CTEQ-TEA parton distributions in a nutshell

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With CTEQ-TEA (Tung Et. Al.) working group

China: A. Ablat, S. Dulat, Y. Fu, T.-J. Hou, I. Sitiwaldi Mexico: A. Courtoy USA: M. Guzzi, T.J. Hobbs, J. Huston, H.-W. Lin, C. Schmidt, K. Xie, C.-P. Yuan and other coauthors





DIS workshop, Grenoble, France

RESEARCH PROJECTS AND RESULTS https://cteq-tea.gitlab.io/

- CTEQ-TEA publications from INSPIRE
- LHAPDF grids for parton distributions
 - CT18 (N)NLO, CT18 QED, CT18 FC, ...
 - Subtracted heavy-quark PDFs in the S-ACOT-MPS scheme
- Public codes

— ...

- ePump (Hessian updating for PDFs with tolerance > 1)
- LHAexplorer (fast surveys of data using L2 sensitivities)
- Fantômas (Bezier parametrizations)
- mp4lhc/mcgen (MC PDFs, combination of PDFs)

M. Guzzi, Tuesday

A. Courtoy, Wednesday

Toward a new generation of CT202X PDFs

- 1. Multiple preliminary NNLO fits with LHC Run-2 (di)jet, vector boson, $t\bar{t}$ data
 - based on the selections of experiments recommended in 2305.10733, 2307.11153
- 2. Work on implementation of N3LO contributions
- 3. Next-generation PDF uncertainty quantification: Bézier curves, META combination, ML stress-testing, multi-Gaussian approaches, ...
- 4. Physics applications
 - a. QCD+QED PDFs for a neutron
 - b. PDF dependence of forward-backward asymmetry
 - c. An L2 sensitivity study using xFitter
 - d. Pion PDFs

Work in progress

QCD cross sections @N3LO



DIS: The CTEQ-TEA code implements complete flavor decompositions of DIS SFs at N3LO using approximate zero-mass Wilson coefficients with a rescaling variable (the **Intermediate-Mass VFN scheme**, cf. the figure)

Boting Wang's and Keping Xie's Theses, SMU

 Imminent implementation of massive N3LO heavyquark coefficients to obtain N3LO DIS cross sections in the SACOT-MPS General-Mass VFN scheme

Factorization schemes	Mass dependence in the FC terms	Mass dependence of the FE and subtraction terms	Introduce heavy-quark PDFs at large Q
FFN	Exact	N/A	no
ZM	None	None	yes
\mathbf{IM}	Approximate	Approximate	yes
 GM	Exact	Approximate	yes

- **DGLAP evolution** is performed at N3LO with APFEL/APFEL++.
- Drell-Yan: Ongoing work to include N3LO DY effects using NNLO ApplFast + N3LO/N2LO K-factor tables

NNLO fits with new data at 8 and 13 TeV

 χ^2/N_{pt} for CT18+new data (CT18 in parentheses) NNLO fits; 68% CL



Fits with 1 type of new data

A fit with all 3 types

Example



The most precise new experiments tend to have an elevated χ^2/N_{pt} , in the same pattern as observed for CT18

 χ^2/N_{pt} increases for experiments 124 and 125 (NuTeV), 126 and 127 (CCFR) and 203 (E866 DY), 266 and 267 (CMS 7TeV Ach), 268 (ATLAS 7TeV W, Ach).

 χ^2/N_{pt} decreases for experiments 249 (CMS 8 TeV Ach), 250 (LHCb 8 TeV W/Z)

Pulls on the gluon PDF by the new data type





After including DY, $t\bar{t}$, and inc. jet data simultaneously, we get a softer gluon. Note that new DY and $t\bar{t}$ data favor a softer gluon, new inc. jet data prefer a harder gluon.

Mild changes in the gluon uncertainty

PRELIMINARY



2024-04-09

Inclusive jet vs. dijet data sets: impact on the gluon for various QCD scales



+ dijets: significant scale, dependence, varied pulls on g(x, Q)



The impact of the Inc. jet data on g(x, Q) is relatively independent of the scale choice. The final fit uses $\mu_{R,F} = p_T^j$, giving better χ^2 .

The impact of dijet data substantially depends on scale choices, especially in the case of CMS8 TeV dijet.

