

Fragmentation Functions of light charged hadrons

Emanuele R. Nocera

Higgs Centre for Theoretical Physics - University of Edinburgh

JLab Theory Center – 29th January 2018

Outline

1 Fragmentation Functions: the basics

- ▶ factorisation, evolution
- ▶ higher-order corrections, theoretical constraints
- ▶ statistical representation of uncertainties
- ▶ FFs: why should we bother? Are current FF sets good?

2 The NNFF1.0 analysis

- ▶ data set and fit settings
- ▶ the NNPDF methodology: parametrisation and uncertainty representation
- ▶ results: fit quality, perturbative stability, dependence on the data set/kinematic cuts
- ▶ is the NNFF1.0 set better than currently available sets?

3 Summary and outlook

- ▶ global fits, simultaneous fits

DISCLAIMER

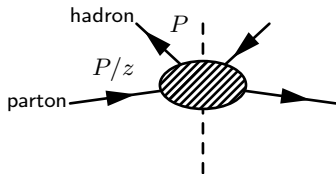
This is not a review talk on Fragmentation Functions
Focus on topics which I've worked on recently

[[JHEP 1503 \(2015\) 046](#); [EPJ C77 \(2017\) 516](#); [PoS DIS2017 \(2018\) 231](#)]

1. Fragmentation Functions: the basics

Hadrons in the final state: Fragmentation Functions

FFs allow for a proper field-theoretic definition as matrix elements of bilocal operators



collinear transition
of a parton i into a hadron h
with fractional momentum z
no local OPE \implies no lattice formulation

[Rev.Mod.Phys. 67 (1995) 157]

$$D_i^h(z) = \frac{1}{12\pi} \sum_X \int dy^- e^{-i\frac{P^+}{z}y^-} \text{Tr} [\gamma^+ \langle 0 | \psi(y) \mathcal{P} | h(P) X \rangle \langle h(P) X | \mathcal{P}' \bar{\psi}(0) | 0 \rangle]$$

with light-cone coordinates and appropriate gauge links \mathcal{P} , \mathcal{P}'

$$y = (y^+, y^-, \mathbf{y}_\perp), \quad y^+ = (y^0 + y^z)/\sqrt{2}, \quad y^- = (y^0 - y^z)/\sqrt{2}, \quad \mathbf{y}_\perp = (y^x, y^y)$$

All these definitions have ultraviolet divergences which must be renormalised
in order to define finite FFs to be used in the factorisation formulas
(FFs, like PDFs, are scheme dependent)

The definition above can be generalised to include longitudinal/transverse polarisations

Factorisation of physical observables [Adv.Ser.Direct.HEP 5 (1988) 1]

- 1 A variety of sufficiently inclusive processes allow for a factorised description

short-distance part
hard interaction of partons
process-dependent kernels

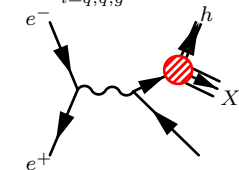
factorisation
← scheme & scale μ →

long-distance part
nucleon structure
universal PDFs/FFs

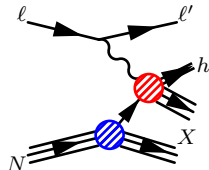
- 2 Physical observables are written as a convolution of coefficient functions and FFs

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

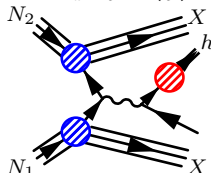
$$f \otimes g = \int_x^1 \frac{dy}{y} f\left(\frac{x}{y}\right) g(y)$$



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



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



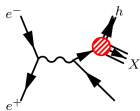
$N_1 + N_2 \rightarrow h + X$
high- p_T hadron production in
proton-proton collisions (PP)

- 3 Coefficient functions allow for a perturbative expansion

$$C_{If}(y, \alpha_s) = \sum_{k=0} a_s^k C_{If}^{(k)}(y), \quad a_s = \alpha_s / (4\pi)$$

- 4 After factorisation, all quantities (including FFs) depend on μ

Factorisation of physical observables

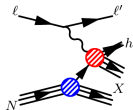


$e^+ + e^- \rightarrow h + X$
single-inclusive
annihilation (SIA)

$$\frac{d\sigma^h}{dz} = F_T^h(z, Q^2) + F_L^h(z, Q^2) = F_2^h(x, Q^2)$$

$$F_{k=T,L,2}^h = \frac{4\pi\alpha_{\text{em}}^2}{Q^2} \langle e^2 \rangle \left\{ D_{\Sigma}^h \otimes C_{k,q}^S + n_f D_g^h \otimes C_{k,g}^S + D_{\text{NS}}^h \otimes C_{k,q}^{\text{NS}} \right\}$$

up to NNLO [PLB 386 (1996) 422; NPB 487 (1997) 233; PLB 392 (1997) 207]



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

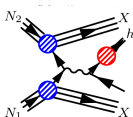
$$\frac{d\sigma^h}{dx dy dz} = \frac{2\pi\alpha_{\text{em}}^2}{Q^2} \left[\frac{1+(1-y)^2}{y} 2F_1^h + \frac{2(1-y)}{y} F_L^h \right]$$

$$2F_1^h = e_q^2 \left\{ q \otimes D_q^h + \frac{\alpha_s}{2\pi} \left[q \otimes C_{qq}^1 \otimes D_q^h + q \otimes C_{gq}^1 \otimes D_g^h + g \otimes C_{qg}^1 \otimes D_q^h \right] \right\}$$

$$F_L^h = \frac{\alpha_s}{2\pi} \sum_{q,\bar{q}} e_q^2 \left[q \otimes C_{qq}^L \otimes D_q^h + q \otimes C_{gq}^L \otimes D_g^h + g \otimes C_{qg}^L \otimes D_q^h \right]$$

up to NLO [NPB 160 (1979) 301; PRD 57 (1998) 5811]

partial NNLO [PRD 95 (2017) 034027]



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

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

$$= \sum_{i,j,k} \int \frac{dx_a}{x_a} \int \frac{dx_b}{x_b} \int \frac{dz}{z^2} f^{i/p_a}(x_a) f^{j/p_b}(x_b) D^{h/k}(z) \hat{\sigma}^{ij \rightarrow k} \delta(\hat{s} + \hat{t} + \hat{u})$$

up to NLO [PRD 67 (2003) 054004; PRD 67 (2003) 054005]

Evolution of FFs: DGLAP equations [NPB 126 (1977) 298]

- ① A set of $(2n_f + 1)$ integro-differential equations (n_f =number of active flavours)

$$\frac{\partial}{\partial \ln \mu^2} D_i(x, \mu^2) = \sum_j^{n_f} \int_x^1 \frac{dz}{z} P_{ji}(z, \alpha_s(\mu^2)) D_j\left(\frac{x}{z}, \mu^2\right)$$

- ② Often written in a convenient basis of FFs

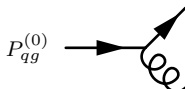
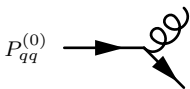
$$D_{\text{NS};\pm} = (D_q \pm D_{\bar{q}}) - (D_{q'} \pm D_{\bar{q}'}) \quad D_{\text{NS};v} = \sum_q^{n_f} (D_q - D_{\bar{q}}) \quad D_{\Sigma} = \sum_q^{n_f} (D_q + D_{\bar{q}})$$

$$\frac{\partial}{\partial \ln \mu^2} D_{\text{NS};\pm,v}(x, \mu^2) = P^{\pm,v}(x, \mu_F^2) \otimes D_{\text{NS};\pm,v}(x, \mu^2)$$

$$\frac{\partial}{\partial \ln \mu^2} \begin{pmatrix} D_{\Sigma}(x, \mu^2) \\ D_g(x, \mu^2) \end{pmatrix} = \begin{pmatrix} P^{qq} & 2n_f P^{gq} \\ \frac{1}{2n_f} P^{qg} & P^{gg} \end{pmatrix} \otimes \begin{pmatrix} D_{\Sigma}(x, \mu^2) \\ D_g(x, \mu^2) \end{pmatrix}$$

- ③ With perturbative computable (time-like) splitting functions

$$P_{ji}(z, \alpha_s) = \sum_{k=0} a_s^{k+1} P_{ji}^{(k)}(z), \quad a_s = \alpha_s / (4\pi)$$



Splitting functions: LO and NLO

$$P_{\text{qq}}^{(0)}(x) = C_F(2p_{\text{qq}}(x) + 3\delta(1-x))$$

$$P_{\text{ps}}^{(0)}(x) = 0$$

$$P_{\text{qg}}^{(0)}(x) = 2n_f p_{\text{qg}}(x)$$

$$P_{\text{gg}}^{(0)}(x) = 2C_F p_{\text{gg}}(x)$$

$$P_{\text{ss}}^{(0)}(x) = C_A(4p_{\text{ss}}(x) + \frac{11}{3}\delta(1-x)) - \frac{2}{3}n_f\delta(1-x)$$

