The package PAKPDF 1.1 of parametrizations of parton distribution functions in the proton

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A FORTRAN package containing parametrizations of parton distribution functions (PDFs) in the proton is described. It allows an easy access to PDFs provided by several recent parametrizations and to some parameters characterizing particular parametrization. Some comments about the use of various parametrizations are also included.

PROGRAM SUMMARY

Title of program: PAKPDF version 1.1

Catalogue number: ACGU

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Licensing provisions: none

Computer for which the program is designed: (i) IBM 3090, (ii) VAX, and any computer with a FORTRAN 77 compiler

Operating systems under which the program has been tested: (i) MVS; (ii) VMS

Programming language used: FORTRAN 77

Memory required required to execute with typical data: 45000 words

No. of bits in a word: 32

No. of lines in distributed program, including test data, etc.: 15366

Keywords: perturbative quantum chromodynamics (QCD), QCD improved parton model, standard model, Altarelli–Parisi equation, deep inealstic scattering, parton distribution functions (PDFs), structure functions, cross-sections

Nature of physical problem
In the framework of the QCD improved parton model, parton distribution functions play a basic role enabling to relate the theoretically calculated hard partonic cross-section with the experimentally measured one. Their specific features determine the behaviour of hadronic cross-sections at high energies. The accurate knowledge of PDFs is important especially in precision studies of the standard model, in estimating possible sources of background in search for new physics and in predictions for forthcoming colliders. A collection of all recent parametrizations of parton distribution functions allows an easy and fast access to various PDFs in a wide kinematic range.

Method of solution
Solutions of the Altarelli–Parisi equation with input distributions appropriately determined from experimental data have been parametrized in an analytic form with Q^2-dependent parameters or through the look-up tables containing grids in (x, Q^2) variables with an interpolating procedure. The collection of parametrizations has a modular form consisting of several procedures with a unified calling format.

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LONG WRITE-UP

1. Introduction

The QCD improved parton model provides a comprehensive framework for describing general high energy processes in current and planned accelerators [1–4]. In this framework parton distribution functions (PDFS) play a basic role enabling to connect a theoretically calculated partonic hard cross-section $\hat{\sigma}$ with the experimentally measured cross-section σ. For example, in a typical hadron–hadron collision process A + B → C + X the relation is the following:

$$\sigma_{AB \to CX} = f_A^a \otimes \hat{\sigma}_{ab \to C} \otimes f_B^b, \tag{1}$$

where f_A^a is the distribution function of parton a in the hadron A, $\hat{\sigma}_{ab \to C}$ is the hard scattering cross-section for the partonic process a + b → C, and $\otimes$ denotes a convolution integral. It is obvious from eq. (1) that specific features of PDFs play a key role in determining the behaviour of hadronic cross-sections at high energies. The detailed, up-to-date knowledge of parton distributions is especially required in the following studies:

• precise tests of the standard model;
• the study of signals and backgrounds in search for new physics;
• predictions made for forthcoming colliders (HERA, LHC and SSC).

Perturbative QCD predicts the Q^2 evolution of the parton distributions by means of the Altarelli–Parisi (AP) equation [1], which describes well the Q^2-dependence of measured structure functions within the range of available energies. However, the size and shape of the distributions are not specified by QCD. Some ideas from Regge (soft) physics (see e.g. ref. [2]) happen to be very helpful in determining the x shape of PDFs. The extrapolation to smaller x, however, is still not very well understood. Partons with very small x, well beyond the currently measured range, will be very important at forthcoming colliders. Available theoretical guidelines were up to now mainly qualitative and only recently more quantitative studies have appeared [5–7].

The determining source of information on parton distribution comes from experimental data, mainly from structure functions measured in deep inelastic scattering (DIS). Data from modern high statistics DIS experiments [8,9] (CDHSW, BCDMS, EMC and NMC) accompanied with the new analysis [10] of the SLAC-MIT experiments allowed to get accurate structure functions data. They can be used for constraining parton distributions in a wide range of x (around $0.01 < x < 0.75$) and Q^2 (around $1 < Q^2 < 280$ GeV^2).