PRELIMINARY

χ^2/N_{pt} for fits that add one inclusive jet or dijet data set to the CT18 (without LHC jets) baseline at a time

Inclusive jets		χ^2/N_{pt} using $\mu_{R,F} \propto HT$ or p_T^j					
Experiment	N _{pt}	HT/2	HT	2 <i>HT</i>	$p_T^j/2$	p_T^j	$2p_T^j$
ATL8IncJet	171	1.7	1.74	1.87	1.75	1.66	1.7
ATL13IncJet	177	1.42	1.36	1.4	1.52	1.31	1.28
CMS13IncJet	78	1.2	1.16	1.2	1.08	1.09	1.1
Dijets	χ^2/N_{pt} using $\mu_{R,F} \propto HT$ or $p_T^* = p_T^j \exp(0.3y^*)$						
		λ	, pi	3 F ^K , F)
Experiment	N _{pt}	м _{jj} /2	M _{jj}	2 <i>M_{jj}</i>	$p_T^*/2$	p_T^*	$2p_T^*$
Experiment ATL7DiJet	N _{pt} 90	<i>M_{jj}</i> /2 0.81	<i>M_{jj}</i> 0.79	2 <i>M_{jj}</i> 0.87	$p_T^*/2$	p_T^*	$2p_T^*$
Experiment ATL7DiJet CMS7DiJet	N _{pt} 90 54	<i>M_{jj}</i> /2 0.81 1.55	<i>M_{jj}</i> 0.79 1.55	2 <i>M_{jj}</i> 0.87 1.63	p _T */2	<i>p</i> _{<i>T</i>} *	$2p_T^*$
Experiment ATL7DiJet CMS7DiJet CMS8DiJet	N _{pt} 90 54 122	<i>M_{jj}</i> /2 0.81 1.55 0.95	<i>M</i> _{jj} 0.79 1.55 1.2	2 <i>M</i> _{jj} 0.87 1.63 1.9	p _T */2	<i>p</i> _T *	2 <i>p</i> [*] _T 1.01

Dijet data are dominated by the CMS 8 TeV dataset

Dijet data sets tend to have larger uncertainties than inc. jets, facilitating better χ^2 for similar constraints on PDFs

PDFs from fits with inclusive jet and dijet data



2024-04-09

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Impact of A_{FB} in the high-mass Drell-Yan process

- *A_{FB}* at the LHC is sensitive to the energy dilution factor D (probability of $k_a^0 < k_{\overline{a}}^0$ in the Collins-Soper frame)
- $A_{FB}^{h} = \frac{N_{F}^{h} N_{B}^{h}}{N_{F}^{h} + N_{B}^{h}} \approx (1 2D) A_{FB}^{q}$
- A_{FB} at high invariant mass region probes \overline{u}/u , \overline{d}/d at x > 0.2









- CT18, MSHT20, and NNPDF4.0 predict very different \overline{q}/q at x > 0.2
- The article quantified the potential effect of high-mass A_{FB} on large-x antiquarks See also NNPDF (2209.08115), Fiaschi et al. (2211.06188)

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recent CT studies of APV

- parity-violating DIS may access quark-level EW couplings
- 20 GeV JLab data may constrain nucleon PDFs
- NC SFs like F₃ (right) can inform high-x valence distributions; may indirectly constrain nucleon sea

CT18As NNLO, 68% CL f(x, μ^2 =4 GeV²) and (5 $F_2^{p,\gamma Z}$ -2 F_2^N) (x_B =0.15, Q²=4 GeV²)





- PVDIS may also allow constraints to strange PDF
- APV depends on interference structure functions
- combination with (isoscalar) deuteron structure function strongly correlated with s(x)
- needs high luminosity; control over deuteron (offshell) corrections; thorough study of systematics

more detail in 2306.09360

2305.10497 (Accepted by JHEP) Neutron's photon PDF





- We have determined the neutron's photon PDF using a similar methodology as for the proton one.
- The structure function is determined using pQCD at high Q2 and HERMES and CLAS/CB data a low Q2
- We estimated many low-Q2 uncertainties, including the isospin symmetry violation and the QED evolution effects. We also explored implications for W-boson production, etc.
- CT18qed and MSHT20qed are in a good agreement
- In comparison to the first generation of photon PDFs, the uncertainty is significantly reduced.

