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**EXTRACTION OF PARTON DISTRIBUTIONS AND α_s
FROM DIS DATA WITHIN THE BAYESIAN TREATMENT
OF SYSTEMATIC ERRORS**

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Abstract

Alekhin S.I. Extraction of parton distributions and α_s from DIS data within the Bayesian treatment of systematic errors: IHEP Preprint 96-79. – Protvino, 1996. – p. 12, figs. 9, tables 2, refs.: 30.

We have performed the NLO QCD global fit of BCDMS, NMC, H1 and ZEUS data with full account of point-to-point correlations using the Bayesian approach to the treatment of systematic errors. Parton distributions in the proton associated with experimental uncertainties, including both statistical and systematic ones were obtained. The gluon distribution in the wide region of x was determined and it turned out to be softer than in the global analysis using prompt photon data. We also obtained the robust estimate of $\alpha_s(M_Z) = 0.1146 \pm 0.0036$ (75% *C.L.*) based on Chebyshev's inequality, which is compatible with the earlier determination of α_s from DIS data, but with less dependence on high twist effects.

Аннотация

Алехин С.И. Определение партонных распределений и α_s из данных по ГНР на основе байесовского описания систематических ошибок: Препринт ИФВЭ 96-79. – Протвино, 1996. – 12 с., 9 рис., 2 табл., библиогр.: 30.

В работе представлены результаты глобального фита данных коллабораций BCDMS, NMC, H1 и ZEUS, выполненного в рамках NLO QCD с учетом взаимных корреляций на основе байесовского описания систематических ошибок. Получены партонные распределения в протоне и их неопределенности учитывающие и статистические и систематические ошибки данных. Глюонное распределение, определенное в широком диапазоне x , оказалось мягче, чем в глобальных фитах, использующих данные по рождению прямых фотонов. Получена также устойчивая оценка $\alpha_s(M_Z) = 0.1146 \pm 0.0036$ (75% *C.L.*), основанная на неравенстве Чебышева, которая совместима с предыдущими оценками α_s из анализа данных по ГНР, но менее зависима от вклада высших твистов.

Introduction

Recently it has been argued [1] that parton distributions functions (PDFs) obtained from the global data analysis (e.g. [2,4]) have the principal shortcomings arising from the absence of experimental errors associated with the parameters of these distributions. Indeed, the only and often used way to evaluate the spread of predictions given by these PDFs is to compare results of calculations with the various parametrizations input. It is evident that if different authors use the same theoretical model and similar data sets this procedure cannot account for real uncertainties occurring due to statistical and systematic fluctuations of data used to extract PDFs. These uncertainties can be evaluated using the propagation of these fluctuations into the dispersion of PDFs parameters or PDFs themselves. The conclusive treatment of systematic errors, which are usually dominating, is often limited since they are presented in the publications as the combinations from separate sources. For the recent deep inelastic scattering (DIS) data from HERA as well as older ones from SPS full error matrix are fortunately available. Deep inelastic scattering of charged leptons remains the cleanest source of information on PDFs among the other relevant processes and the careful analysis of these data including propagation of systematics can be valuable for exploring the nucleon structure. The handling with statistical fluctuations is well understood on the basis of probability theory, meanwhile the elaborating of systematic ones is the subject of various approaches.

In one of them, based on the classical treatment of probability, one considers the systematic shifts as additional unknown methodical parameters arising due to a poor knowledge of experimental apparatus. Within this approach one usually tries to determine these parameters using some statistical estimator, say χ^2 minimization, to fit the data with these parameters left free. The obtained values are further considered as a reasonable approximation to the true values and data are corrected to account for these systematic shifts. As to systematic errors of theoretical model parameters, they are evaluated inverting full error matrix, including both physical and methodical parameter derivatives. In most cases, the only kinds of the systematic errors which can be determined in the pure classical approach are the systematics connected to the general normalization of the data.

Other methodical parameters are strongly correlated with each other and with physical parameters which leads to their huge errors and unreasonable central values. This situation can be readily explained qualitatively: as far as one turned out to be unable to determine the parameters of the apparatus using the special tests and measurements it is doubtful that one can do it using some cross section measurements indirectly related to the resolving of the methodical ambiguities.