It should be emphasized, that although the relation between structure functions and parton distributions is intimate, those quantities are not identical. Structure functions are physical quantities which are measured in a specific deep inelastic experiment (i.e. they are process dependent). On the other hand, parton distribution functions are theoretical objects which (if properly defined) are universal – i.e. they do not dependent on the physical process to which they are applied. However, beyond the leading order they start to be renormalization-scheme dependent. In the QCD improved parton model, structure functions can be expressed through parton distributions. For example, the electromagnetic F_2 structure function for ep scattering has the following form (in leading order):

$$F_2(x, Q^2) = \sum_q e_q^2 xq(x, Q^2), \tag{2}$$

where $q(x, Q^2)$ is the quark distribution function and e_q denotes the charge of a quark q.

In order to determine parton distributions, a "global analysis" is usually performed. The term "global analysis" refers to the quantitative comparison of experimental data from a wide range of physical processes with the QCD predictions (e.g. eq. (1)), for the purpose of extracting a set of universal parton distribution functions. In more details, the standard procedure goes as follows:

- a reference momentum value Q_0^2 is chosen (usually around 4 GeV^2) and the parton distributions at that value are parametrized with the help of a simple formula, e.g.: $q(x, Q_0^2) = Ax^a(1-x)^b$;
- these distributions are then evolved numerically, using the AP equation, to obtain (through, e.g. eq. (1)) values for the quantities measured in the experiment;

- a global numerical fit is next performed to determine the "best" values for the parameters appearing in the formulas for PDFs at Q_0^2 scale;
- finally, input distributions at Q_0^2 with the "best" parameters are evolved to higher Q^2 values and a set of PDFs in a desired (x, Q^2) range is obtained.

In general a further step is added: the resulting distributions are parametrized by some analytic formulas with Q^2-dependent parameters or a look-up table grid in (x, Q^2). The *parametrizations* of parton distribution functions obtained in this way allow an easy and fast access to PDFs at any (x, Q^2) point. However, one should remember that such parametrizations can, at best, summarize our knowledge concerning the parton dis-

Table 1
Summary of parametrizations

Parameter	IPAR	ISET	Type	N_f	Λ_4 (GeV)	x range	Q^2 range (GeV^2)	Remarks	Ref.
DO	1	1	LO	4	0.200	5×10^{-3}–1	4–10^6	soft gluons, set 1	[12]
		2	LO	4	0.400	5×10^{-3}–1	4–10^6	hard gluons, set 2	
		3	LO	4	0.177	10^{-3}–1	4–1.67×10^6	updated ver., set 1.1	[13]
EHLQ	2	1	LO	6	0.200	10^{-4}–1	5×10^8	$R = \sigma_L/\sigma_T = 0.1$	[14]
		2	LO	6	0.290			$R = R_{QCD}$	
DFLM	3	1	LO	6	0.200	5×10^{-5}–0.95	10–10^8	average	[15]
		2	NLO	6	0.300			average, DIS	
GRV	4	1	LO	5	0.200	10^{-5}–1	0.25–10^8		[16]
		2	NLO	5	0.200	10^{-5}–1	0.30–10^8	$\overline{MS}$ scheme	
MT	5	0	LO	6	0.144	10^{-5}–1	4–10^8	set SL	[17]
		± 1	NLO	6	0.212			DIS/$\overline{MS}$, set S	
		± 2	NLO	6	0.237			DIS/$\overline{MS}$, set SN	
		± 3	NLO	6	0.194			DIS/$\overline{MS}$, set B1	
		± 4	NLO	6	0.191			DIS/$\overline{MS}$, set B2	
		± 5	NLO	6	0.155			DIS/$\overline{MS}$, set E	
HMRS	6	1	NLO	5	0.100	10^{-5}–1	5–1.3×10^6	$\overline{MS}$, set E	[18]
		2	NLO	5	0.190			$\overline{MS}$, set B	
KMRS	7	1	NLO	5	0.190	10^{-5}–1	$5 \times 1.3 \times 10^6$	$\overline{MS}$, set B0	[19]
		2	NLO	5	0.190			$\overline{MS}$, set B-	
		3	NLO	5	0.190			$\overline{MS}$, set B-5	
		4	NLO	5	0.190			$\overline{MS}$, set B-2	
MRS	8	1	NLO	5	0.135	10^{-5}–1	5–1.3×10^6	$\overline{MS}$, set B135	[20]
		2	NLO	5	0.160			$\overline{MS}$, set B160	
		3	NLO	5	0.200			$\overline{MS}$, set B200	
		4	NLO	5	0.235			$\overline{MS}$, set B235	

tributions at the time they were constructed from the existing data.