LO: 1973

$$P_{\text{ns}}^{(1)+}(x) = 4C_A C_F \left(p_{\text{qq}}(x) \left[\frac{67}{18} - \zeta_2 + \frac{11}{6}H_0 + H_{0,0} \right] + p_{\text{qg}}(-x) \left[\zeta_2 + 2H_{-1,0} - H_{0,0} \right] \right. \\ \left. + \frac{14}{3}(1-x) + \delta(1-x) \left[\frac{17}{24} + \frac{11}{3}\zeta_2 - 3\zeta_3 \right] - 4C_F n_f \left(p_{\text{qq}}(x) \left[\frac{5}{6} + \frac{1}{3}H_0 \right] + \frac{2}{3}(1-x) \right) \right. \\ \left. + \delta(1-x) \left[\frac{1}{12} + \frac{2}{3}\zeta_2 \right] + 4C_F^2 \left(2p_{\text{qq}}(x) \left[H_{1,0} - \frac{3}{4}H_0 + H_2 \right] - 2p_{\text{qg}}(-x) \left[\zeta_2 + 2H_{-1,0} - H_{0,0} \right] - (1-x) \left[1 - \frac{3}{2}H_0 \right] - H_0 - (1+x)H_{0,0} + \delta(1-x) \left[\frac{3}{8} - 3\zeta_2 + 6\zeta_3 \right] \right) \right)$$

$$P_{\text{ns}}^{(1)-}(x) = P_{\text{ns}}^{(1)+}(x) + 16C_F \left(C_F - \frac{C_A}{2} \right) \left(p_{\text{qg}}(-x) \left[\zeta_2 + 2H_{-1,0} - H_{0,0} \right] - 2(1-x) - (1+x)H_0 \right)$$

$$P_{\text{ps}}^{(1)}(x) = 4C_F n_f \left(\frac{20}{9} \frac{1}{x} - 2 + 6x - 4H_0 + x^2 \left[\frac{8}{3}H_0 - \frac{56}{9} \right] + (1+x) \left[5H_0 - 2H_{0,0} \right] \right)$$

$$P_{\text{qg}}^{(1)}(x) = 4C_A n_f \left(\frac{20}{9} \frac{1}{x} - 2 + 25x - 2p_{\text{qg}}(-x)H_{-1,0} - 2p_{\text{qg}}(x)H_{1,1} + x^2 \left[\frac{44}{3}H_0 - \frac{218}{9} \right] \right. \\ \left. + 4(1-x) \left[H_{0,0} - 2H_0 + xH_1 \right] - 4\zeta_2 x - 6H_{0,0} + 9H_0 \right) + 4C_F n_f \left(2p_{\text{qg}}(x) \left[H_{1,0} + H_{1,1} + H_2 - \zeta_2 \right] + 4x^2 \left[H_0 + H_{0,0} + \frac{5}{2} \right] + 2(1-x) \left[H_0 + H_{0,0} - 2xH_1 + \frac{29}{4} \right] - \frac{15}{2} - H_{0,0} - \frac{1}{2}H_0 \right)$$

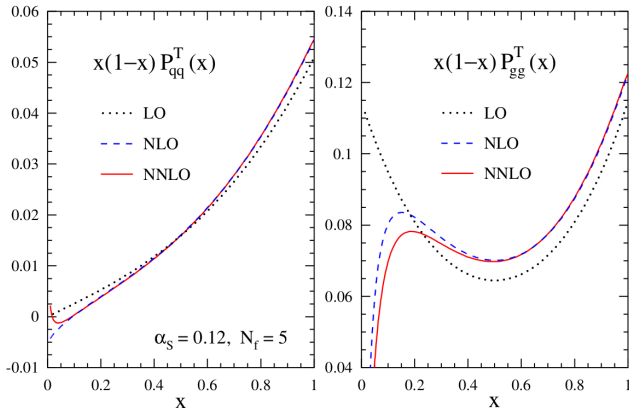
$$P_{\text{gg}}^{(1)}(x) = 4C_A C_F \left(\frac{1}{x} + 2p_{\text{gg}}(x) \left[H_{1,0} + H_{1,1} + H_2 - \frac{11}{6}H_1 \right] - x^2 \left[\frac{8}{3}H_0 - \frac{44}{9} \right] + 4\zeta_2 - 2 \right. \\ \left. - 7H_0 + 2H_{0,0} - 2H_1 x + (1+x) \left[2H_{0,0} - 5H_0 + \frac{37}{9} \right] - 2p_{\text{qg}}(-x)H_{-1,0} \right) - 4C_F n_f \left(\frac{2}{3}x - p_{\text{qg}}(x) \left[\frac{2}{3}H_1 - \frac{10}{9} \right] \right) + 4C_F^2 \left(p_{\text{gg}}(x) \left[3H_1 - 2H_{1,1} \right] + (1+x) \left[H_{0,0} - \frac{7}{2} + \frac{7}{2}H_0 \right] - 3H_{0,0} + 1 - \frac{3}{2}H_0 + 2H_1 x \right)$$

$$P_{\text{ss}}^{(1)}(x) = 4C_A n_f \left(1 - x - \frac{10}{9}p_{\text{ss}}(x) - \frac{13}{9} \left(\frac{1}{x} - x^2 \right) - \frac{2}{3}(1+x)H_0 - \frac{2}{3}\delta(1-x) + 4C_A^2 \left(27 \right. \right. \\ \left. \left. + (1+x) \left[\frac{11}{3}H_0 + 8H_{0,0} - \frac{27}{2} \right] + 2p_{\text{ss}}(-x) \left[H_{0,0} - 2H_{-1,0} - \zeta_2 \right] - \frac{67}{9} \left(\frac{1}{x} - x^2 \right) - 12H_0 \right. \right. \\ \left. \left. - \frac{44}{3}x^2 H_0 + 2p_{\text{ss}}(x) \left[\frac{67}{18} - \zeta_2 + H_{0,0} + 2H_{1,0} + 2H_2 \right] + \delta(1-x) \left[\frac{8}{3} + 3\zeta_3 \right] \right) + 4C_F n_f \left(2H_0 \right. \right. \\ \left. \left. + \frac{21}{3x} + \frac{10}{3}x^2 - 12 + (1+x) \left[4 - 5H_0 - 2H_{0,0} \right] \right)$$

NLO: 1980

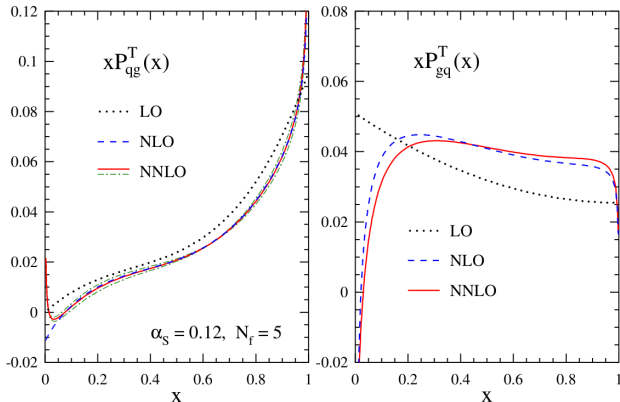
Properties of splitting functions

- 1 At LO [*Sov. J. Nucl. Phys.* 15 (1973) 438; *NPB* 126 (1977) 298; *NPB* 136 (1978) 445]
time-like and space-like splitting functions are equal, provided $P_{qq}^{S,(0)} \leftrightarrow P_{qq}^{T,(0)}$
- 2 At NLO [*NPB* 175 (1980) 27, *PLB* 97 (1980) 497, *PRD* 48 (1993) 116]
time-like and space-like splitting functions are related by analytic continuation
- 3 at NNLO [*PLB* 638 (2006) 61, *PLB* 659 (2008) 290, *NPB* 854 (2012) 133]
an uncertainty still remains on the exact form of $P_{qq}^{(2)}$ (it does not affect its log behavior)



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Properties of splitting functions

Must be careful with fixed-order splitting functions as $z \rightarrow 0$ ($m = 1, \dots, 2k + 1$)