Another, much more productive approach, is based on the Bayesian treatment of systematic uncertainties. In this approach they are considered as random variables with the postulated/evaluated probability distribution function and systematic errors are evaluated within general statistical procedures alongside with the statistical errors. For the analysis of the modern DIS data as a rule having a number of noticeable systematic errors this approach is the unique possibility to account for the point-to-point correlation of data. This is the Bayesian approach that we use in our paper to obtain the complete propagation of systematic uncertainties of DIS data into the uncertainties of the resulting PDFs.

1. Theoretical and experimental input

1.1. Data used in the fit

As a subject of our analysis we use the data for deep inelastic muon/electron hydrogen/deuterium scattering [9,10,11,12] cut to reduce the effects of high twists in the following way

$$W > 4 \text{ GeV}, \quad Q^2 > 9 \text{ GeV}^2,$$

where W and Q^2 are common DIS variables. The number of data points for each experiment after the cut is presented in Table 1. For data of ZEUS collaboration asymmetric systematic errors were averaged. As to BCDMS data we suppose the total correlation of systematic errors for proton and deuterium cross sections.

Table 1. The number of data points (NDP) and χ^2/NDP for the analysed data sets.

Experiment	BCDMS	NMC	H1	ZEUS	total
NDP	558	190	147	166	1061
χ^2/NDP	0.97	1.43	0.91	2.00	1.20

1.2. Probability model of the data

If the experimental data with K sources of multiplicative systematics are explicitly described by a theoretical model they can be presented in the Bayesian approach as

$$y_i = (f_i + \mu_i \sigma_i) \cdot \left(1 + \sum_{k=1}^K \lambda_k \eta_i^k\right),$$

where $f_i = f_i(\theta^0)$ is the value predicted by the theoretical model with parameter θ^0 , μ_i and λ_k are independent random variables, σ_i and η_i^k – statistic and systematic errors from the k -th source for i -th measurement, $i = 1 \dots N$, $k = 1 \dots K$, N is the total number of points in the data set. If the data come from the data sample with a large number of events in every bin, μ are normally distributed, as to λ , the only assumption we are making is that they have zero average and unity dispersions. Within this ansatz individual measurements are correlated and their correlation matrix C_{ij} is given by

$$C_{ij} = \sum_{k=1}^K f_i \eta_i^k f_j \eta_j^k + \delta_{ij} \sigma_i^2$$

where δ_{ij} is the Kronecker symbol. To obtain the estimator of the parameter θ^0 we minimize the quadratic form

$$\chi^2(\theta) = \sum_{i,j=1}^N [f_i(\theta) - y_i] E_{ij} [f_j(\theta) - y_j], \quad (1)$$

where E_{ij} is inverted correlation matrix. We should note that through this paper we treat the normalization errors within this formalism as well as other systematics are regarded as multiplicative, which is almost always the case for counting experiments. The minimization was made with the help of MINUIT package [5] supplied with the modules improving the numerical stability of calculations [6].

If λ_k are normally distributed and $\eta_i^k \ll 1$, $\{y_i\}$ set obeys the multidimensional Gaussian distribution with correlations and $\hat{\theta}$ has the minimal possible dispersion. The systematic errors calculated as the propagation of uncertainties in apparatus parameters or Monte-Carlo corrections are well believed to be Gaussian distributed. At the same time we have shown [7] that even this is not the case this estimator has reduced dispersion comparing with the simplest χ^2 without account of correlations. One should underline that as far as we use the correct covariance matrix built using predicted averages for the measurements our estimator would be asymptotically unbiased and hence does not suffer from the bias discussed in [8].

1.3. QCD input

Physical model for describing the considered data is based on the parton model with pQCD evolution of the light quarks and gluon distributions in the proton defined at initial value of $Q_0^2 = 9 \text{ GeV}^2$. These distributions were evolved using DGLAP equations [14] in the NLO within \overline{MS} factorization scheme [15]. As to the contributions of c -quark and b -quark they were calculated using the LO formula from [16] setting $m_c = 1.5 \text{ GeV}$, $m_b = 4.5 \text{ GeV}$ and the renormalization/factorization scale equal to $\sqrt{Q^2 + 4m_{c,b}^2}$. Our QCD evolution program was tested as suggested in [17] and demonstrated numerical precision of $O(0.1\%)$ in the kinematic region covered by the analysed data. Adjusting the functional form of PDFs we've started from rather general and widely used expressions