This paper gives a description of a collection (package) of procedures which calculate PDFs using recent parametrizations of parton distribution functions for the proton. The main aim of this package is to collect in one place and one format these parametrizations, which represent the present knowledge (theoretical and experimental) about parton distributions in the proton. In addition, the user is provided with an easy access (in the form of a call to the procedure) to useful information relevant to a particular parametrization (range of validity, value of the A_{QCD} parameter,...).

The outline of the paper is as follows. In section 2 more details about collected parametrizations are given. The structure of the package is described in section 3. In section 4 the main procedures are described in detail. Finally, section 5 contains an example of the output from the package and final remarks.

2. The parametrizations

The following parametrizations have been incorporated in the package (also see table 1):

DO   Duke and Owens (1984) [12], Owens (1991) [13];

EHLQ   Eichten, Hinchliffe, Lane and Quigg (1984) [14];

DFLM   Diemoz, Ferroni, Longo and Martinelli (1988) [15];

GRV   Glück, Reya and Vogt (1991) [16];

MT   Morfin and Tung (1990) [17];

HMRS   Harriman, Martin, Roberts and Stirling (1990) [18];

KMRS   Kwiecinski, Martin, Roberts and Stirling (1990) [19];

MRS   Martin, Roberts and Stirling (1990) [20].

These parametrizations differ in many aspects: the choice of experimental data taken for determination of the input distributions, the treatment of experimental errors and corrections, the selection of functional forms for the input distribu-

tions, the order of the approximation (leading order (LO) or next-to-leading order (NLO)), the treatment of the heavy-quark sector, assumptions about the behaviour at small x – to mention only a few (a detailed comparison between various parametrizations can be found in ref. [11,21,22]).

The parametrizations can be divided into two main groups. The first two (DO and EHLQ) were obtained in the leading order QCD approach and are based on the experimental data which existed before 1984. The remaining (DFLM, MT, GRV, HMRS, KMRS and MRS) use the next-to-leading order formalism and recent data from the high statistics neutrino and muon experiments. Because the old data are not in full agreement with the new data, the older parametrizations (DO (old sets), EHLQ and to some extent also DFLM) do not reproduce the best current data [11]. The new parametrizations (MT, GRV, HMRS, KMRS and MRS) describe current deep inelastic data well. Some of them, i.e. KMRS and MT, include various options (as specific sets) for the behaviour of PDFs in the region of small x. This feature is very important for the studies at the forthcoming colliders (HERA, LHC, SSC), where the bulk of data will come from processes in which partons carry a small part of the longitudinal momentum, i.e. small x.

In all applications within the leading order QCD formalism it is sufficient to use the LO parton distributions. It is important, however, that these distributions agree with existing data. As was discussed above, older LO parametrizations (DO (old sets) and EHLQ) do not reflect accurately recent data and therefore are not recommended. Instead, the LO set of the recent MT, GRV parametrizations or the new (updated) set of DO parametrization are preferred.

For applications which require higher accuracy, the next-to-leading order formalism is usually used. When the NLO hard cross-sections are taken (for example, in eq. (1)) also the NLO parton distributions should be used in order not to loose consistency (and accuracy). In this case it is also important to make a consistent choice of the renormalization scheme in the hard cross-section formula and in the definition of the parton distributions (i.e. DIS scheme or $\overline{MS}$ scheme).

It follows from comparative studies of various parametrizations [21,22] that between the different NLO parametrizations the HMRS(B) (or KMRS(B0)) and the MT(S) parametrizations should be preferred for high energy studies. Within a particular parametrization (for example, MT or KMRS) the use of various sets can be helpful in estimating the range of uncertainty due to the fact that existing data do not completely determine all the parton distributions and that the behaviour of PDFs beyond the currently measured region is not precisely defined by QCD (especially at small x).

