Simplified QCD fit method
for BSM analysis of HERA data

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Abstract

The high-precision HERA data can be used as an input to a QCD analysis within the DGLAP formalism to obtain the detailed description of the proton structure in terms of the parton distribution functions (PDFs). However, when searching for Beyond Standard Model (BSM) contributions in the data one should take into account the possibility that the PDF set may already have been biased by partially or totally absorbing previously unrecognised new physics contributions. The ZEUS Collaboration has proposed a new approach to the BSM analysis of the inclusive $ep$ data based on the simultaneous QCD fits of parton distribution functions together with contributions of new physics processes. Unfortunately, limit setting procedure in the frequentist approach is very time consuming in this method, as full QCD analysis has to be repeated for numerous data replicas. We describe a simplified approach, based on the Taylor expansion of the cross section predictions in terms of PDF parameters, which allowed us to reduce the calculation time for the BSM limits by almost two orders of magnitude.

1 Introduction

The H1 and ZEUS collaborations measured inclusive $e^{\pm}p$ scattering cross sections at HERA from 1994 to 2000 (HERA I) and from 2002 to 2007 (HERA II), collecting together a total integrated luminosity of about 1 fb$^{-1}$. All inclusive data were recently
combined to create one consistent set of neutral current (NC) and charged current (CC) cross-section measurements for $e^\pm p$ scattering with unpolarised beams. The inclusive cross sections were used as input to a QCD analysis within the DGLAP formalism, resulting in a PDF set denoted as HERAPDF2.0.

The ZEUS collaboration has recently used the HERA combined data to set limits on possible deviations from the Standard Model due to a finite radius of the quarks. To take into account the possibility that the new physics contributions can affect PDF determination, resulting in the bias of the QCD fit results, the limit-setting procedure was based on a simultaneous QCD fit of PDF parameters and the quark radius. The 95% C.L. limits on the effective quark-radius squared, $R^2_q$, were

$$-(0.47 \cdot 10^{-16} \text{ cm})^2 < R^2_q < (0.43 \cdot 10^{-16} \text{ cm})^2.$$ 

Taking into account the possible influence of quark radii on the PDF parameters turned out to be important - for fixed PDFs the obtained limits would be too strong by about 10%.

These limits on the effective quark-radius squared were derived in a frequentist approach using the technique of replicas. The replicas are sets of cross-section values that are generated by varying all cross sections randomly according to their known statistical and systematic uncertainties. For each value of the true quark-radius squared, $R^2_{q, \text{True}}$, considered in the limit setting procedure, about 5000 replicas were generated and used as an input to a QCD fit with the PDF parameters and the quark radius squared treated as free parameters. With a single QCD fit to the full HERA data set taking on average about 1.5 hour of CPU time, 200 000 fits performed for setting the final limits in the quark radius analysis required over 30 years of CPU time. Even when using a high performance computing cluster, processing time is a limiting factor for possible extensions of the analysis to other models.

## 2 Standard QCD+BSM fit

As described in the $R_q$ paper, the PDFs of the proton are described at a starting scale of $1.9 \text{ GeV}^2$ in terms of $N_{\text{par}} = 14$ parameters. These parameters, denoted $p_k$ in the following (or $p$ for the set of parameters), together with the possible contribution of BSM phenomena (quark form factor $R^2_q$ or CI coupling $\eta$) are fit to the data using a $\chi^2$ method, with the $\chi^2$ formula given by:

$$\chi^2(p, s, \eta) = \sum_i \left[ m^i + \sum_j \gamma_j^i m^i s_j - \mu_0^i \right]^2 \left( \delta_i^{\text{stat}} + \delta_i^{\text{uncor}} \right) (\mu_0^i)^2 + \sum_j s_j^2. \quad (1)$$

Here $\mu_0^i$ and $m^i$ are the measured cross-section value and the pQCD+BSM cross-section prediction at the point $i$. The quantities $\gamma_j^i$, $\delta_i^{\text{stat}}$ and $\delta_i^{\text{uncor}}$ are the relative correlated systematic, relative statistical and relative uncorrelated systematic uncertainties of the input data, respectively. The components $s_j$ of the vector $s$ represent the correlated systematic shifts of the cross sections (given in units of $\gamma_j^i$), which
are fit to the data together with PDF parameter set $p$ and the CI coupling $\eta$. The summations extend over all data points $i = 1, \ldots, N_{\text{data}}$ and all correlated systematic uncertainties $j = 1, \ldots, N_{\text{sys}}$.