$$xq_i(x, Q_0) = A_i x^{a_i} (1-x)^{b_i} (1 + \gamma_1^i \sqrt{x} + \gamma_2^i x), \quad (2)$$

and then reduced the number of free parameters keeping the quality of data description. The resulting functional form of PDFs at Q_0 looks like

$$\begin{aligned} xd_V(x, Q_0) &= \frac{1}{N_d^V} x^{a_d} (1-x)^{b_d}, \quad xd_S(x, Q_0) = \frac{A_S}{N_S} x^{a_{sd}} (1-x)^{b_{sd}}, \\ xu_V(x, Q_0) &= \frac{2}{N_u^V} x^{a_u} (1-x)^{b_u} (1 + \gamma_2^u x), \quad xu_S(x, Q_0) = \frac{A_S}{N_S} \eta_u x^{a_{su}} (1-x)^{b_{su}}, \\ xG(x, Q_0) &= A_G x^{a_G} (1-x)^{b_G}, \quad xs_S(x, Q_0) = \frac{A_S}{N_S} \eta_s x^{a_{ss}} (1-x)^{b_{ss}}. \end{aligned}$$

We did not consider N_u^V, N_d^V and A_G as free parameters, they were calculated from other parameters using partons' number/momentum conservation. As to N_S it is defined by the relation

$$2 \int_0^1 x [u_s(x, Q_0) + d_s(x, Q_0) + s_s(x, Q_0)] dx = A_S.$$

Forecasting the final results we note that after trial fits it has been found that η_u is well compatible with unity and it is fixed at this value. We fixed $\eta_s = 0.5$, which is compatible with recent CCFR findings [13] and also adopted $a_{su} = a_{sd} = a_{ss}$, $b_{ss} = (b_{su} + b_{sd})/2$ since our data do not allow for a separate determination of these parameters.

We calculate strong coupling constant $\alpha_s(Q)$ from the fitted parameter $\alpha_s(M_Z)$ by numerical solving of the NLO renormalization equation

$$\frac{1}{\alpha_s(Q)} - \frac{1}{\alpha_s(M_Z)} = \frac{\beta_0}{2\pi} \ln\left(\frac{Q}{M_Z}\right) + \beta \ln\left[\frac{\beta + 1/\alpha_s(Q)}{\beta + 1/\alpha_s(M_Z)}\right],$$

where

$$\beta_0 = 11 - \frac{2}{3}n_f, \quad \beta = \frac{2\pi\beta_0}{51 - \frac{19}{3}n_f}.$$

This approach prevents one from the uncertainties occurring for the approximate solutions based on the expansion in the inverse powers of $\ln(Q)$, which are ~ 0.001 at the scale of evolution from M_Z to $O(GeV)$ (cf. [18]), i.e. is comparable with the standard deviation of $\alpha(M_Z)$. The number of the active fermions n_f is changing from 4 to 5 due to b-quark threshold at the $Q = m_b$ keeping continuity of $\alpha_s(Q)$.

1.4. Corrections to the basic formula and data

1.4.1. Target mass correction

In addition to the pure pQCD evolution we applied to the calculated value of F_2 the so-called target mass corrections [19] using the relation

$$F_2^{TMC}(x, Q) = \frac{x^2}{\tau^{3/2}} \frac{F_2(\xi, Q)}{\xi^2} + 6 \frac{M^2}{Q} \frac{x^3}{\tau^2} \int_{\xi}^1 dz \frac{F_2(z, Q)}{z^2},$$

where

$$\xi = \frac{2x}{1 + \sqrt{\tau}}, \quad \tau = 1 + \frac{4M^2 x^2}{Q^2}$$

and M is the nucleon mass. The contribution to this correction of the order of M^4/Q^4 presented in [19] turned out to be negligible for all considered data. Target mass correction is most essential for the BCDMS data, where it ranges from -1% to $+7\%$, having the average module related to the statistical error as large as 0.16. We should note that our way of introducing this correction differs from the one applied in [20] and consisting of the substitution $F_2(x, Q) \rightarrow F_2(\xi, Q)$. Due to this difference in our case the correction exhibits crossover from negative to positive values at $x \approx 0.5$ instead of $x \approx 0.4$ like in [20] and differs in the magnitude. For the NMC data this correction is significantly smaller (range – $[-1\%, 0\%]$, relative average – 0.05) and for ZEUS and H1 data is absolutely negligible.