In particular, the approach to the small x region in various parametrizations is different. Large differences in the predictions for the experimentally not yet accessible small-x region ($x \leq 0.01$ or so) come mainly from the assumptions about input distributions, i.e. how flat or steep an input for $xG(x, Q_0^2)$ and $x\bar{q}(x, Q_0^2)$ has been chosen as $x \rightarrow 0$. Various shapes of parton distributions in different sets of the MT parametrization come mainly from different assumptions about the functional form (in x) of parton distributions. The sets, obtained during detailed and careful phenomenological analysis, constitute a collection of allowed (by experimental data) behaviour of parton distributions at small x. The behaviour of PDFs at small x in the KMRS parametrization relies on ideas coming from Regge theory and from studies of shadowing effects. Two extreme possibilities for the small-x behaviour of gluon and sea quark distributions were assumed at Q_0^2: $xG(x, Q_0^2)$, $x\bar{q}(x, Q_0^2) \sim x^0$ and $x^{-0.5}$. Shadowing corrections were included by modifying the initial distributions in the region of $x < x_0 = 10^{-2}$ and by including a non-linear term in the evolution equation. The GRV analysis represents an alternative approach to the small-x region (and generally to the evolution of parton distributions). In this approach a low-value μ^2 (around 0.3 GeV^2) of the input scale Q_0^2 is chosen in order to allow for a valence-like input which vanishes as $x \rightarrow 0$. The gluon and sea quark distributions are produced radiatively by evolving the initial valence-like structure at μ^2 to $Q^2 > \mu^2$. The resulting predictions for PDFs at $x \leq 10^{-2}$ and $Q^2 > \mu^2$ are mainly due to the QCD dynam-

ics and not to the input assumptions for small x. They are usually steeper as $x \rightarrow 0$ than the ones obtained in the "conventional" approach.

The uncertainties connected with the choice of the Λ_{QCD} value can best be studied with the MRS parametrization. It is built around the KMRS(B0) set with slightly different Λ_{QCD} values and powers of the $(1 - x)$ term in the formula for the input gluon distribution.

For the sake of simple and fast applications the new set of the DO parametrization (Set 1.1), provided by J. Owens [13] can be used. It is based on the recent data from DIS, dilepton production and direct photon plus jet production. All parton distributions, obtained in LO approach, are parametrized in a convenient analytical form (the same as the old DO sets). It is meant to replace the old Set 1 of the DO parametrization.

Although the aim of the package is to collect parametrizations which properly describe present data, three older parametrizations were included for backward compatibility. The DO (sets 1,2), EHLQ and DFLM parametrizations were extensively used in the past and it can be helpful to have those sets available for comparative studies.

3. Structure of the package

Each parametrization is specified by two INTEGER numbers: the parametrization code (IPAR) and the set code (ISET). The correspondence between this notation and the original one as well as a short description of every parametrization set is given in table 1. The package contains two user-oriented subroutines:

- PDSET – allows to get/set values of several parameters characterizing a particular parametrization,
- PDVAL – returns parton distribution functions at (x, Q^2) calculated in a chosen parametrization; momentum weighted distributions (i.e. $xp(x, Q^2)$, where p stands for parton distribution) are returned;

and several internal ones:

- PDDO, PDEHLQ, PDDFLM, PDGRV, PDMT, PDHMRS, PDKMRS, PDMRS – contain codes of individual parametrizations,

- PDWARI, PDWARR, PDWARC – are warning procedures,
- PDDAT – is a block data segment with default values.

4. Description of procedures

In the following the detailed description of user-oriented subroutines is given:

(1) SUBROUTINE PDVAL (IPAR, ISET, X, Q2, XPDF, IRET)

Purpose: to get values of PDFs in a chosen parametrization.

Arguments:
IPAR: (INTEGER, input) specifies parametrization.
ISET: (INTEGER, input) specifies set in the parametrization IPAR.
X: (REAL * 8, input) value of the Bjorken x variable.
Q2: (REAL * 8, input) square of the momentum scale, in GeV^2.
XPDF: (REAL * 8, output) $(-6:6)$ vector with momentum weighted $(X * p(X, Q^2))$ PDFs;
the assignment of flavours in the XPDF vector is as follows [23]:
IPDF = 0, 1, 2, 3, 4, 5, 6,
flavour = G, d, u, s, c, b, t,
with negative values of IPDF corresponding to antiquarks.
IRET: (INTEGER, output) return error/warning code;
= 0, no errors;
errors:
= − 1: X < 0;
= − 2: X > 1;
warnings:
= 1: parametrization code is not valid (default value taken);
= 2: X out of (XMIN, XMAX) range (limit value usually taken);
= 3: Q2 out of (Q2MIN, Q2MAX) range (limit value taken).