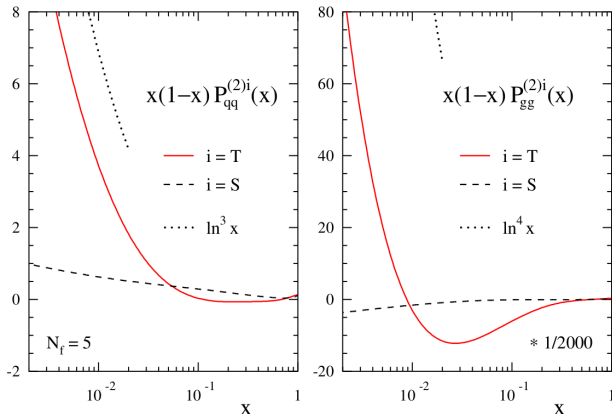
SPACE-LIKE CASE

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

TIME-LIKE CASE

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

Soft gluon logarithms diverge more rapidly in the TL case than in the SL case: as z decreases, the unresummed SGLs spoil the convergence of the FO series for $P(z, a_s)$ if $\log \frac{1}{z} \geq \mathcal{O}(a_s^{-1/2})$



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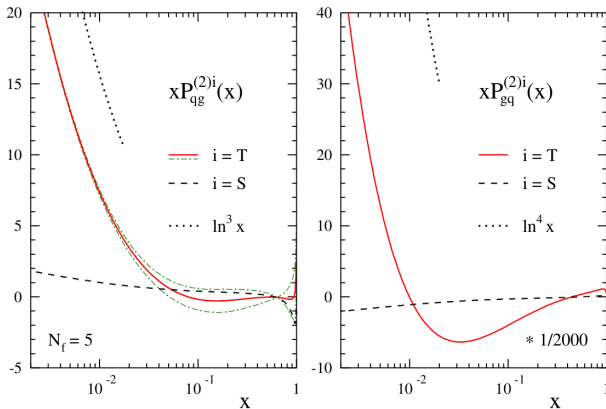
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Theoretical constraints

1 Momentum sum rule

$$\sum_h \int_0^1 dz z D_i^h(z, \mu^2) = 1 \quad \forall \text{ parton } i$$

2 Charge sum rule

$$\sum_h \int_0^1 dz e_h D_i^h(z, \mu^2) = e_i \quad \forall \text{ parton } i$$

where $e_{h(i)}$ is the electric charge of the hadron h (parton i)

3 Charge conjugation symmetry

$$D_{q(\bar{q})}^{h^+} = D_{\bar{q}(q)}^{h^-} \quad D_g^{h^+} = D_g^{h^-} \quad \forall \text{ hadron species } h^\pm$$

4 Isospin symmetry of the strong interaction

$$D_u^{\pi^+} = D_d^{\pi^-} \quad D_d^{\pi^+} = D_u^{\pi^-}$$

approximate, as $m_u \sim m_d$, but no phenomenological evidences of violation

5 Positivity of cross sections

implies that FFs should be positive-definite at LO

Determining FFs from data: a global QCD analysis

Determine the probability density $\mathcal{P}[D]$ in the space of FFs $[D]$

$$\mathcal{P}(D|data) = \mathcal{L}(data|D)\pi(D)$$

Project the infinite-dim. space of FFs $[D]$ onto the finite-dim. space of parameters $\{\mathbf{a}\}$

$$\mathcal{P}(D|data) = \mathcal{L}(data|D)\pi(D) \longleftrightarrow \mathcal{P}(\mathbf{a}|data) = \mathcal{L}(data|\mathbf{a})\pi(\mathbf{a})$$

$$\mathcal{L}(data|\mathbf{a}) = \exp\left[-\frac{1}{2}\chi^2\right] \quad \text{Gaussian likelihood}$$

$$\pi(\mathbf{a}) = \prod_i \theta(a_i - a_i^{\min})\theta(a_i^{\max} - a_i) \quad \text{uninformative flat prior}$$

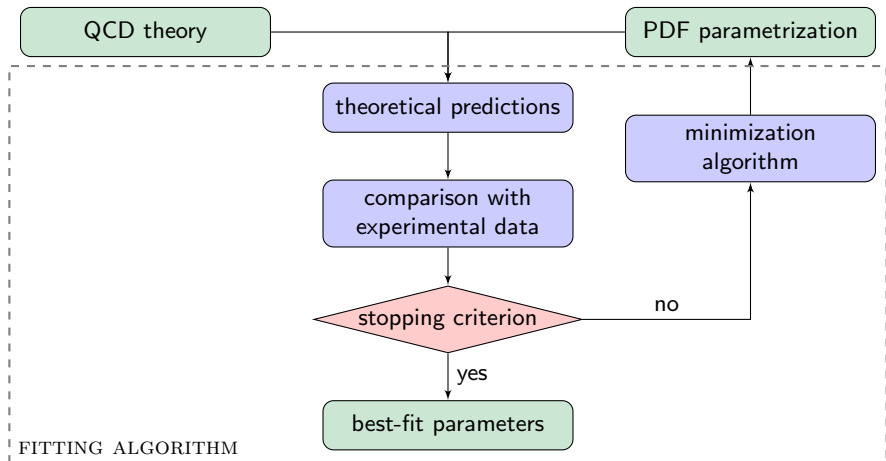
For any observable \mathcal{O} depending on a set of FFs $[D]$

its expectation value and uncertainty are functional integrals over the space of FFs

$$E[\mathcal{O}] = \langle \mathcal{O}[D] \rangle = \int d^n a \mathcal{P}(\mathbf{a}|data) \mathcal{O}[\mathbf{a}] \quad \text{expectation value}$$

$$V[\mathcal{O}] = \sigma_{\mathcal{O}}^2[D] = \int d^n a \mathcal{P}(\mathbf{a}|data) (\mathcal{O}[\mathbf{a}] - E[\mathcal{O}])^2 \quad \text{variance}$$

A global FF determination: the underlying strategy



Assume a reasonable PDF parametrisation

Obtain theoretical predictions for various processes and compare predictions to data

Determine the best-fit parameters via minimization (maximum likelihood)
of a proper figure of merit (usually the log-likelihood χ^2)

Maximum likelihood: Hessian method

- 1 Expand the χ^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 $\{\mathbf{a}\}$

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

- 3 Determine σ_{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 χ^2 ; for Gaussian uncertainties:

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

Maximum likelihood: Hessian method

- 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

Maximum likelihood: Monte Carlo method

- 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_{rep} fits instead of one**

Maximum likelihood: 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 χ^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) \rightarrow genetic algorithms
- 2 need for a computationally efficient minimisation
(non-trivial relationship between FFs and observables) \rightarrow adaptive algorithms
- 3 need to define a criterion for minimisation stopping
(avoid learning statistical fluctuations of the data) \rightarrow partition and cross-validation

Covariance Matrix Adaption Evolution Strategy [N. Hansen, Springer (2016)]

Nested sampling [Astrophys.J. 638 (2006) L51; Mon.Not.Roy.Astron.Soc. 398 (2009) 1601]

Basic idea: compute

$$Z = \int \mathcal{L}(\text{data}|\mathbf{a})\pi(\mathbf{a})d^m a = \int_0^1 \mathcal{L}(X)dX$$

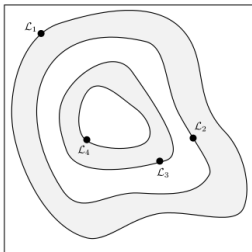
The algorithm traverses ordered isolikelihood contours in the variable X such that X follows the progression $X_i = t_i X_{i-1}$

The variable t_i is estimated statistically

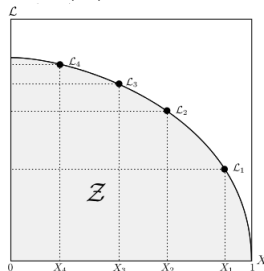
The algorithm can be optimised iteration by iteration

One can sample only in the regions where the likelihood is larger (*importance sampling*)

$\mathcal{L}(\text{data}|\mathbf{a})$ in a space

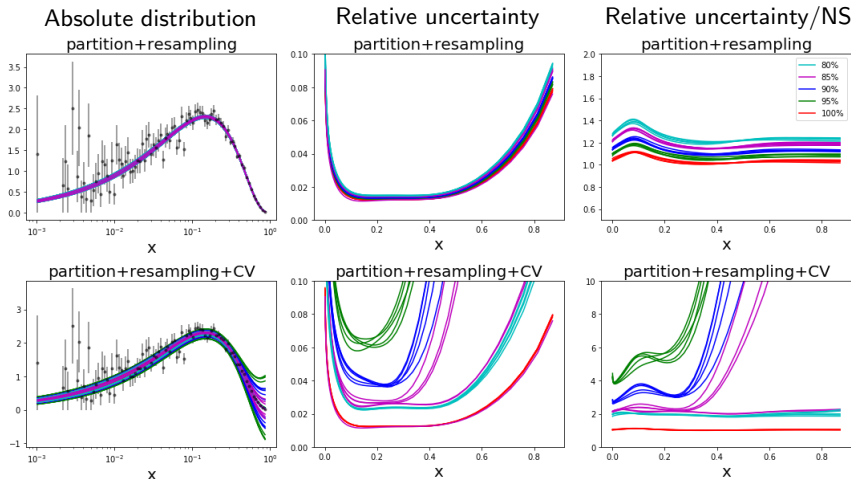


$\mathcal{L}(X)$ in X space



Comparing maximum likelihood and sampling methods

Toy example: $data(x) = Nx^\alpha(1-x)^\beta$



Results are independent from the parametrisation and from the shape of the data
A quantitative explanation of these results require a proper Bayesian formulation