1.4.2. Reduction to the common $R = \sigma_L/\sigma_T$

All the data on F_2 were reduced to the common value of $R = \sigma_L/\sigma_T$ comprised the NLO contribution from light quarks and gluon, the LO contribution from c -quark and b -quark, and the target mass correction included (see [21] for the compilation of the relevant formula). The value of R was calculated during the fit for every new set of the PDFs parameters (its final form is presented on Fig.1). This reduction is most essential at the smallest x accessible in an experiment, mainly, due the maximum sensitivity of the data to the value of R in these regions. The value of this correction is different for the considered data sets. For the BCDMS data the value of this correction is in the range of $[-3.5\%, 0\%]$ (the average relative module – 0.10). This collaboration calculated R from pQCD predictions, but used the larger gluon distributions than in our final set. The NMC data are renormalized by 0.10 statistical error in average (range – $[-1.5\%, 2\%]$). For the ZEUS data, which exhibit the most sensitivity to the choice of R due to the large span in lepton scattering variable y , this correction calculated with the final set of our PDFs ranges from -3% to 0% with the average relative module of 0.04 and as to the H1 data they are affected to the same extent.

Resuming we should note that this correction, being not very large in average, is significant for separate data points on the edge of the experimental acceptance. Since at small x the value of R heavily depends on the $G(x, Q)$, our approach imposes the additional constraints on its value. The residual influence of different ansatzes for R used in the calculation of radiative corrections in different experiments is believed to be small.

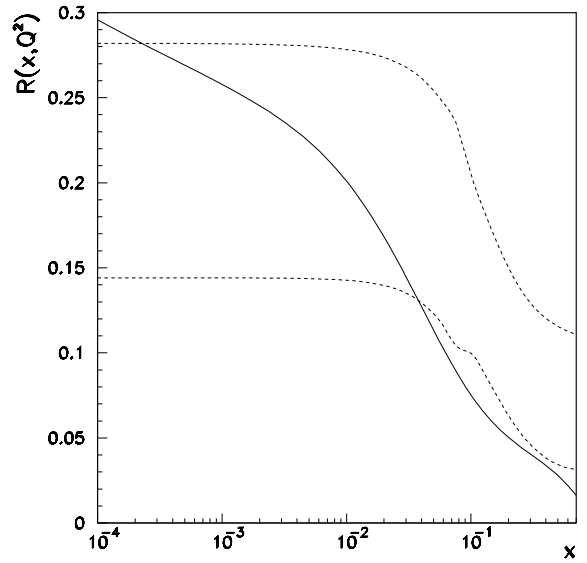


Fig. 1. $R = \sigma_L/\sigma_T$ calculated using our resulting PDFs (solid line) and the band of R_{SLAC}^{1990} [22] (dashed lines) at $Q^2 = 9 \text{ GeV}^2$.

1.4.3. Fermi motion correction for deuterium

Deuterium data were corrected for Fermi motion using procedure [23] with the Paris wave function for deuterium [24]. This correction was also calculated iteratively to obtain fully consistent set of PDFs. The value of $R = \sigma_L/\sigma_T$ for deuteron was adopted to be unchanged under this correction, we have proved that this adoption is of minor importance for the final results. For the calculation of the relevant integrals we used program [25], which exhibited better numerical stability than standard procedures based on the simple Gauss algorithm. This correction being maximum at large x ranges from -2% to $+15\%$ for the BCDMS data and from -2% to -1% for the NMC data, whereas its average relative module is about 0.6 for the both experiments.

2. Results

The central values and the full experimental errors of the adjustable parameters obtained after the minimization of (1) are presented in Table 2 (full correlation matrix of the fitted parameters is available by the request to the author).

Table 2. The fitted parameters of PDFs with the full experimental errors including statistics and systematics.

