fitted FFs with a probability of  $\sim 68\%$
- data uncertainty

# Closure testing NNFF1.0



$$\chi^2/N_{\text{dat}} = 0.0001 \text{ (L0)}$$

$$\chi^2/N_{\text{dat}} = 1.0262 \text{ (L1)}$$