NNLO Parton Distributions for the LHC

Sergey Alekhin
II. Institut für Theoretische Physik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany;
Institute for High Energy Physics, 142281 Protvino, Russia
E-mail: sergey.alekhin@desy.de

Johannes Blümlein
Deutsches Elektronensynchrotron DESY, Platanenallee 6, D–15738 Zeuthen, Germany
E-mail: Johannes.Bluemlein@desy.de

Sven-Olaf Moch
II. Institut für Theoretische Physik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany
E-mail: sven-olaf.moch@desy.de

We consider some trends, achievements and a series of remaining problems in the precision determination of parton distribution functions. For the description of the scaling violations of the deep-inelastic scattering data, forming the key ingredients to all PDF fits, a solid theoretical framework is of importance. It is provided by the fixed flavor number scheme in describing the heavy-quark contributions which is found in good agreement with the present experimental data in a very wide range of momentum transfers. In this framework also a consistent determination of the heavy-quark masses is possible at high precision. The emerging Drell-Yan data measured at hadron colliders start to play a crucial role in disentangling the quark species, particularly at small and large values of $x$. These new inputs demonstrate a good overall consistency with the earlier constraints on the PDFs coming from fixed-target experiments. No dramatic change is observed in the PDFs in case of a consistent account of the higher-order QCD corrections and when leaving enough flexibility in the PDF shape parameterization.
After a long period of phenomenological studies, contemporary particle physics has reached the level of percent accuracy for the parton distribution functions (PDFs). However, some important features still need further clarification [1]. This concerns in particular the asymptotic behavior for small and large values of Bjorken $x$. The first issue is in turn related to the theoretical foundations for the description of small-$x$ deep-inelastic scattering (DIS) processes, including the heavy-quark contributions to the structure functions due to charm and bottom. The latter provide very essential constraints on the PDFs in the small-$x$ region. The heavy quark contribution to deep-inelastic scattering (DIS) is commonly considered within two competitive factorization schemes, one with a fixed number of flavors (FFN) and another variable number of flavors (VFN). A detailed comparison of these two approaches was performed in Ref. [1] and the FFN scheme was found to provide a better description of the existing HERA data on DIS charm production. Indeed, the superiority of the FFN scheme versus a VFN scheme within the kinematic region covered by HERA had been observed already very early on, cf. Ref. [2].

The FFN scheme turns out to provide a more consistent setting for the heavy quark masses than in the case of the VFN scheme \(^1\). Present theoretical calculations in the FFN scheme include the next-to-next-to-leading order (NNLO) Wilson coefficients [4], which are modeled using the available asymptotics in different kinematic regimes between heavy-quark production at threshold and the high-energy limit. The asymptotic expressions of these two regimes are matched using the factorized form of the massive Wilson coefficients expressed in terms of massless coefficient functions and the massive operator matrix elements (OMEs), which are valid at momentum transfers $Q^2 \gg m_h^2$, where $m_h$ denotes heavy quark mass [5–8]. At NNLO one needs for this purpose the 3-loop OMEs, which are known exactly in part [5–7, 10–12] and are available in main terms in form of an approximation [4] based on the fixed number of Mellin moments, calculated in Ref. [9]. Such approximations are commonly less accurate at small $x$, however their uncertainty can be validated using exact results, e.g., the recently calculated pure-singlet OME [5]. It turns out, that the exact pure-singlet term is well within the uncertainties quoted for the approximate form obtained earlier from the first five non-vanishing Mellin moments [9], see Fig. 1. Moreover, the exact pure-singlet term can be employed to derive the gluon OME using the Casimir-scaling approximation. The expressions for the NNLO massive Wilson coefficients in the FFN scheme comprise all these ingredients \(^2\).

An important improvement in this formalism concerns definition of the heavy-quark mass.

\(^1\)See also Ref. [3] for an updated comparison with the use of recent HERA data on the heavy-quark production

\(^2\)The 3-loop massive OMEs obtained in this way can be also used to compute NNLO PDFs in the VFN scheme, see e.g. Ref. [6].
While the perturbative calculations are usually based on the pole mass-scheme, one rather turns to the $\overline{\text{MS}}$ running-mass for reasons of perturbative stability [13]. Good agreement with the existing data is achieved by using this framework.

The value for the $c$-quark $\overline{\text{MS}}$ mass obtained in the recent ABMP16 fit [14]

$$m_c(m_c) = 1.252 \pm 0.018(\text{exp.}) \pm 0.010(\text{th.})$$

is in a very good agreement with other precision determinations, e.g. based on the $e^+e^-$ data [15].