Valence	a_u	0.745 ± 0.024	Sea	A_S	0.159 ± 0.036
	b_u	3.823 ± 0.069		a_{sd}	-0.1885 ± 0.0072
	γ_2^u	0.56 ± 0.28		b_{sd}	7.5 ± 1.3
	a_d	0.876 ± 0.066		η_u	1.0 ± 0.12
	b_d	5.32 ± 0.22		b_{su}	10.61 ± 0.96
Glue	a_G	-0.267 ± 0.043		η_s	0.5 ± 1.0
	b_G	8.2 ± 1.5		$\alpha_s(M_Z)$	0.1146 ± 0.0018

To decrease the model dependence of our predictions, calculating the covariance matrix we released parameters η_u and η_s , keeping their central values intact. The resulting χ^2 values are presented in Table 1. On the average the model describes the data fairly well. One can heavily ascribe rather large χ^2 obtained for the NMC and ZEUS data to the shortcoming of the theoretical model, as far as the BCDMS and H1 data having comparable statistics and lying in the nearby kinematic regions are described by this model perfectly. The most probable explanation is that some systematic errors in these experiments are not Gaussian distributed. The average bias of the data against our model, calculated as

$$B = \left\langle \frac{f - y}{\sqrt{\sigma^2 + f \sum_{k=1}^K (\eta^k)^2}} \right\rangle$$

turned out to be 0.10, i.e. is statistically insignificant. The principal difference of our analysis from other global fits is that we do not renormalize data and as far the BCDMS data are usually shifted down, our resulting F_2 curves are slightly higher than others at large x . The data on F_2 reduced to the common value of R together with our curves are

presented on Figs.2–5, where the error bars correspond to the squared sum of statistics and systematics. The selected set of PDFs is presented on Figs.6–9.

Fig. 2. The description of BCDMS data with our PDFs. The data and curves are scaled by factor 1.2^{11-i} , where i runs from 1 for the highest x bin to 11 for the lowest one.

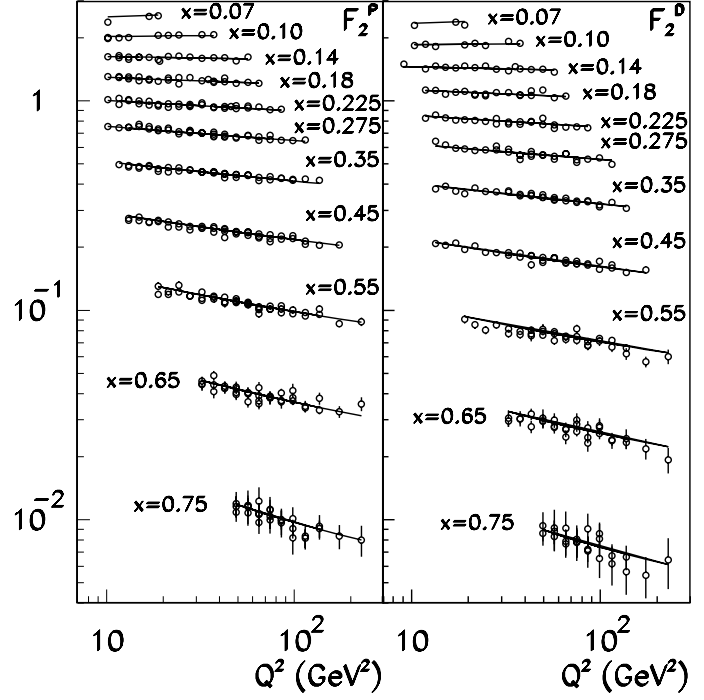
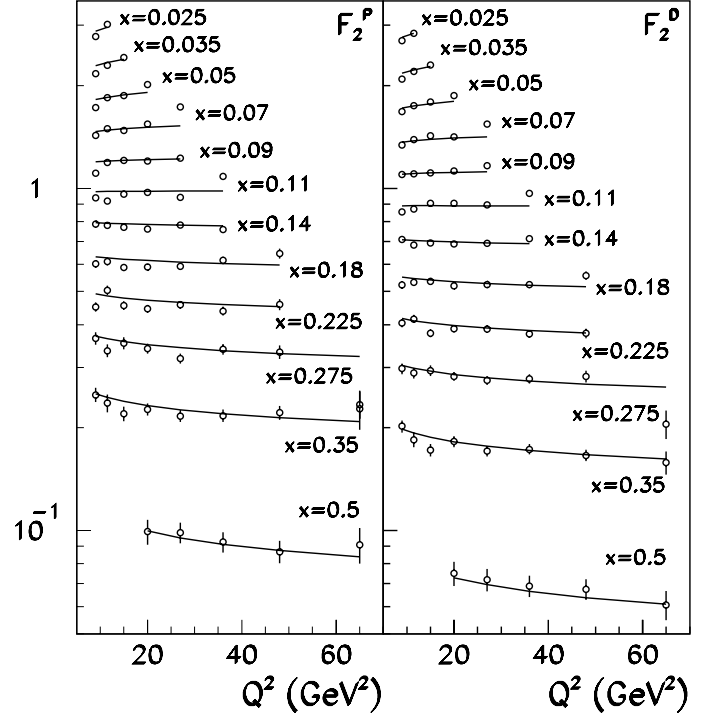