Available FF sets (status 2017)

| | | DHESS | HKNS | JAM | NNFF |
|---------------|--|------------------------------------|-----------------------------------|-----------------------|-----------------------------|
| DATA | SIA | ✓ | ✓ | ✓ | ✓ |
| | SIDIS | ✓ | ✗ | ✗ | ✗ |
| | PP | ✓ | ✗ | ✗ | ✗ |
| METH. | statistical treatment | Iterative Hessian 68% - 90% | Hessian $\Delta\chi^2 = 15.94$ | Iterative Monte Carlo | Monte Carlo |
| | parametrisation | standard | standard | standard | neural network |
| THEORY | pert. order | (N)NLO | NLO | NLO | LO, NLO, NNLO |
| | HF scheme | ZM(GM)-VFN | ZM-VFN | ZM-VFN | ZM-VFN |
| | hadron species | $\pi^\pm, K^\pm, p/\bar{p}, h^\pm$ | $\pi^\pm, K^\pm, p/\bar{p}$ | π^\pm, K^\pm | $\pi^\pm, K^\pm, p/\bar{p}$ |
| latest update | PRD 91 (2015) 014035 PRD 95 (2017) 094019 | PTEP 2016 (2016) 113B04 | PRD 94 (2016) 114004 | EPJ C77 (2017) 516 | |

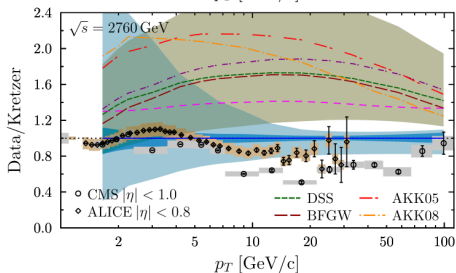
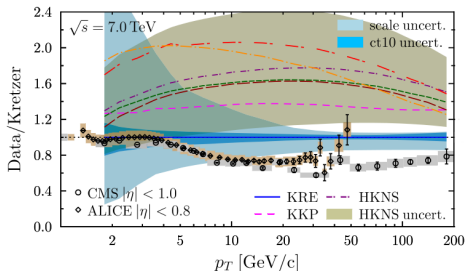
+ some others (including analyses for specific hadrons)

| | | | |
|----------------------------|------------------|--------------------------------|------------------|
| BKK95 [ZPB 65 (1995) 471] | π^\pm, K^\pm | AESS11 [PRD 83 (2011) 034002] | η |
| BKK96 [PRD 53 (1996) 3553] | K^0 | SKMNA13 [PRD 88 (2013) 054019] | π^\pm, K^\pm |
| DSV97 [PRD 57 (1998) 5811] | Λ^0 | LSS15 [PRD 96 (2016) 074026] | SIDIS only |
| BFGW00 [EPJ C19 (2001) 89] | h^\pm | | |

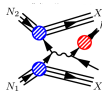
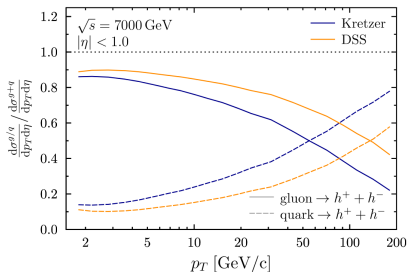
Focus on π and K which constitute the largest fraction in measured yields

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]



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

Predictions from all available FF sets are not compatible with CMS and ALICE data, not even within scale and PDF/FF uncertainties
 → How well do we know the gluon FF?

Fragmentation functions: why should we bother?

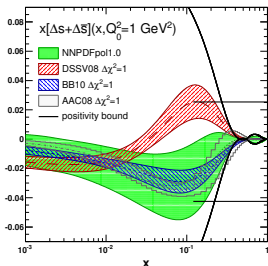
Example 2: The strange polarised parton distribution at $Q^2 = 2.5 \text{ GeV}^2$ ($\Delta_s = \Delta_{\bar{s}}$)

NNPDFpol1.0 [NPB 874 (2013) 36]
 $\int_0^1 dx [\Delta s + \Delta \bar{s}] = -0.13 \pm 0.09$

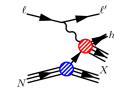
JAM17 [PRL 119 (2017) 132001]
 $\int_0^1 dx [\Delta s + \Delta \bar{s}] = -0.03 \pm 0.10$

First moment constrained by
 $a_3 = \int_0^1 dx [\Delta u^+ - \Delta d^+] = 1.2701 \pm 0.0025$

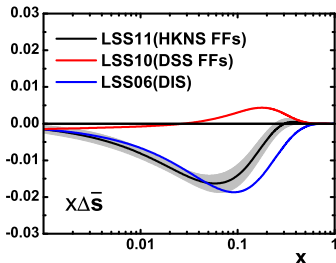
$a_8 = \int_0^1 dx [\Delta u^+ + \Delta d^+ - 2\Delta s^+] = 0.585 \pm 0.176$



directly from SIDIS Kaon data



indirectly from DIS + SU(3)



$$\frac{d\sigma}{dx dy} = \frac{2\pi\alpha_{\text{em}}^2}{Q^2} [(2-y)g_1]$$

$$\frac{d\sigma^h}{dx dy dz} = \frac{2\pi\alpha_{\text{em}}^2}{Q^2} \left[\frac{1+(1-y)^2}{y} 2g_1^h + \frac{2(1-y)}{y} g_L^h \right]$$

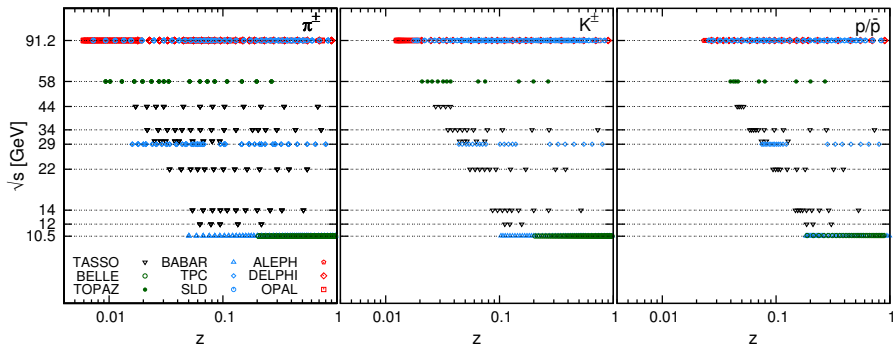
If SIDIS data is used to determine Δ_s , K^\pm FFs for different sets lead to different results. Such results may differ significantly among them and w.r.t. the results obtained from DIS
 → How well do we know kaon FFs?

Figure taken from [PRD D84 (2011) 014002]

2. The NNFF1.0 analysis

[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]

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

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

The NNPDF methodology: parametrisation

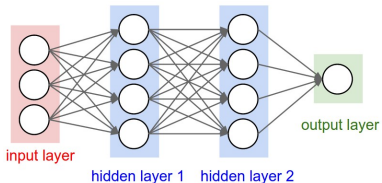
- ① Neural network (NN), *i.e.* a generator of random functions in the space of FFs

$$zD_i^h(z, Q_0^2) = \mathcal{F}_i^h(z, \{\mathbf{c}\}) \quad \mathcal{F}_i^h(z, \{\mathbf{c}\}) \text{ is a feed-forward neural network}$$

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

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

- ② What a feed-forward NN exactly is?