The dependence of the pQCD+BSM cross-section prediction at the point $i$ on the PDF parameters $p$ and the CI coupling $\eta$ can be written as:

$$m^i = Q(x_i, Q^2_i, p, \eta),$$ (2)

where $x_i$ and $Q^2_i$ are the kinematic variables corresponding to the point $i$.

## 3 Replica generation

Equation (2) relating model parameters and cross-section predictions is also used for the replica generation. For each replica, the generated value of the cross section at the point $i$, $\mu^i$, is calculated as

$$\mu^i = \left[ m^i_{\text{True}} + \sqrt{\delta^2_{\text{stat}} + \delta^2_{\text{uncor}} \cdot \mu^i_0 \cdot r_i} \right] \cdot \left( 1 + \sum_j \gamma^j \cdot r_j \right),$$ (3)

where variables $r_i$ and $r_j$ represent random numbers from a normal distribution generated for each data point $i$ and for each source of correlated systematic uncertainty $j$, respectively. A set of cross-section values $m^i_{\text{True}}$ is calculated using the nominal PDF predictions (based on the set $p_0$ of the PDF parameters fit to the actual data without taking CI contribution into account) and the assumed CI coupling value $\eta^{\text{True}}$. It can be written as

$$m^i_{\text{True}} = Q(x_i, Q^2_i, p_0, \eta^{\text{True}}).$$ (4)

The set of nominal Standard Model predictions can be defined as

$$m^i_0 = Q(x_i, Q^2_i, p_0, 0).$$ (5)

In the simplified approach described below, these predictions will be used as the reference cross section values.

## 4 Simplified QCD fit approach

The proposed approach is based on the assumption that PDF parameters resulting from the QCD fit fluctuate only within relatively small uncertainties from replica to replica. Therefore, we assume that the dependence of the cross-section predictions on the PDF parameters can be approximated by a first order (linear) Taylor expansion, valid for small parameter variations. For each data point $i$, we define a vector of
derivatives:

\[
\theta^i_{0 k} = \left. \frac{\partial m^0_i}{\partial p_k} \right|_{\chi^2 = \chi^2_{\text{min}}} = \left. \frac{\partial Q(x_i, Q^2_i, p, 0)}{\partial p_k} \right|_{p = p_0},
\]

where \(k = 1, \ldots N_{\text{par}}\). These derivatives can be calculated numerically in the linear approximation as:

\[
\theta^i_{0 k} = \left. \frac{\partial Q(x_i, Q^2_i, p, 0)}{\partial p_k} \right|_{p = p_0} \approx \frac{Q(x_i, Q^2_i, p_0^+ k, 0) - Q(x_i, Q^2_i, p_0^- k, 0)}{\sigma_k}.
\]

Here \(\sigma_k\) is the uncertainty of the fitted PDF parameter \(p^k_0\) (\(k\)-th parameter of the vector \(p_0\)) and the two parameter vectors \(p_0^{+ k}\) and \(p_0^{- k}\) describe parameter sets resulting from changing parameter \(p^k_0\) by \(\pm \frac{1}{2} \sigma_k\):

\[
p_0^{+ k} = (p^1_0, \ldots, p^k_0 + \frac{\sigma_k}{2}, \ldots, p^{N_{\text{par}}}_0),
\]

\[
p_0^{- k} = (p^1_0, \ldots, p^k_0 - \frac{\sigma_k}{2}, \ldots, p^{N_{\text{par}}}_0).
\]

The simplified formula for the model predictions has a form

\[
\tilde{Q}(x_i, Q^2_i, p, 0) = m^0_i + \sum_k \theta^i_{0 k} \cdot \Delta p^k,
\]

where \(\Delta p^k\) is the shift of the PDF parameter \(p^k\) with respect to the nominal fit result, \(\Delta p^k = p^k - p^k_0\). By substituting exact formula (2) by the approximate formula (10) we can significantly speed-up calculation of the model predictions \(m^i\) in the PDF fitting procedure.