The inclusive DIS data have a limited potential to disentangle the distributions of the quark species, particularly at small $x$. This is due to the fact that the HERA data consist only of proton data. Meanwhile, however, the Drell-Yan (DY) data from the LHC are of sufficient quality to determine the different flavor distributions very well up to energies of 13 TeV. These data probe the PDFs in a wide range of $x$, down to $x \sim 10^{-4}$ and provide a variety of constraints on the quark distributions due to the production of both, $W^\pm$- and $Z$-bosons. The impact of this input on the PDF determination is demonstrated for instance in ABMP16 fit [14], which includes a wide collection of the $W^\pm$- and $Z$-production data from the ATLAS, CMS and LHCb experiments at the LHC and from the DØ experiment at Tevatron. By discarding these data sets in a test variant of the ABMP16 fit we find an essential deterioration in the determination of the quark distributions, leading to a greatly expanded uncertainty in the iso-spin asymmetry $(\bar{d} - \bar{u}) / (\bar{d} + \bar{u})$ at small $x$. In the absence of DY data this piece is essentially unconstrained, see Fig. 2. Therefore, in earlier PDF parameterizations, it was commonly set to zero for $x \to 0$. The collider DY data prefer a sizable negative value at $x \sim 10^{-4}$ and a symmetric non-strange sea is observed at $x \lesssim 10^{-5}$ only [16].

In general, the available DY data a very consistent. However, with rising experimental accuracy some tension between different experiments or even within one experiment may emerge. In particular, this concerns the recent ATLAS data on $W^\pm$- and $Z$-production at a center-of-mass (c.m.s.) energy of 7 TeV [17]. This sample is in good agreement with the earlier data obtained by the same collaboration from the low-luminosity run [18]. It is in part related to the $W^\pm$-production, see Fig. 3. Meanwhile, the $Z$-production cross sections at central rapidity moved somewhat higher than the earlier ones. The tension is at the level of 1-2$\sigma$. It makes it difficult to describe the recent ATLAS data with the PDFs tuned to the previous release. Moreover, the epWZ16 PDFs extracted by ATLAS from data of Ref. [17], in combination with the inclusive DIS sample from HERA,

\[\text{Figure 2: The 1σ band for the NNLO quark iso-spin asymmetry } (\bar{d} - \bar{u}) / (\bar{d} + \bar{u}) \text{ in the 3-flavor scheme at the scale of } \mu = 3 \text{ GeV as a function of Bjorken } x \text{ obtained in variants of the ABMP16 PDF fit [14] with the data on production of } W^\pm \text{- and } Z \text{-bosons (right-titled hash), } Z \text{-bosons (right-titled hash), and both } W^\pm \text{- and } Z \text{-boson (shaded area) excluded from the fit.}\]
Figure 3: The pulls for the ATLAS data on the \(pp \rightarrow W^± + X \rightarrow l^± v + X\) production (a) and (b) and \(pp \rightarrow Z + X \rightarrow l^+ l^- + X\) (c): central region, (d): forward region) at \(\sqrt{s} = 7\) TeV collected at luminosity of 35 pb\(^{-1}\) (2011) \([18]\) (blue squares) and 4.6 fb\(^{-1}\) (2016) \([17]\) (red circles) with cuts on the lepton’s transverse momentum \(P_T > 20\) GeV as a function of the lepton pseudo-rapidity \(\eta\) versus NNLO predictions obtained using FEWZ (version 3.1) \([19, 20]\) and the ABMP16 PDFs.

demonstrate some unusual features, namely the strange sea is greatly enhanced if compared to strange suppression factors of \(\sim 0.5\) as commonly obtained in the PDF fits.

To the most extent such an enhancement can be explained by a particular PDF shape employed in the analysis of Ref. \([17]\). This shape had been suggested for the HERAPDF fit based on the HERA data only long ago. Therefore it contains many constraints due to the limited potential of inclusive DIS in disentangling quark distributions. By applying these constraints the non-strange sea distributions are artificially suppressed and this suppression is compensated in the ATLAS analysis by the strangeness enhancement, which finally leads to an abnormal strange sea suppression factor \([21]\). If instead a flexible enough PDF shape is used, the strangeness preferred by the ATLAS data is in a reasonable agreement with the earlier determinations, although some tension at \(x \sim 0.01\) still persists, see Fig. 4. This tension is evidently related to the impact of the upward shift in the central \(Z\)-production observed for the recent ATLAS measurements, see Fig. 3. However, it is worth noting that the ATLAS data for forward-rapidity demonstrate a different trend, although being statistically less significant.

Besides, the CMS data on \(Z\)-production are also somewhat lower than the ATLAS results, see Ref. \([21]\) for details. Therefore this tension still deserves further clarification. Another problematic aspect of the DY data analysis concerns the accuracy of the tools, which are needed for the computation of the cross sections with account of realistic experimental cuts on the lepton transverse momentum.

The fully exclusive NNLO codes FEWZ \([19, 20]\) and DYNNLO \([22, 23]\), which accomplish these computations, are not in perfect agreement in the relevant kinematical region, see Fig. 5.
In general, the predictions by DYNNLO are lower than the ones by FEWZ by $\sim 1\%$. However, at the edges of the distributions this difference rises to $10\%$. The discrepancies between DYNNLO and FEWZ were partially understood as being due to the numerical integration accuracy [24] and due to effects of experimental cuts on the lepton transverse momentum in higher-order QCD computations [25], but at the moment the theoretical accuracy is limiting the related studies.