Fig. 3. The same as in Fig.2 for the NMC data (i runs from 1 to 12). For the presentation purposes we pictured combined energy data with convenient binning.



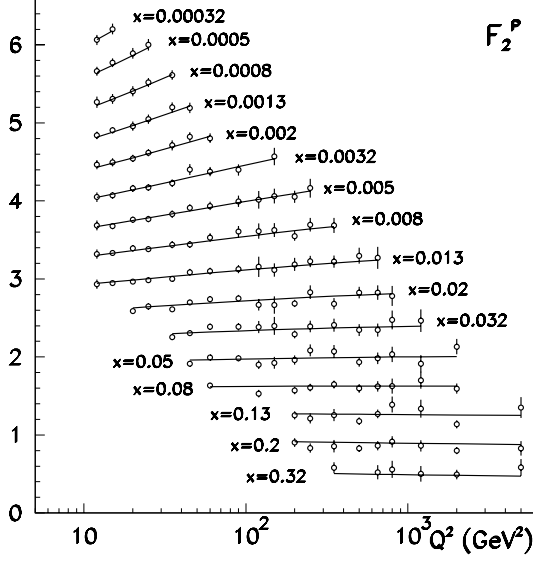


Fig. 4. The description of H1 data with our PDFs. The data and curves are shifted by $5.1 - 0.3i$, where i runs from 1 for the highest x bin to 16 for the lowest one.

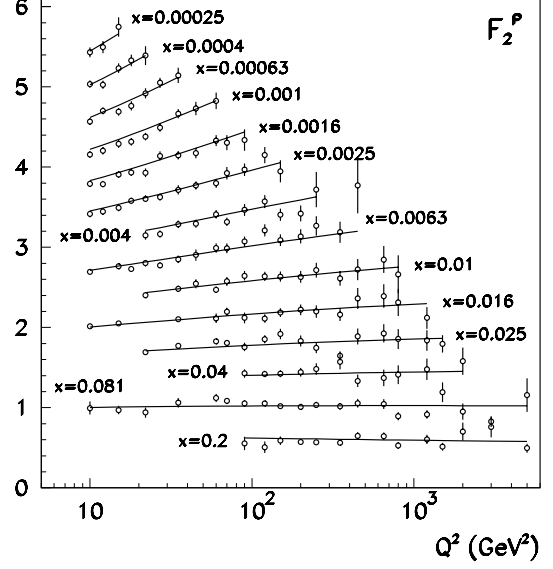


Fig. 5. The description of ZEUS data with our PDFs. The data and curves are shifted by $4.5 - 0.3i$, where i runs from 1 for the highest x bin to 14 for the lowest one.

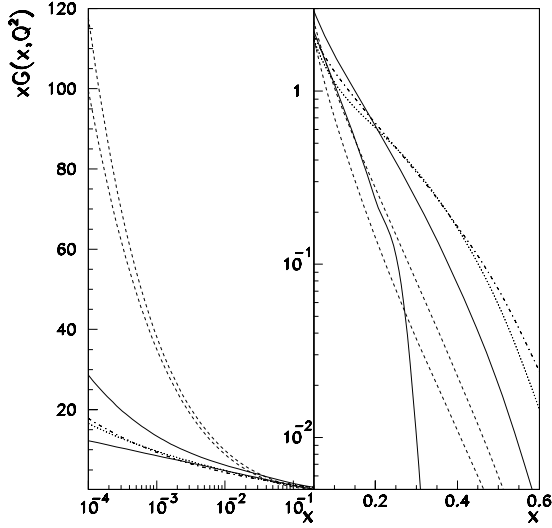


Fig. 6. Gluon distribution obtained in our analysis. Solid lines correspond to $Q^2 = 9 \text{ GeV}^2$, dashed – to $Q^2 = 10000 \text{ GeV}^2$. Dotted line gives MRS(R1) and dashed-dotted – CTEQ4M predictions at $Q^2 = 9 \text{ GeV}^2$.