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

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

- ▶ 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)

⇒ **potentially non-smooth**

⇒ **bias due to the parametrisation reduced as much as possible**

Fit settings

Physical parameters: consistent with the NNPDF3.1 PDF set [EPJ C77 (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)

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

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

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

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

Hadron mass corrections: included exactly à la Albino-Kniehl-Kramer [NPB 803 (2008) 42]

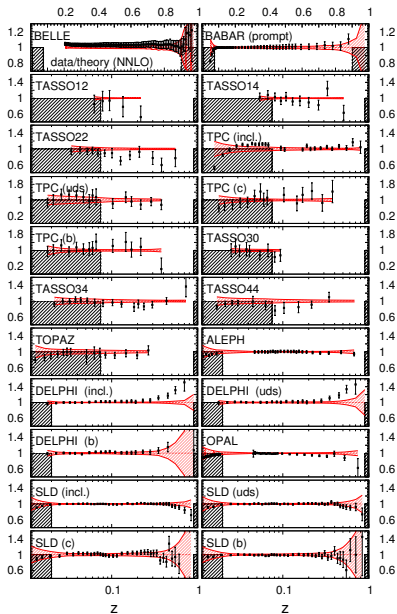
Kinematic cuts: $z \rightarrow 0$: contributions $\propto \ln z$; $z \rightarrow 1$: contributions $\propto \ln(1 - z)$

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

Momentum sum rule: check a posteriori that

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

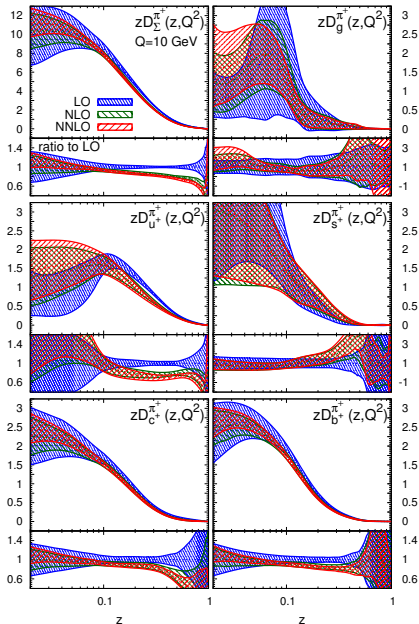
Fit quality: π^+



| Exp. | NNLO theory | | remarks |
|--------------|------------------|-------------------------|----------------------|
| | N_{dat} | χ^2/N_{dat} | |
| BELLE | 70 | 0.09 | lack of correlations |
| BABAR | 40 | 0.78 | ✓ |
| TASSO12 | 4 | 0.87 | small sample |
| TASSO14 | 9 | 1.70 | } data fluctuations |
| TASSO22 | 8 | 1.91 | |
| 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 | tension with OPAL |
| 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 | ✓ |
| TOTAL | 428 | 0.87 | ✓ |

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

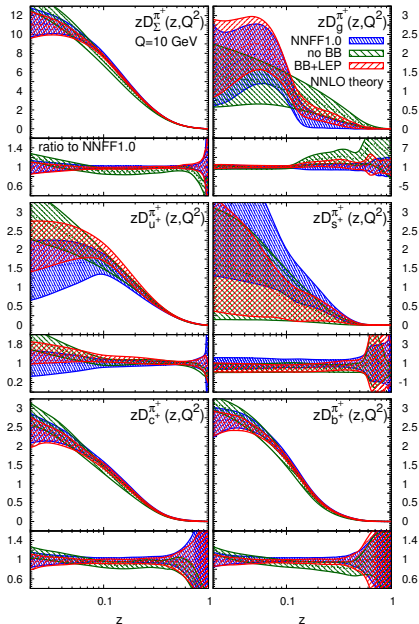
Dependence upon perturbative order: π^+



| Exp. | N_{dat} | LO χ^2/N_{dat} | NLO χ^2/N_{dat} | NNLO χ^2/N_{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 |
| TOTAL | 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: π^+

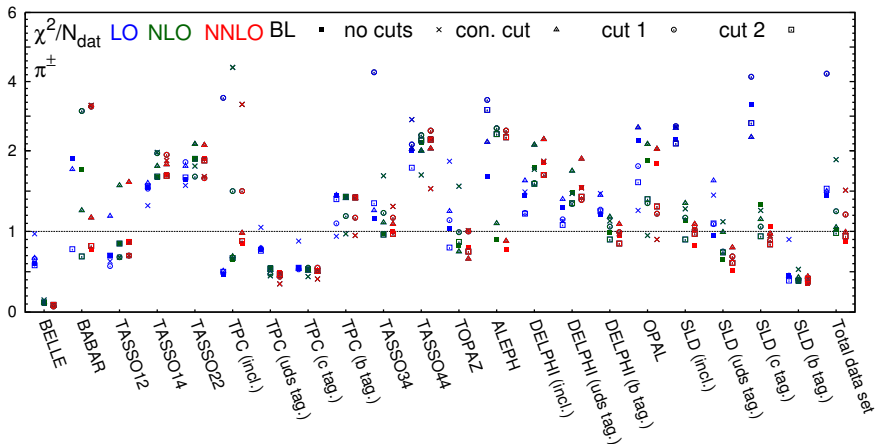


| NNLO theory Exp. | N_{dat} | χ^2/N_{dat} | no BB χ^2/N_{dat} | BB+LEP χ^2/N_{dat} |
|---------------------|------------------|-------------------------|----------------------------------|-----------------------------------|
| BELLE | 70 | 0.09 | [4.92] | 0.09 |
| BABAR | 40 | 0.78 | [144] | 0.88 |
| 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 |
| TOTAL | | 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

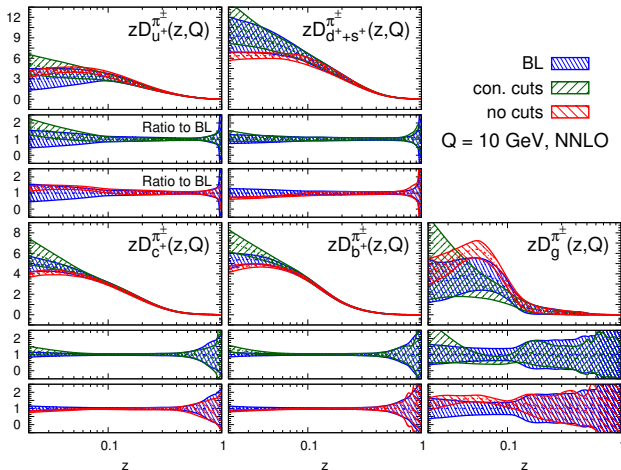
Dependence upon kinematic cuts: π^+

| BL | | no cuts | | con. cut | | cut1 | | cut2 | |
|--------------------|------------|--------------------|------------|--------------------|------------|--------------------|------------|--------------------|------------|
| $z_{\min}^{(m_Z)}$ | z_{\min} | $z_{\min}^{(m_Z)}$ | z_{\min} | $z_{\min}^{(m_Z)}$ | z_{\min} | $z_{\min}^{(m_Z)}$ | z_{\min} | $z_{\min}^{(m_Z)}$ | 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: π^+

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

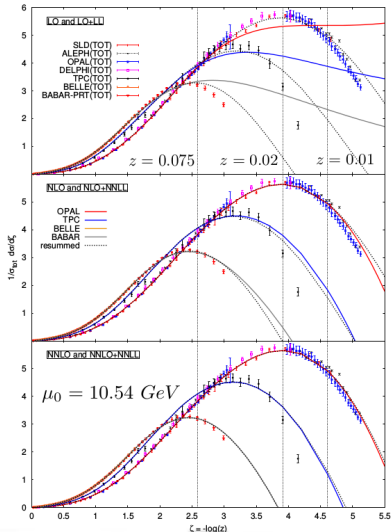


Small- z resummed Fragmentation Functions [PRD 95 (2017) 054003]

436 Total data Points:

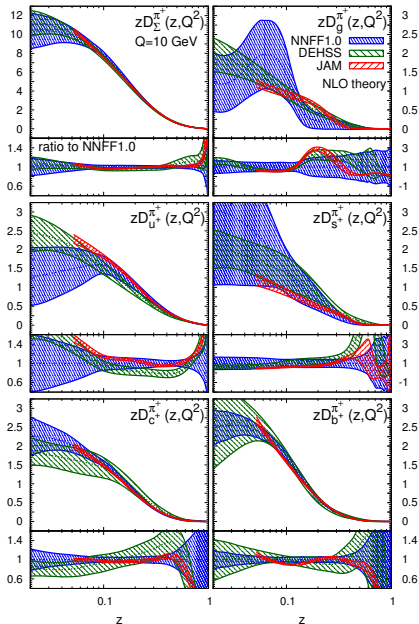
- LEP cut ($z = 0.01$) due to inconsistency between OPAL and ALEPH
- TPC lower cut ($z = 0.02$) based on difference of energy fraction $z = 2 E_h/Q$ and three momentum fraction $x_p = z - 2m_h^2/(zQ^2) + \mathcal{O}(1/Q^4)$ in c.m.s being less than at least 15%

| accuracy | χ^2 | χ^2/dof |
|-----------|----------|---------------------|
| LO | 1260.78 | 2.89 |
| NLO | 354.10 | 0.81 |
| NNLO | 330.08 | 0.76 |
| LO+LL | 405.54 | 0.93 |
| NLO+NNLL | 352.28 | 0.81 |
| NNLO+NNLL | 329.96 | 0.76 |