If several warnings occur, they are returned as e.g.: = 13: both warnings 1 and 3; = 123: all three warnings 1, 2 and 3.

(2) SUBROUTINE PDSET (IACT, IPAR, ISET, CHNAME, VALUE, IRET)

Purpose: to get/set values of some parameters of specified parametrization.

Arguments:
IACT: (INTEGER, input) specifies action:
= 0: write short information about all the parametrizations; IPAR, ISET, CHNAME, VALUE-dummy variables;
= 1: get VALUE of the parameter CHNAME in specified parametrizations: input variables: IPAR, ISET, CHNAME, output variable: VALUE;
= 2: set parameter CHNAME to VALUE in specified parametrizations: input variables: IPAR, ISET, CHNAME, VALUE.
IPAR: (INTEGER, input) specifies parametrization.
ISET: (INTEGER, input) specifies set in the parametrization IPAR.
CHNAME: (CHARACTER, input) name of the parameter (upper case!):
if IACT = 0: dummy variable;
if IACT = 1, i.e. "get" option:
= NFL: number of flavours provided by the parametrization;
= ORD: order of pert. calculations; $1 \equiv LO$, ± 2 $\equiv NLO(DIS, \overline{MS})$;
= LAMBDA: value of the Λ_{QCD} (for 4 flavours);
= MTOP: top quark mass, in GeV;
= XMIN: lower limit of X variable range;
= XMAX: upper limit of X variable range;
= Q2MIN: lower limit of Q2 variable range, in GeV^2;
= Q2O: starting value of Q2 evolution $(\simeq Q2MIN)$, in GeV^2;
= Q2MAX: upper limit of Q2 variable range, in GeV^2;
= NOUT: unit no. for output messages (default = 6);

if IACT = 2, i.e. "set" option:
= MTOP: mass of the top quark;
= NOUT: unit no. for output messages; VALUE
 = 0 – no warnings appear.
VALUE: (REAL * 8) value of specified parameter CHNAME;
for IACT = 0 – dummy;
for IACT = 1 – output;
for IACT = 2 – input.
IRET: (INTEGER, output) return error/warning code;
= 0: no errors: parameter found/valid value;
errors:
= –1: parametrization code is not valid;
= –2: parameter is not found;
= –3: wrong value of parameter (also IACT).

For completeness, below is the format of procedures containing the FORTRAN code for individual parametrizations. Those routines can be used as stand-alone procedures but, for example, warning and errors messages will not be issued.

(3) SUBROUTINE *subname* (ISET, X, Q2, XPDF)

Purpose: to calculate PDFs in a parametrization identified by *subname*, where *subname* = PDDO, PDEHLQ, PDDFLM, PDGRV, PDMT, PDHMRS, PDKMRS, PDMRS.

Arguments:
ISET: (INTEGER, input) specifies set in the parametrization *subname*,
X: (REAL * 8, input) value of the Bjorken x variable.
Q2: (REAL * 8, input) square of the momentum scale, in GeV^2.
XPDF: (REAL * 8, output) (–6:6) vector with momentum weighted (X * p(X, Q2)) PDFS;
the assignment of flavours in the XPDF vector is as follows [23]:
IPDF = 0, 1, 2, 3, 4, 5, 6;
flavour = G, d, u, s, c, b, t;
with negative values of IPDF corresponding to antiquarks.

Finally, several general remarks concerning the whole package:
• it is an extended and modified version of the package described in ref. [25];
• the flavour codes of partons follow the Particle Data Group numbering convention [23]; in particular, the code for the up quark is 2 and for the down quark 1;
• parton distributions returned in the XPDF vector satisfy the momentum conservation sum rule at every Q^2, i.e.

$$\int_0^1 dx \sum_0^6 xp_i(x, Q^2) = 1,$$

where $xp_i(x, Q^2) = XPDF(i)$ at (x, Q^2).
• the default parametrization is the MT parametrization, set "S", i.e. IPAR = 5, ISET = 1;
• the DO, MT and GRV parametrizations can be used to X values lower than XMIN but results may be unreliable (an appropriate warning will be issued);
• in the parametrizations which provide the top quark distribution (EHLQ, DFLM and MT) it is possible to change (through PDSET) the value of the top quark mass; the modification of the top quark distribution is achieved by a simple rescaling of the momentum scale: $m_{old}Q_{old} = m_{new}Q_{new}$:
• the convention for message codes is the following:
IRET = 0 – no errors,
 > 0 – warnings,
 < 0 – errors;
• all procedures and commons begin with PD, i.e. PDVAL;

5. Final remarks

An example of the numerical results obtained from the PAKPDF package is presented in fig. 1. The predictions for the gluon distribution at Q^2 = 10 GeV^2 coming from various parametrizations are compared. Because of the dependance on the order of QCD calculations and renormalization scheme (in NLO order) of PDFs, the LO

and NLO ($\overline{MS}$) distributions are compared on separate figures.