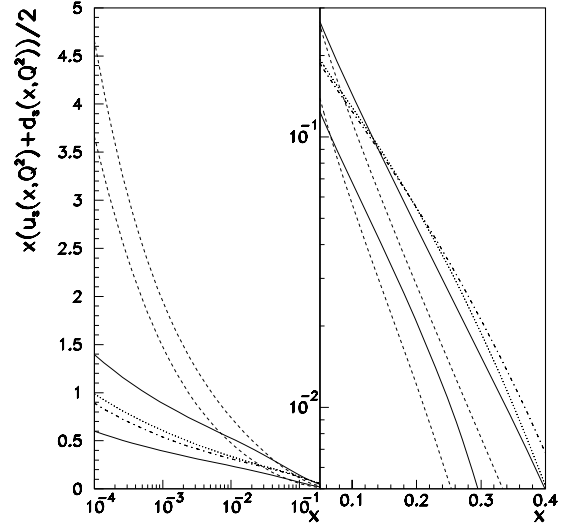


Fig. 7. The same as in Fig.6 for the non-strange sea.

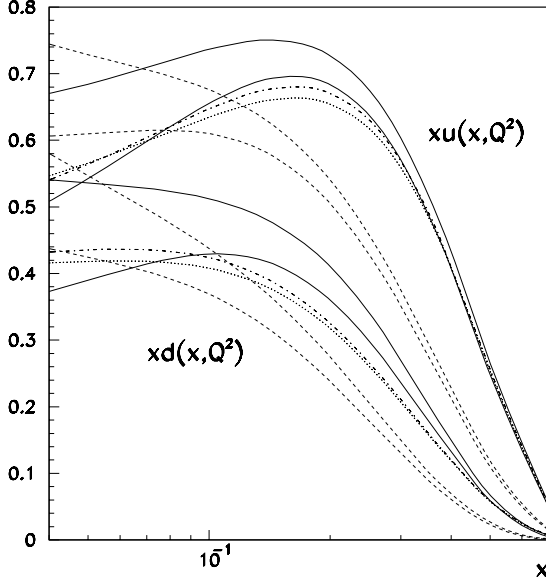


Fig. 8. The same as in Fig.6 for the valence quarks.

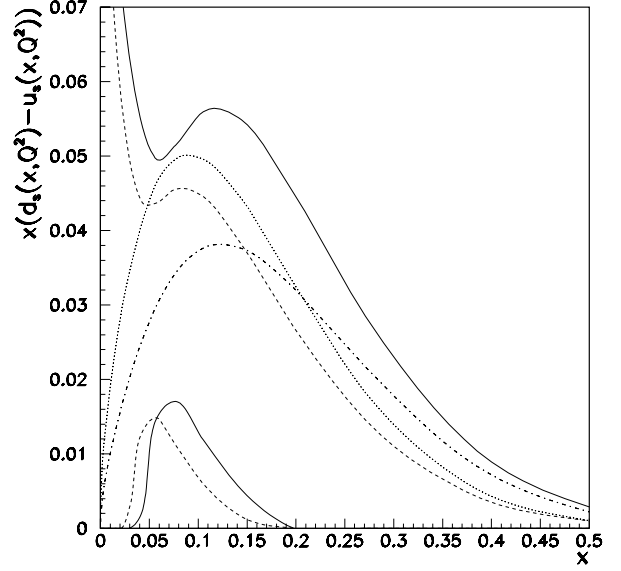


Fig. 9. The same as in Fig.6 for the non-strange sea asymmetry.