The proposed procedure was tested by comparing results of the full QCD fit and the simplified fit on a large sample of Standard Model replicas (generated without BSM contribution, i.e. with \(\eta^{\text{True}}\) set to 0). Possible CI contribution was also not considered in the fit (\(\eta\) parameter fixed to 0). Parameter values resulting from the full QCD fit and from the simplified fit on the large set of the Standard Model replicas are compared in Fig. 1. Parameters \(C_{uu}, C_{ud}, C_{U}\) and \(C_D\) describing high-\(x\) behaviour of valence \(u\), valence \(d\), see \(u\) and see \(d\) quarks respectively, are considered. Distributions of the fitted parameter values agree in general, but there are also visible differences between the two methods and a systematic bias for \(C_d\) and \(C_D\) parameters. However, when comparing the reduced cross-section values calculated from the fitted PDFs, as illustrated in Fig. 2, the two approaches agree very well. The simplified fit reproduces results of the full fit with percent level accuracy and no systematic bias. The agreement of the replica data with the predictions of DGLAP evolution equations, as indicated by the \(\chi^2\) value of the fit, is well reproduced while the processing time is reduced by a factor of almost 50, as shown in Fig. 3.
Figure 1: Comparison of the chosen PDF parameter values from the full QCD fit and from the simplified fit on the large set of the Standard Model replicas. Parameters describing high-x behaviour of valence and sea quark distributions are shown, as indicated in the plot labels.
Figure 2: Comparison of the reduced cross-section predictions from the full QCD fit and from the simplified fit on the large set of the Standard Model replicas. Cross sections for NC and CC $e^\pm p$ DIS at $x = 0.25$ and $Q^2 = 8000$ GeV$^2$ are considered, as indicated in the plot labels.
Figure 3: Comparison of the full QCD fit performance with the simplified fit procedure for the large set of the Standard Model replicas, for the $\chi^2$ values resulting from the fit (left) and for the CPU time required (right; note the logarithmic scale).

5 Simplified QCD+BSM fit

The procedure described above can be easily extended to different CI scenarios. Exact description of the pQCD+BSM cross-section predictions as a function of the coupling parameter $\eta$ can still be preserved. This is because the dependence of the model predictions on the coupling $\eta$ is restricted to linear and quadratic terms only.

For each data point $i$, two additional cross-section values (in addition to the reference value $m^0_i$ defined by formula 5) can be defined:

$$m^+_i = Q(x_i, Q^2_i, p_0, +\Delta \eta),$$
$$m^-_i = Q(x_i, Q^2_i, p_0, -\Delta \eta),$$

where $\Delta \eta$ is a fixed (but otherwise arbitrary) step value (e.g., $\Delta \eta = 1 \text{ TeV}^{-2}$). These values can be then used to calculate the cross section terms linear and quadratic in CI coupling:

$$m^1_i = \frac{m^+_i - m^-_i}{2 \Delta \eta},$$
$$m^2_i = \frac{m^+_i + m^-_i - 2 m^0_i}{2 (\Delta \eta)^2}.$$  

The cross section prediction can be then written as

$$m^i = Q(x_i, Q^2_i, p_0, \eta) = m^0_i + m^1_i \cdot \eta + m^2_i \cdot \eta^2.$$
two vectors of derivatives, corresponding to \( m^i_+ \) and \( m^i_- \) values (\( k = 1, \ldots N_{\text{par}} \)):

\[
\theta^i_+ = \frac{\partial m^i_+}{\partial p_k} \bigg|_{\chi^2 = \chi^2_{\text{min}}} = \frac{\partial Q(x_i, Q^2_i, p, +\Delta \eta)}{\partial p_k} \bigg|_{p=p_0},
\]

\[
\theta^i_- = \frac{\partial m^i_-}{\partial p_k} \bigg|_{\chi^2 = \chi^2_{\text{min}}} = \frac{\partial Q(x_i, Q^2_i, p, -\Delta \eta)}{\partial p_k} \bigg|_{p=p_0}.
\]

These derivatives can also be calculated numerically, based on the linear approximation, see formula (7) above.