Taming PDF uncertainties in CT202X PDFs

Several efforts to refine PDF uncertainty quantification:

- understand conceptual underpinnings of the multivariate inverse problem. Much can be learned from non-HEP statistics applications
- suppress aleatory and perturbative uncertainties (e.g., from higher-order contributions)
- comprehensively estimate epistemic uncertainties (e.g., due to the PDF parametrization forms)



CT approach: "Bayesian exploration with Gaussian emulation"

preliminary PDFs for alternative parametrizations

final uncertainty with one parametrization

Preliminary fits explore experimental, theoretical, parametrization, methodological uncertainties

The final Hessian error set (50-60) approximates the total uncertainty due to the above factors.

P. Nadolsky, DIS 2024

Fantômas + mp4lhc 2.0: pion PDFs with advanced parametrization uncertainties



P. Nadolsky, DIS 2024

J. Huston et al., a study of tolerances in progress (cf. backup) L2 sensitivity: Jing et al., 2306.03918

CT and MSHT both use analytic minimization to determine the central PDF (by definition, at their best χ^2). This is different for the Monte-Carlo method of NNPDF.

The uncertainty is determined by allowing an excursion from that central value. For a 68% CL error on average, CT18 uses $\Delta \chi^2 \lesssim 37$. For MSHT it is closer to $\Delta \chi^2 \approx 10$.



Conceptually, uncertainties based on χ^2 are traced to the likelihood-ratio test:



: If two PDFs T_1 , T_2 with the same priors have the same $\chi^2 = -2 \ln P(D|T_i)$, they have the same confidence level

This fundamental Bayesian test justifies the technique of Lagrange Multiplier scans (on the left) as well as its fast approximation called "L2 sensitivity" (next slide).

It also explains why $\Delta \chi^2 = 1$ does not capture the full uncertainty.

[Many typical χ^2/dof are >1.1 for >4000 points, or very unlikely from the pure statistical fluctuations. They reflect tensions among the experiments. In addition, the choice of PDF parametrization forms may change the PDFs without changing the χ^2].

CT and MSHT use different criteria to account for the full uncertainty.



- Comparisons of strengths of constraints from individual data sets in 8 PDF analyses using the common L_2 sensitivity metric. [Definitions in the backup.]
- An interactive website (<u>https://metapdf.hepforge.org/L2/</u>) to plot such comparisons [2070 figures in total; a code L2LHAexplorer to plot L2 sensitivities for LHAPDF grids] 2024-04-09 P. Nadolsky, DIS 2024

L. Kotz, 2401.11350

xFitter+L2LHAexplorer

L2 sensitivities were computed using xFitter

- PDF sets (NNLO, $\alpha_s(M_Z) = 0.118$, $Q = 2 \text{ GeV}, T^2 = 10$):
 - CT18
 - CT18As
 - MSHT20
- Data sets (included in xFitter):
 - ATLAS Drell-Yan ($\sqrt{s} = 7 \text{ TeV}$)
 - ATLAS jet production ($\sqrt{s} = 2.76 \text{ TeV}$)
 - CMS W+c production ($\sqrt{s} = 7 \text{ TeV}$)
 - H1+ZEUS combined *c* and *b* production
 - H1 jet production
 - HERA I+II DIS
 - LHCb *c* and *b* production ($\sqrt{s} = 7 \text{ TeV}$)
 - ZEUS jet production



HERA I+II combined inclusive DIS [in CT18 and MSHT20]



Left column: differences in χ^2 definition and heavy-quark scheme. Same PDFs and m_Q .

Right column: differences in χ^2 definition only. Same PDFs and m_0 .

LHCb c and b @7 TeV; $p_T^{\text{meson}} \ge 2 \text{ GeV}$ [Not in CT18 or MSHT20]



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ML models for PDF generation

Kriesten and Hobbs, arXiv:2312.02278



- autoencoder-based models can efficiently represent PDFs in dimensionally reduced form
- through careful choice of network topology, can impose interpretable structure on latent space

- physics constraints may include PDFs' Mellin-space behavior (i.e., integrated moments)
- trained models (like VAIM at right) can generatively predict PDFs from moments
- → new ML tool to mutually compare PDFs, explore statistical properties (e.g., out-of-distribution behavior)

Near-future plans

- 1. Final selection of experiments for NNLO PDFs planned for the next year
- 2. Work on N3LO contributions
- 3. Next-generation PDF uncertainty quantification
- 4. Recent and imminent PDF releases
 - a. QCD+QED PDFs for protons and neutrons
 - b. Subtracted S-ACOT-MPS PDFs
 - c. Fantômas 1.0 pion PDFs (Hessian)
 - d. Release of the Fantômas PDF parametrization package in xFitter