There exists a similar collection of various parametrizations of PDFs in the proton called PDFLIB [24]. The main differences between these two packages (PAKPDF and PDFLIB) can be summarizes as follows:

• The aim of PDFLIB was to collect all existing parametrizations (about 50 different sets); many of those sets, however, do not describe recent data, i.e. these are older sets based on low statistics data. The goal of the PAKPDF package was to collect only recent, up-to-date parametrizations obtained in different analyses and based on present data. As a result the size of the package is considerably smaller than that of PDFLIB.

• In PAKPDF there is explicit checking of the allowed (x, Q^2) range for a chosen parametrization; in case of trouble a warning/error code is returned.

• PAKPDF provides access to several parameters characterizing the chosen parametrization, like Λ_{QCD}, number of flavours, order of QCD analysis, validity range in (x, Q^2).

• PDFLIB allows to calculate the QCD (running) coupling constant α_s at a given scale and order of QCD approach.

• In PAKPDF values of parton distributions are returned in a vector XPDF ($-6:6$) with the flavour code convention as advocated by the Particle Data Group (a similar convention is used in recent versions of some Monte Carlo programs: PYTHIA55, JETSET72,...). In PDFLIB values of parton distributions are returned through several parameters of a calling procedure, which correspond to different flavours.

• A package similar to PAKPDF – which is devoted to the proton – exist for the parametrizations of PDFs in the photon – PHOPDF [26]; an analogous format of procedures makes it easy to use both packages in some studies (e.g. photoproduction).

In a future version of PAKPDF a procedure calculating predictions for various DIS structure functions from collected parametrizations will be provided.
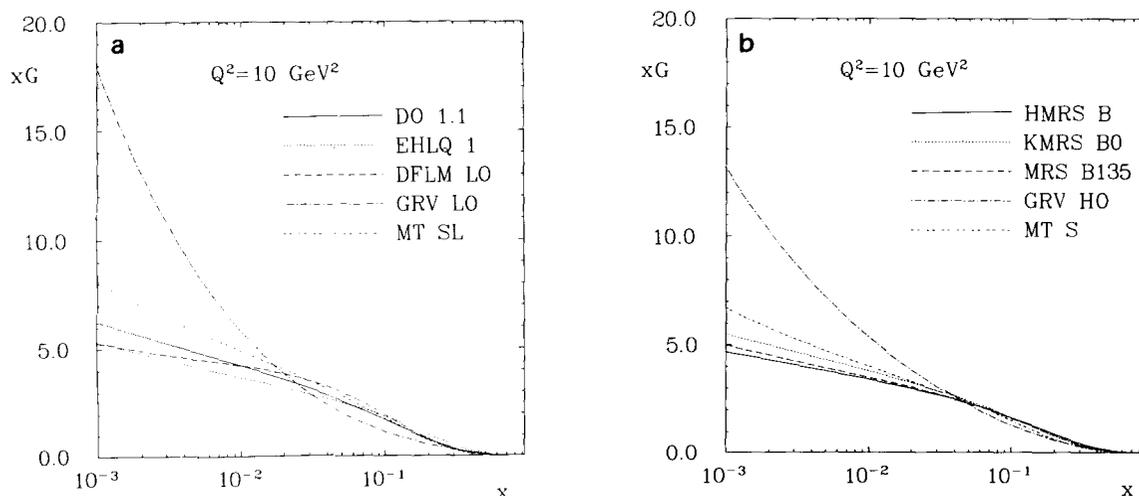
Acknowledgements

Fig. 1. Comparison of gluon distributions at $Q^2 = 10$ GeV^2 obtained in (a) LO analyses and (b) NLO ($\overline{MS}$) analyses. Only representative sets of the parametrizations are shown.

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