To summarize, \( 3 + 3N_{\text{par}} \) reference values have to be stored for each data point \( i \) (three cross section values and three derivative values for each PDF parameter). These values are calculated using the full cross section formula (2) and the PDF parameters fit to the nominal data. We can then introduce a simplified description of the CI model predictions:

\[
\tilde{Q}(x_i, Q^2_i, p, \eta) = m^i_0 + \sum_k \theta^i_0 k \Delta p^k + \left( m^i_1 + \sum_{k'} \theta^i_{1 k} \Delta p^{k'} \right) \eta
\]

\[
+ \left( m^i_2 + \sum_{k''} \theta^i_{2 k''} \Delta p^{k''} \right) \eta^2,
\]

where \( \Delta p^k = p^k - p^k_0 \) and \( \theta^i_0 k, \theta^i_{1 k}, \theta^i_{2 k} \) are combinations of calculated derivatives, corresponding to cross-section terms linear and quadratic in the coupling:

\[
\theta^i_{1 k} = \frac{\theta^i_{+ k} - \theta^i_{- k}}{2 \Delta \eta}
\]

\[
\theta^i_{2 k} = \frac{\theta^i_{+ k} + \theta^i_{- k} - 2 \theta^i_0 k}{2 (\Delta \eta)^2}
\]

The simplified cross-section function \( \tilde{Q}(x_i, Q^2_i, p, \eta) \) defined by the formula (18) can then replace the full cross-section calculation (including QCD evolution of PDFs) given by \( Q(x_i, Q^2_i, p, \eta) \) of formula (2) in the QCD+CI fit procedure for replicas generated for any \( \eta^{\text{true}} \), assuming the deviations from nominal Standard Model predictions are small.

The presented approach was tested for the quark form-factor model. Shown in Fig. 4 is the correlation between the \( R^2_q \) value obtained from the full QCD+\( R_q \) fit and those obtained, for the same replicas, using the simplified approach. The replica sets were generated for the Standard Model (\( R_q = 0 \)) and for the quark form-factor model with the quark radius corresponding to the ZEUS limit of \( R_q = 0.43 \cdot 10^{-16} \text{ cm} \). As for the cross-section predictions, \( R^2_q \) values fitted with the simplified method agree almost perfectly with the full QCD+\( R_q \) fit results. Only for a small fraction of replicas some differences are visible, which are much smaller than the width of the \( R^2_q \) distribution. The quality of the fit, as described by the resulting \( \chi^2 \) value, is also very similar for both fit methods, as illustrated in Fig. 5. When the simplified
Figure 4: Comparison of the quark radius squared, $R_q^2$, resulting from the full QCD+$R_q$ fit and from the simplified fit to the same replica. Results are shown for the set of the Standard Model replicas (left) and for the replicas generated with the assumed $R_q^2$ corresponding to the limit set in the ZEUS analysis [2] (right).

Figure 5: Comparison of the $\chi^2$ values resulting from the full QCD+$R_q$ fit and from the simplified fit to the same replica. Results are shown for the set of the Standard Model replicas (left) and for the replicas generated with the assumed $R_q^2$ value corresponding to the limit set in the ZEUS analysis [2] (right).
method is used for the limit setting procedure, the probability distribution and the resulting limit on the quark radius squared also agrees very well with the results of [2], see Fig. 6.

![Figure 6: Results of the limit setting procedure in the frequentist approach, based on the QCD fits to multiple data replicas. The probability of obtaining $R_{q}^{2, \text{Fit}}$ values smaller than that obtained for the actual data, $R_{q}^{2, \text{Data}}$, is shown as a function of the assumed value for the quark-radius squared, $R_{q}^{2, \text{True}}$. The solid blue circles correspond to the published ZEUS results [2] obtained with the full QCD+$R_{q}$ fit to the replica sets generated for different values of $R_{q}^{2, \text{True}}$, while the open green circles show the results based on the simplified fit described in this paper. The dashed lines represent the cumulative Gaussian distributions fitted to the replica points.](image)

6 Conclusions

The simplified procedure for fitting PDF parameters and BSM couplings to the HERA inclusive data has been developed. The procedure reproduces the results of the full QCD fit very well and allows to shorten the computation time by a factor of 50. This opens the possibility to extend the quark form-factor analysis [2] of the HERA inclusive data [1] to other CI-like scenarios.
References

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