Slide: courtesy of D. P. Anderle

Comparison with other FF determinations: π^+



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)

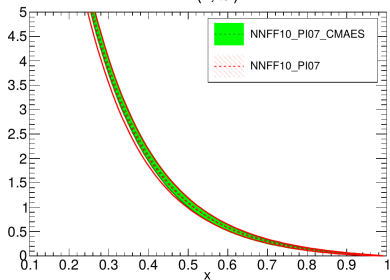
$D_g^{\pi^+}$: slight disagreement
different shapes, larger uncertainties
DEHSS: data; JAM: parametrisation

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

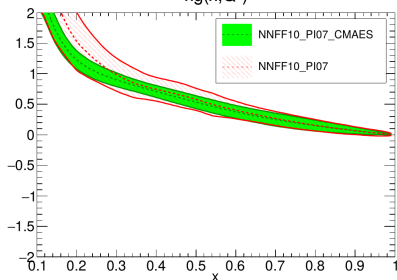
$D_{c^+}^{\pi^+}$, $D_{b^+}^{\pi^+}$: good overall agreement
excellent with JAM, same uncertainties
slightly different shape w.r.t. DEHSS (dataset)

Dependence upon the minimisation algorithm

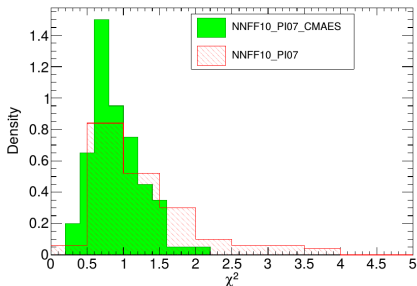
$\chi\Sigma(x, Q^2)$



$xg(x, Q^2)$



χ^2 distribution for ALEPHPI



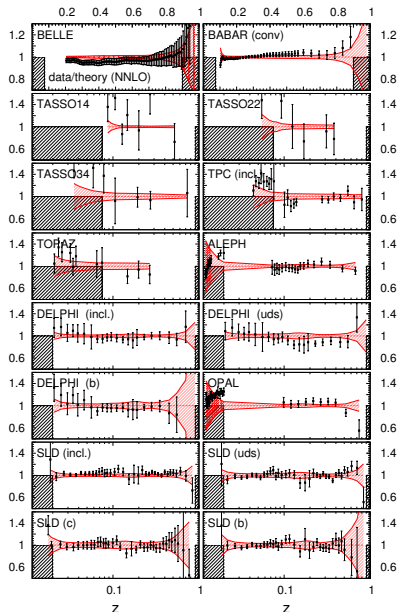
Singlet and Gluon FFs at $Q = 5$ GeV

| | NNFF10.PI07_CMAES | NNFF10.PI07 |
|--|-------------------|-----------------|
| $\chi^2_{\text{tot}}/N_{\text{dat}}$ | 0.93 | 0.92 |
| $\langle E_{\text{tr}} \rangle \pm \sigma_{\text{tr}}$ | 1.97 ± 0.28 | 1.97 ± 0.71 |
| $\langle E_{\text{val}} \rangle \pm \sigma_{\text{val}}$ | 2.16 ± 0.37 | 2.91 ± 1.72 |
| $\langle \text{TL} \rangle \pm \sigma_{\text{TL}}$ | 3065 ± 1673 | 5560 ± 9394 |

Fit quality: K^+

| Exp. | N_{dat} | NNLO theory | |
|------------|------------------|-------------------------|-------------------------------|
| | | χ^2/N_{dat} | remarks |
| BELLE | 70 | 0.32 | lack of correlations |
| BABAR | 43 | 0.95 | ✓ |
| TASSO12 | 3 | 1.02 | } small sample |
| TASSO14 | 9 | 2.07 | |
| 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 | ✓ |
| TOTAL | 385 | 0.73 | ✓ |

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

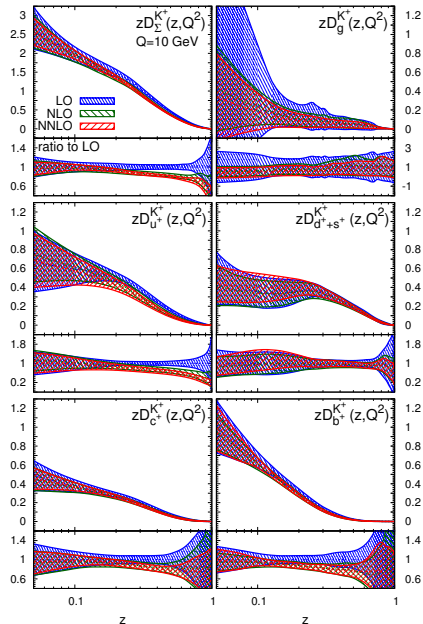


Dependence upon perturbative order: K^+

| Exp. | N_{dat} | LO χ^2/N_{dat} | NLO χ^2/N_{dat} | NNLO χ^2/N_{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 |
| TOTAL | 385 | 1.02 | 0.78 | 0.73 |

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

| i | N^{i+1}/N^i | 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 |



Comparison with other FF determinations: K^+

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

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

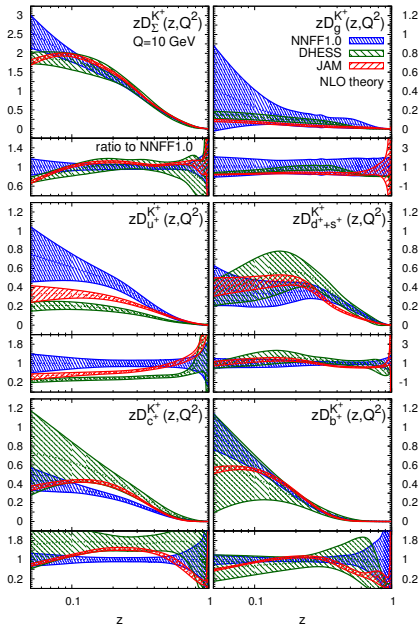
$D_{\Sigma}^{\pi^+}$: excellent agreement (both c.v. and unc.)
bulk of the dataset

$D_g^{\pi^+}$: 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

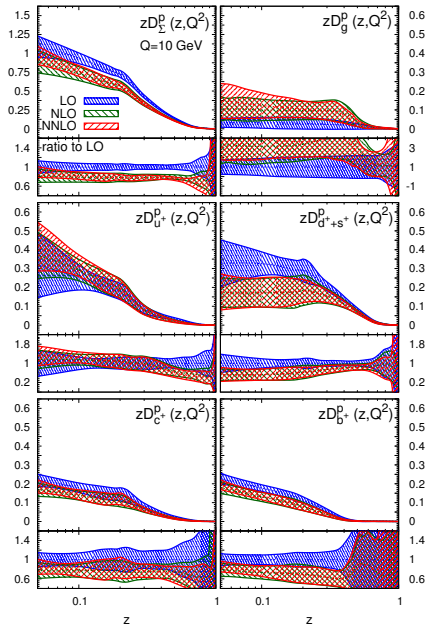
$D_{d^+}^{\pi^+} + D_{s^+}^{\pi^+}$: fair mutual agreement
differences in dataset and parametrisation
comparable uncertainties in the data region

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



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

| Exp. | N_{dat} | LO χ^2/N_{dat} | NLO χ^2/N_{dat} | NNLO χ^2/N_{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 |
| TOTAL | 360 | 1.31 | 1.13 | 0.98 |



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

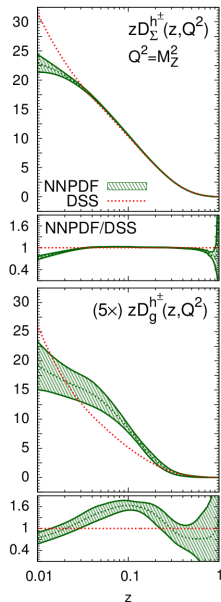
Fragmentation functions of unidentified charged hadrons

Combine the information from identified π^\pm , K^\pm and p/\bar{p} FFs with that from residual light charged hadrons [PoS DIS2017 231]