The strange sea is not shown since from the analysed data we can obtain only a weak upper limit for this value. As we have mentioned above the distribution of our PDFs parameters defined mainly by the distribution of systematic uncertainties may differ from Gaussian and then for the robust error bands estimate one should better use Chebyshev's inequality. The bands presented on these pictures correspond to two standard deviations, which corresponds to the 75% robust confidence level. Although we do not use in our analysis prompt photon data, which are often considered as an unique source of gluon distribution at moderate x , through the kinematic region of $x = [0.0001, 0.5]$ gluon distributions is determined rather precisely and better than in the earlier analysis [12,26]. One could achieve this due to the measurement of F_2 at small x , which defines gluon distribution in this region and provides momentum constraint to determine it at larger x as well. As to the quark distributions they are determined much more precisely. We should, however, point out that the obtained PDFs and their errors are certainly model dependent. Say, releasing the condition $a_{su} = a_{sd} = a_{ss}$ significantly increases the errors of sea distributions at the small x . Analogous effect arises if one adds more polynomial terms to the initial PDFs. The model dependence is inevitable in such analysis since one cannot determine the continual functional form of a distribution having the limited set of measurements and without additional constraints. In our case this model dependence is more pronounced for the quark distributions because the considered data are well known to have limited potential in the discrimination of sea and valence quarks meanwhile the gluon distribution and $\alpha_s(M_Z)$ are less model dependent. It is well understood as far as the latter are defined from the F_2 derivatives, less sensitive to the variation of separate quark distributions. At small x and large Q one can observe shrinking the error bands of gluon distribution. This reflects a well known property of the DGLAP equation based on the dominance of the singular terms and leading to the focusing of any input gluon distribution to the universal form [27].

For the comparison we also present the parametrizations MRS(R1) [2] and CTEQ4M [4] on these figures. This comparison is limited because of the lack of the error bands for their PDFs, but any way is more conclusive than the comparison of two curves without any error bands moreover that one can suppose the error bands for MRS and CTEQ PDFs to be smaller than ours since these groups use more data in the fit. We observe the statistically significant difference of our gluon distribution with those given by MRS and CTEQ sets at large x , which can be ascribed to using in these analysis the data on prompt photon production. The interpretation of these data has been recently recognized to suffer from the large ambiguities [28] and the alternative analysis of prompt photon data with the improved theoretical treatment of these ambiguities give much lower gluon distribution at moderate x [29], compatible with ours. As to the discrepancies in d -quark and, to less extent, u -quark distributions at moderate x , the additional investigation showed that they are partially explained by the influence of target mass and Fermi motion corrections. One can note that the larger values of quark distributions in this region of x can help to explain the excess of the recent data on jet production from Fermilab collider over NLO QCD predictions in the region of $E_T = 200 - 400 \text{ GeV}$, where the basic contribution comes from quark-quark scattering (viz [2,4]). In addition to the above, all these discrepancies can also originate due to the possible numerical inaccuracies in MRS's and CTEQ's QCD evolution codes reported recently [17] and difference in the α_s values. The difference in the sea value at $x \sim 0.3$ seems to be statistically insignificant and can disappear after inclusion of more data in the analysis.

For the value of $\alpha_s(M_Z)$ the robust estimate is

$$\alpha_s(M_Z) = 0.1146 \pm 0.0036 \text{ (75\% C.L.)},$$

compatible with [30], but less sensitive to the higher twist contribution. This estimate is not essentially biased if the PDFs functional form is changed from (2) to our final form and hence we can conclude that these estimates are, in the good approximation, model independent.

3. Conclusion

The Bayesian treatment of systematic errors is the clear and efficient method in the analysis of data with numerous sources of systematic errors and in particular data on DIS scattering. This approach allows for a straightforward and correct account of point-to-point correlations contrary to widely used 'simplification' consisting of combining statistic and systematic errors in quadrature. The certain suspicions that the estimator using covariance matrix suffer from the bias proved to be irrelevant if one uses the estimator inspired by the maximum likelihood function. First time the quark and gluon distributions from the global fit with the full account of experimental errors are obtained. These PDFs can be extremely useful for further phenomenological studies. Having estimation of PDFs' error bands one can conclusively compare the results of various global fits, PDFs extracted from different processes and evaluate the statistical significance of theoretical uncertainties

in the fitted formula. At last, calculation of cross sections for other processes, based on PDFs are more meaningful if one can account for PDFs' uncertainties.

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