Backup

Post-CT18 Drell-Yan data's impact 2305.10733 (PRD23')

ID	Experiment		- 14 27		
			CT18	CT18A	CT18As
215	ATLAS 5.02 TeV W, Z	27	0.81	0.71	0.71
211	ATLAS 8 TeV W	22	2.45	2.63	2.51
214	ATLAS 8 TeV Z 3D [†]	188	1.12	1.14	1.18
212	CMS 13 TeV Z	12	2.38	2.03	2.71
216	LHCb 8 TeV W	14	1.34	1.36	1.43
213	LHCb 13 TeV Z	16	1.10	0.98	0.83
248	ATLAS 7 TeV W, Z	34	2.52	2.50	2.30
To	tal 3994/3953/3959 poin	nts	1.20	1.20	1.19





- Many new Drell-Yan (nDY) data came out after the release of CT18 PDFs.
- We found that most of the nDY data sets are consistent with the ATLAS 7 WZ precision data (16') and prefer enhanced strangeness at x ~ 0.02
- Only one exception: ATL8W has an opposite pull on d, \bar{d}
- CMS13Z and ATL8W have a similar χ^2/N_{pt} as ATL7WZ
- The more flexible strangeness parameterization in CT18As can relax the tension, but not completely resolve it.

Impact of new high-precision LHC 13 TeV $t\bar{t}$ data on the CT2X gluon PDF

Impact of LHC 13 TeV $t\bar{t}$ production on CT PDFs (Ablat, Guzzi, Xie, Dulat, Hou, Sitiwaldi, Yuan, PRD109 2024; arXiv:2307.11153)



Theory predictions:

- MATRIX (Catani, Grazzini et al. PRD 2019)
- FastNNLO (Czakon, et al. 1704.08551)

Blue band: CT18NNLO 90% C.L. Hatched bands: CT18 + new top-quark data Green: $\mu_R = \mu_F = H_T/2$ Red: $\mu_R = \mu_F = H_T/4$

Differences related to different scale choices and are well within the CT18 PDF error band.

nTT2 baseline consists of 1D abs ttbar Xsec from:

- ATLAS all hadronic, ytt
- ATLAS lepton + jets, {ytt, Mtt, yBtt, HTtt} stat. comb.
- CMS dilepton, ytt
- CMS lepton + jets, Mtt

What is the L₂ sensitivity?

- The L₂ sensitivity is a way of visualizing the pulls of fitted experiments on the best-fit PDF f_a(x, Q), for a particular parton flavor x, as a function of x and Q
 - or, when plotted for a PDF luminosity, as a function of the final-state mass M_X
- The best-fit value for a particular $f_a(x, Q)$ is determined by the sum of these pulls
- Both the L₂ and LM methods explore the parametric dependence of the χ^2 function in the vicinity of the global minimum
- The L₂ sensitivity streamlines comparisons among independent PDF analyses using published error PDFs
- The L₂ sensitivity has been used internally by CT (in CT18), by the PDF4LHC21 benchmarking group (to determine which data sets should be in the reduced PDF fit used for benchmarking), and now by ATLASpdf, CT, and MSHT

Tolerance hypersphere in the PDF space

2-dim (i,j) rendition of N-dim (26) PDF parameter space

Hessian method: Pumplin et al., 2001

A symmetric PDF error for a physical

observable X is given by

$$\Delta X = \vec{\nabla} X \cdot \vec{z}_m = \left| \vec{\nabla} X \right|$$

$$= \frac{1}{2} \sqrt{\sum_{i=1}^{N} \left(X_i^{(+)} - X_i^{(-)} \right)^2}$$





Correlation cosine for observables X and Y: hep-ph/0110378 $\cos \varphi = \frac{\nabla X \cdot \nabla Y}{\Delta X \Delta Y} = \frac{1}{4\Delta X \Delta Y} \sum_{i=1}^{N} \left(X_i^{(+)} - X_i^{(-)} \right) \left(Y_i^{(+)} - Y_i^{(-)} \right) \xrightarrow{(b)}{Orthonormal eigenvector basis}$

L_2 sensitivity, definition

 $S_{f,L_2}(E)$ for experiment *E* is the estimated $\Delta \chi_E^2$ for this experiment when a PDF $f_a(x_i, Q_i)$ increases by the +68% c.l. Hessian PDF uncertainty