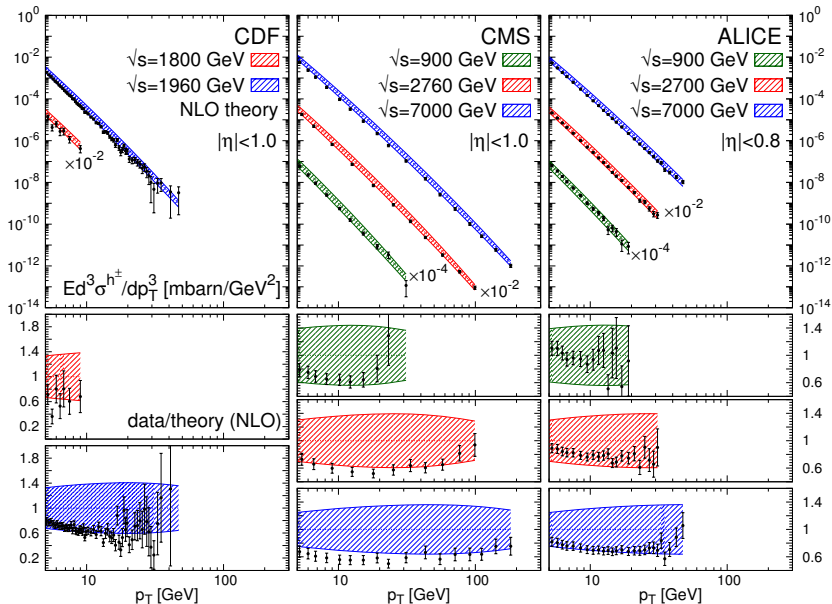
Preliminary analysis done consistently with NNFF1.0 (NLO)

Additional F_L data (non-vanishing $\mathcal{O}(\alpha_s)$ contribution at LO)

| Experiment | Observable | \sqrt{s} [GeV] | N_{dat} | χ^2/N_{dat} |
|---------------|-----------------------|------------------|------------------|-------------------------|
| TASSO14 | F_2 (incl.) | 14.00 | 15 (20) | 1.23 |
| TASSO22 | F_2 (incl.) | 22.00 | 15 (20) | 0.51 |
| TPC | F_2 (incl.) | 29.00 | 21 (34) | 1.65 |
| TASSO35 | F_2 (incl.) | 35.00 | 15 (20) | 1.14 |
| TASSO44 | F_2 (incl.) | 44.00 | 15 (20) | 0.68 |
| ALEPH | F_2 (incl.) | 91.20 | 32 (35) | 1.04 |
| DELPHI | F_L (incl.) | 91.20 | 19 (21) | 0.36 |
| | F_2 | 91.20 | 21 (27) | 0.65 |
| | F_2 (uds tagged) | 91.20 | 21 (27) | 0.17 |
| | F_2 (b tagged) | 91.20 | 21 (27) | 0.82 |
| | F_L (incl.) | 91.20 | 20 (22) | 0.72 |
| OPAL | F_L (b tagged) | 91.20 | 20 (22) | 0.44 |
| | F_2 (incl.) | 91.20 | 20 (22) | 2.41 |
| | F_2 (uds tagged) | 91.20 | 20 (22) | 0.90 |
| | F_2 (c tagged) | 91.20 | 20 (22) | 0.61 |
| | F_2 (b tagged) | 91.20 | 20 (22) | 0.21 |
| SLD | F_L (incl.) | 91.20 | 20 (22) | 0.31 |
| | F_2 | 91.28 | 34 (40) | 0.75 |
| | F_2 (uds tagged) | 91.28 | 34 (40) | 1.03 |
| | F_2 (c tagged) | 91.28 | 34 (40) | 0.62 |
| | F_2 (b tagged) | 91.28 | 34 (40) | 0.97 |
| Total dataset | | | 471 (527) | 0.83 |



Fragmentation functions of unidentified charged hadrons



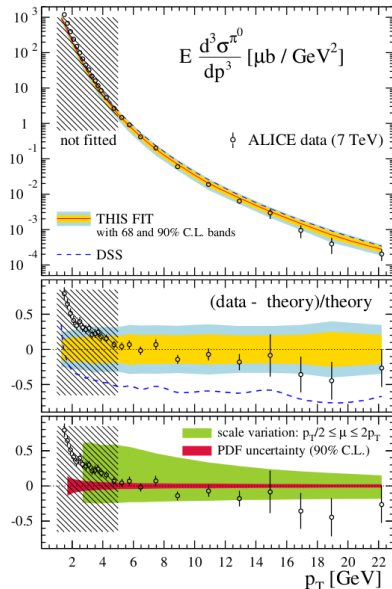
3. Summary and outlook

More global fits

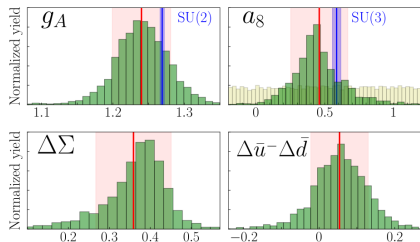
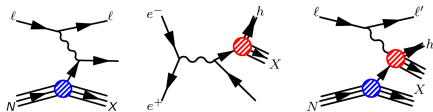
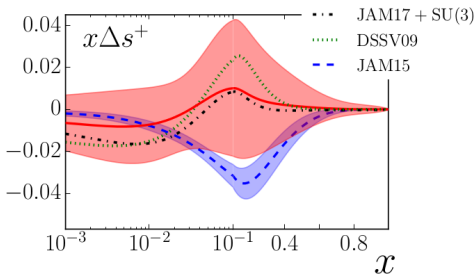
pions: $\chi^2_{\text{tot}}/N_{\text{dat}} = 1.19$

[PRD 91 (2015) 014035; PRD 95 (2017) 094019]

| experiment | data type | norm. N_i | # data in fit | χ^2 | |
|--------------------|--------------------------|----------------------|---------------|----------|------|
| TPC [48] | incl. | 1.043 | 17 | 17.3 | |
| | uds tag | 1.043 | 9 | 2.1 | |
| | c tag | 1.043 | 9 | 5.9 | |
| | b tag | 1.043 | 9 | 9.2 | |
| TASSO [49] | 34 GeV | incl. | 1.043 | 11 | 30.2 |
| | 44 GeV | incl. | 1.043 | 7 | 22.2 |
| SLD [19] | incl. | 0.986 | 28 | 15.3 | |
| | uds tag | 0.986 | 17 | 18.5 | |
| | c tag | 0.986 | 17 | 16.1 | |
| | b tag | 0.986 | 17 | 5.8 | |
| ALEPH [16] | incl. | 1.020 | 22 | 22.9 | |
| DELPHI [17] | incl. | 1.000 | 17 | 28.3 | |
| OPAL [18, 20] | uds tag | 1.000 | 17 | 33.3 | |
| | b tag | 1.000 | 17 | 10.6 | |
| | incl. | 1.000 | 21 | 14.0 | |
| | u tag | 0.786 | 5 | 31.6 | |
| | d tag | 0.786 | 5 | 33.0 | |
| | s tag | 0.786 | 5 | 51.3 | |
| | c tag | 0.786 | 5 | 30.4 | |
| | b tag | 0.786 | 5 | 14.6 | |
| BABAR [28] | incl. | 1.031 | 45 | 46.4 | |
| BELLE [29] | incl. | 1.044 | 78 | 44.0 | |
| HERMES [30] | π^+ (p) | 0.980 | 32 | 27.8 | |
| | π^- (p) | 0.980 | 32 | 47.8 | |
| | π^+ (d) | 0.981 | 32 | 40.3 | |
| | π^- (d) | 0.981 | 32 | 59.1 | |
| COMPASS [31] prel. | π^+ (d) | 0.946 | 199 | 174.2 | |
| | π^- (d) | 0.946 | 199 | 229.0 | |
| PHENIX [21] | π^0 | 1.112 | 15 | 15.8 | |
| STAR [33-36] | $0 \leq \eta \leq 1$ | π^0 | 1.161 | 7 | 5.7 |
| | $0.8 \leq \eta \leq 2.0$ | π^0 | 0.954 | 7 | 2.7 |
| | $ \eta < 0.5$ | π^\pm | 1.071 | 8 | 4.3 |
| | $ \eta < 0.5$ | $\pi^+, \pi^-/\pi^+$ | 1.006 | 16 | 17.2 |
| | ALICE [32] | 7 TeV | π^0 | 0.766 | 11 |
| TOTAL: | | | 973 | 1154.6 | |



Simultaneous fits [PRL 119 (2017) 132001]



$g_A = 1.24 \pm 0.04$ $a_8 = 0.46 \pm 0.21$
 confirmation of SU(2) symmetry to $\sim 2\%$
 $\sim 20\%$ SU(3) breaking $\pm 20\%$

$$\Delta s^+ = -0.03 \pm 0.09$$

$$\Delta\Sigma = 0.36 \pm 0.09 \quad \Delta u - \Delta d = 0.05 \pm 0.08$$

| process | target | N_{dat} | χ^2 |
|--------------------------|-----------------------|------------------|---------------|
| DIS | $p, d, {}^3\text{He}$ | 854 | 854.8 |
| SIA (π^\pm, K^\pm) | | 850 | 997.1 |
| SIDIS (π^\pm) | | | |
| HERMES | d | 18 | 28.1 |
| HERMES | p | 18 | 14.2 |
| COMPASS | d | 20 | 8.0 |
| COMPASS | p | 24 | 18.2 |
| SIDIS (K^\pm) | | | |
| HERMES | d | 27 | 18.3 |
| COMPASS | d | 20 | 18.7 |
| COMPASS | p | 24 | 12.3 |
| Total: | | 1855 | 1969.7 |