The DY collider data also help to constrain the large-$x$ region of the quark distributions, in particular for the ratio $d/u$. In this context the DØ measurement of the $W$ charge asymmetry [26] provides the statistically most significant constraint. Since $W$-boson production is not measured directly, the $W$-asymmetry is derived in the DØ analysis from the measurement of the electrons stemming from the $W$ decays. This is possible in a unique way at leading order (LO) only, while account of the higher-order corrections requires additional modeling. This, in particular, causes sensitivity to the $W$-asymmetry obtained by the choice of the PDFs used. It leads to a certain tension between the $W$-asymmetry data and the original $e$-asymmetry ones, if the PDFs are varied. In particular, the predictions of the $W$-asymmetry for the DØ kinematics obtained with the ABMP15 PDFs based on the DØ data on the $e$-asymmetry [27], are in substantial disagreement with the DØ data on $W$-asymmetry, see Fig. 6.

The potential of the DØ measurements on the large-$x$ asymptotics of the $d/u$ ratio was checked in the recent CJ15 PDF fit [28]. An advantage of this analysis is a flexible PDF shape, which allows for a non-vanishing value of $(d/u)|_{x=1}$. The CJ15 analysis combines both the $W$-asymmetry and the $e$-asymmetry DØ data. The large-$x$ $d/u$ ratio is mainly driven by the $W$-asymmetry data due to its statistical significance. The impact of these data

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4In the ATLAS analysis [17] the DYNNLO calculations are used for nominal results and the difference between DYNNLO and FEWZ is taken as a theoretical uncertainty.
is quite sensitive on the theoretical accuracy of the analysis. The $d/u$ ratio obtained with the LO description leads to higher values than the one obtained accounting for the next-to-leading order (NLO) corrections, see Fig. 7. Furthermore, the uncertainties in the $d/u$-ratio do substantially rise in the NLO fit. This is evidently due to the smearing of the predictions by the gluon-initiated contribution and the propagation of the uncertainty of the gluon-distribution into the ratio of $d/u$ extracted from the fit. The theory framework of the CJ15 fit is based on a $K$-factor approximation of the $W$-production cross section, with the NLO predictions represented as a product of the LO approximation and the pre-computed ratio of the NLO and LO cross sections. In case of the $\bar{p}p$ initial state such an approach reproduces the initial LO predictions. Therefore the CJ15 result on $d/u$ should be biased upwards due to the missing NLO corrections, see Ref. [29] for details. The value of $d/u$ preferred by the DØ data on the $e$-asymmetry [27] is substantially lower than the $W$-asymmetry results and even extends to negative values at $x \rightarrow 1$, although with large uncertainties, see Fig. 7.

Comparing it with the NLO determination based on the $W$-asymmetry, we conclude that there is no strong evidence in favor of a non-vanishing $(d/u)|_{x=1}$ from the analysis of the DØ data. Moreover, the $e$-asymmetry data, preferring a smaller value of $d/u$, are less model-dependent than the $W$-asymmetry.

The interpretation of the DØ data in the PDF fit turns out to be essential for the related phenomenology of electroweak single-top production since the latter reaction is to a great extent driven by the quark-initiated subprocesses. Therefore a trend observed for the $d/u$ ratio in the variants of the PDF fit with a different treatment of the DØ experimental input is reflected in the ratio of the top and anti-top production cross sections $R_{t/\bar{t}}$ computed with respective PDFs, see Fig. 7.

For the fit based on the $e$-asymmetry data the value of $R_{t/\bar{t}}$ is larger by $\sim 2\sigma$ than for the one obtained from the LO fit using the $W$-asymmetry data. This is comparable to the spread in the predictions of different PDFs, which can be explained in part by the selection of the DY collider data and their treatment.

In summary, we have considered some current trends, achievements and problems in the precision determination of PDFs. For the DIS data a solid theoretical framework is available with the FFN scheme used for description of the heavy-quark contribution. It provides good agreement with existing experimental data in a wide range of momentum transfers and implies a consistent setting of the heavy-quark masses, which are basic parameters of the Standard Model. The emerging DY data collected at the hadron colliders start to play a crucial role in disentangling quark species,
particularly at small and large values of $x$. These new inputs demonstrate a good overall consistency with the earlier constraints on PDFs coming from the fixed-target experiments. No dramatic change in the PDFs is caused in case of consistent account of the higher-order QCD corrections and using PDF shapes which are flexible enough for fitting the experimental data.

**Figure 7:** Left: The same as in Fig. 2 for the ratio $d/u$ obtained using the CJ15 PDF shape [28] and with addition of the DØ data on $W$- and $e$-asymmetry, described within various approximations (vertical hash: $W$-asymmetry [26] at LO, left-titled hash: the same at NLO, right-tilted hash: $e$-asymmetry [27] at NLO in comparison with the nominal CJ15 PDFs (shaded area). Right: The ratio of single top to anti-top production cross section in $pp$ collisions at c.m.s. energy 7 TeV computed with the PDFs obtained in these variants of the fit in comparison with the ATLAS data [30] and the predictions of ABMP16 [16], CT14 [31], MMHT14 [32], NNPDF3.0 [33] and NNPDF3.1 [34] PDFs.

**References**