Take $X = f_a(x_i, Q_i)$ or $\sigma(f)$; $Y = \chi_E^2$ for experiment E.



$$S_{f,L_2} \equiv \Delta Y(\vec{z}_{m,X}) = \vec{\nabla} Y \cdot \vec{z}_{m,X} = \vec{\nabla} Y \cdot \frac{\nabla X}{|\nabla X|} = \Delta Y \cos \varphi.$$

A fast version of the Lagrange Multiplier scan of χ_E^2 along the direction of $f_a(x_i, Q_i)$!

Estimated χ^2 pulls from experiments (L₂ sensitivity, T. J. Hobbs et al., arXiv:1904.00222)

CT18 NNLO, g(x, 100 GeV)



CT18 NNLO, gluon at Q=100 GeV

15 core-minutes



Experiments with large $\Delta \chi^2 > 0$ [$\Delta \chi^2 < 0$] pull g(x, Q) in the negative [positive] direction at the shown *x*

Estimated χ^2 pulls from experiments (L₂ sensitivity, T. J. Hobbs et al., arXiv:1904.00222)

CT18 NNLO, g(x, 100 GeV)



CT18 NNLO, gluon at Q=100 GeV

Most sensitive e	xperiments
<mark>253</mark> ATL8ZpTbT	109 cdhswf3
542 CMS7jtR7y6T	110 ccfrf2.mi
544 ATL7jtR6uT	147 Hn1X0c
545 CMS8jtR7T	<mark>204</mark> e866ppxf
160 HERAIpII	504 cdf2jtCor2
101 BcdF2pCor	
102 BcdF2dCor	
108 cdhswf2	

Note opposite pulls (tensions) in some x ranges between HERA I+II DIS (ID=160); CDF (504), ATLAS 7 (544), CMS 7 (542), CMS 8 jet (545) production; E866pp DY (204); ATLAS 8 Z pT (253) production; BCDMS and CDHSW DIS

CT18 NNLO g(x, 100 GeV)



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CT and MSHT both use a Hessian technique to determine the central PDF. By definition, this is at the best χ^2 . This is not necessarily true for NNPDF. The uncertainty is determined by allowing an excursion from that central value. CT18 uses $\Delta\chi^2$ =37 for a 68% CL error.





In a global PDF fit, there are tensions between the input data sets, by

definition. These tensions are most easily demonstrated by the use of the L2 sensitivity above. Some data sets pull the gluon up at $x\sim0.01$, some down.

The end result of the pulling is the central PDF. The PDF uncertainty reflects the size of those pulls/tensions.

Typical χ^2 /dof are of the order of 1.1 for >4000 points, or very unlikely from the pure statistical POV. $\Delta\chi^2$ =1 does not capture the full uncertainty.

CT and MSHT use different criteria to define those tensions/define the uncertainty.

The PDF uncertainties for the combination in the PDF4LHC21 exercise is shown below. Same data sets used for all PDF fits. NNPDF3.1'is the smallest and CT18 is the largest, with MSHT20 in-between. NB: MSHT20 nominally does not use a fixed tolerance, but instead cuts off an eigenvector direction when a particular experiment is badly fit. Thus, the uncertainty can be greatly affected by one experiment.





For some special cases, MSHT20 and CT18 were both defined using a $\Delta \chi^2$ of 10 (see above). The uncertainties are equivalent, as may be expected from them both using similar data sets, and in this case having the same criteria for determining the uncertainty. MSHT20-full-tolerance (i.e. the canonical MSHT20) in some cases has a larger uncertainty than MSHT20-T210, and in some cases smaller, indicating that the effective tolerance for the full fit is sometimes less than 10 and sometimes greater.



It is difficult to perform a directly similar comparison to NNPDF, as they don't use the Hessian formalism. However, as part of the PDF4LHC exercise, fits were carried out to a reduced data set, using similar theory parameters, in which equivalent results should be obtained, if the uncertainty criteria were the same.

CT18red and MSHT20red agree for the most part. There are fewer experiments included, so less likely for a particular experiment to truncate the uncertainty from a particular eigenvector.

NNPDF consistently has a consistently smaller uncertainty, indicative that their effective tolerance is smaller than either CT18red or MSHT20red.



. luminosities are compared (above).