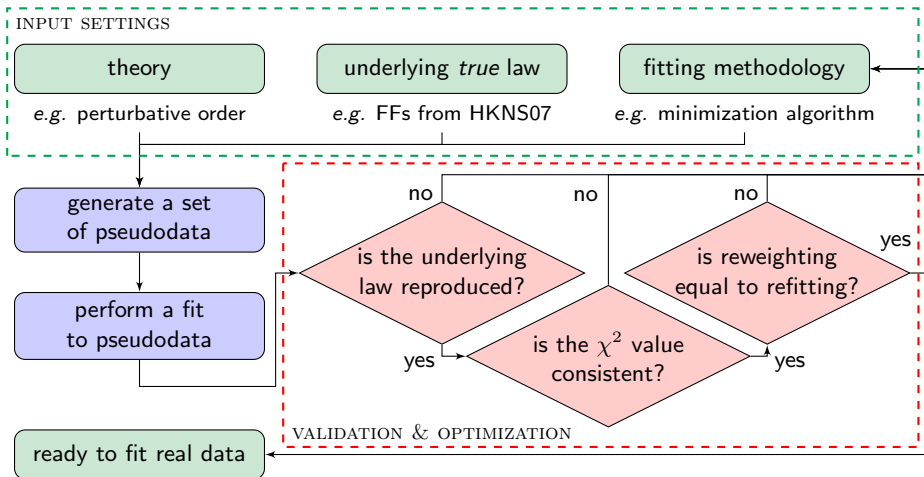
Conclusions

- ➊ 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
- ➋ FFs are poorly known in comparison to PDFs
 - ▶ limited set of available data, observables often require PDFs and FFs simultaneously
 - ▶ are uncertainties faithfully represented?
 - ▶ troubles in describing some observables in pp and SIDIS from current FF sets
- ➌ New analysis based on the NNPDF methodology, NNFF1.0
 - ▶ at LO, NLO and NNLO, based on SIA data for π^\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) larger than in previous determinations
 - ▶ differences in shapes, to be further investigated
 - ▶ good description of the hadron spectra at the LHC within uncertainties
 - ▶ applicability limited by insensitivity to favoured/unfavoured FFs
- ➍ Future improvements
 - ▶ More global fits
 - ▶ Simultaneous fits of FFs and PDFs

4. Additional slides

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

Closure tests: levels

- ① Level 0: generate pseudodata D_i^0 with zero uncertainty (but $(\text{cov})_{ij}$ in the χ^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)

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

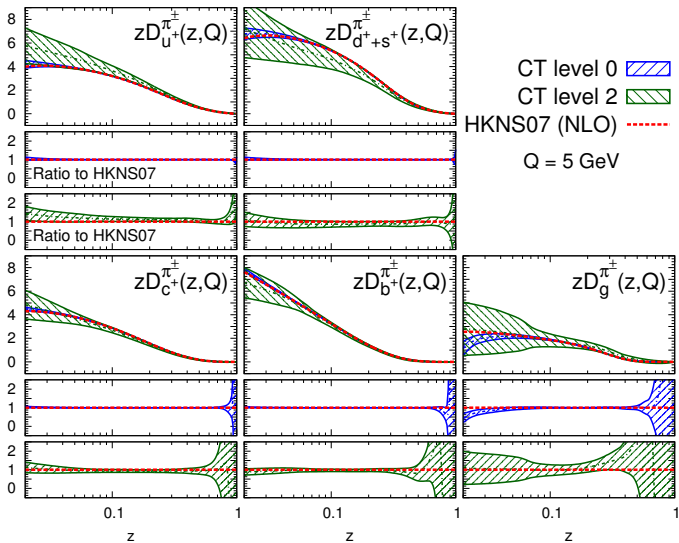
- experimental uncertainties are not propagated into FFs: $\chi^2/N_{\text{dat}} \sim 1$
→ functional uncertainty (a large number of functional forms with equally good χ^2)

- ③ Level 2: generate N_{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

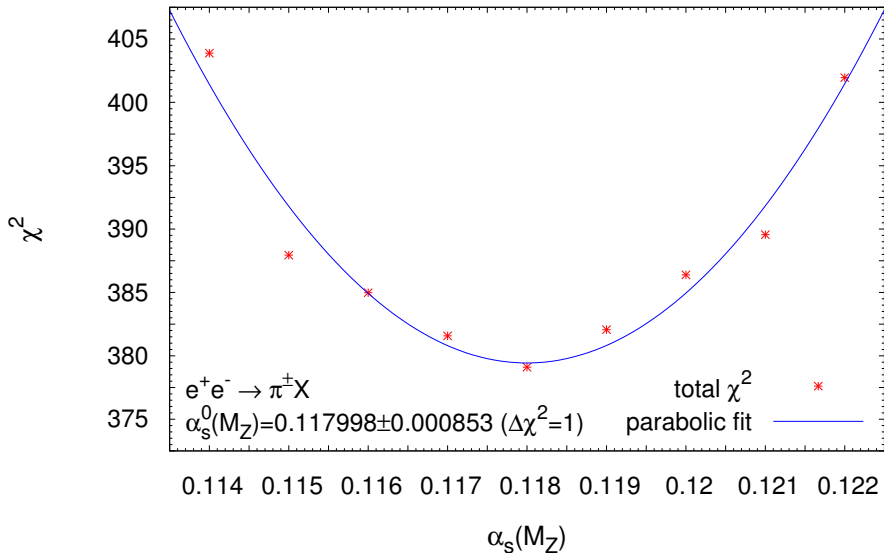
Closure testing NNFF1.0



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

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

Dependence on α_s



Minimisation: adaptive algorithms [N. Hansen, Springer (2016)]

The Covariance Matrix Adaption - Evolution Strategy (CMA-ES)

- 1 Initialisation at the (0)-th generation

$$\mathbf{a}^{(0)} \sim \mathcal{N}(0, \mathbf{C}^{(0)}), \quad \mathbf{C}^{(0)} = \mathbf{I}$$

- 2 Mutation at the (i)-th generation, λ mutants, step-size $\sigma^{(i-1)}$

$$\mathbf{x}_k^{(i)} \sim \mathbf{a}^{(i-1)} + \sigma^{(i-1)} \mathcal{N}(0, \mathbf{C}^{(i-1)}), \quad \text{for } k = 1, \dots, \lambda$$

compute the fitness of each mutant and rank them such that $\chi^2(\mathbf{x}_k) < \chi^2(\mathbf{x}_{k+1})$

- 3 (Non-elitist) recombination

compute the new search centre as a weighted average over the $\mu = \lambda/2$ best mutants

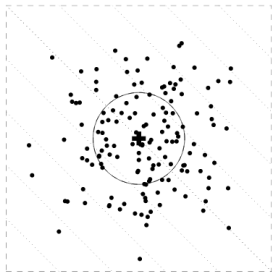
$$\mathbf{a}^{(i)} = \mathbf{a}^{(i-1)} + \sum_{i=1}^{\mu} w_i \left(\mathbf{x}_k^{(i)} - \mathbf{a}^{(i-1)} \right)$$

update \mathbf{C} using information on the parameter space learnt from the mutants

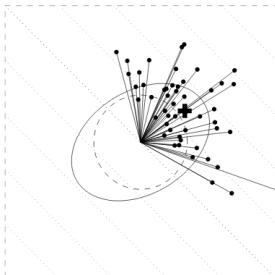
iterate until convergence is reached

Minimisation: the CMA-ES algorithms [N. Hansen, Springer (2016)]

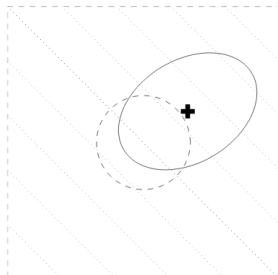
Mutation



Selection



Adaption



The key features of the CMA-ES family of algorithms are the determination of the search distribution covariance matrix $\mathbf{C}^{(i)}$ (and possibly of the step-size σ^i)

These features are optimised by the fit procedure, making use of the information present in the ensemble of mutants to learn preferred directions in parameter space

Internal parameters ($\sigma^{(0)}$, λ , w_i) tuned by trial and error