Determining parton distribution functions accurately and precisely with machine learning

Digital Twins for Nuclear and Particle physics - NPTwins 2024

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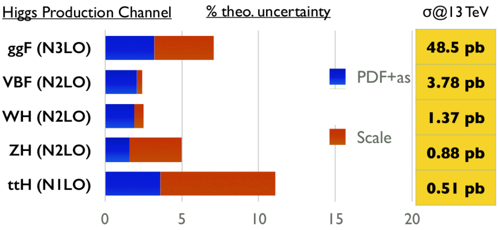
Parton Distribution Functions at the LHC

$$\sigma(Q^2,\tau,\mathbf{k}) = \sum_{ij}\int_\tau^1 \frac{dz}{z}\mathcal{L}_{ij}(z,Q^2)\hat{\sigma}_{ij}\left(\frac{\tau}{z},\alpha_s(Q^2),\mathbf{k}\right) \qquad \mathcal{L}_{ij}(z,Q^2) = (f_i^{h_1}\otimes f_j^{h_2})(z,Q^2)$$

PDF uncertainty is often the dominant source of uncertainty in LHC cross sections

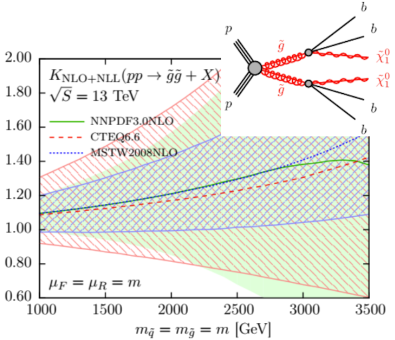
Precision



Unc. [MeV]	Total	Stat.	Syst.	PDF	A_i	Backg.	EW	e	μ	u_T	Lumi	Γ_W	PS
p_T^ℓ	16.2	11.1	11.8	4.9	3.5	1.7	5.6	5.9	5.4	0.9	1.1	0.1	1.5
m_T	24.4	11.4	21.6	11.7	4.7	4.1	4.9	6.7	6.0	11.4	2.5	0.2	7.0
Combined	15.9	9.8	12.5	5.7	3.7	2.0	5.4	6.0	5.4	2.3	1.3	0.1	2.3

[CERN Yellow Report 2016; arXiv:2403.15085]

Discovery



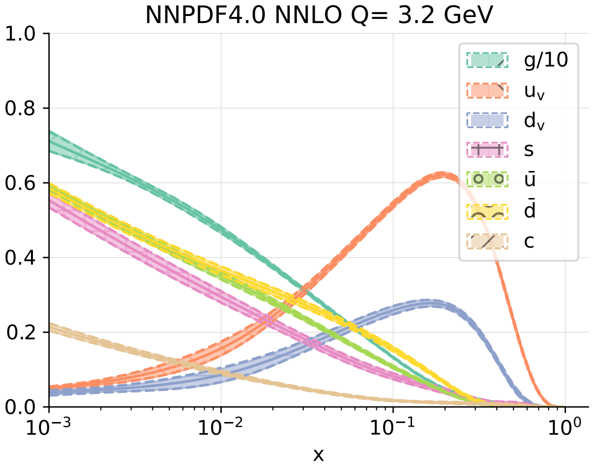
[EPJC 76 (2016) 53]

Parton Distribution Functions

PDFs express the likelihood of a quark or gluon (partons) to enter a collision

That is, $x\times$PDFs are momentum fraction distributions for each parton

Dependence on x is non-perturbative (fit); dependence on Q^2 is perturbative (DGLAP)



[Plot from the PDG Review of Particle Physics]

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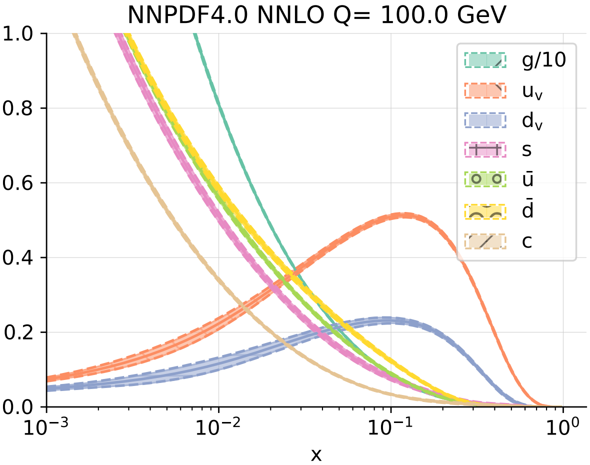


[Plot from the PDG Review of Particle Physics]

PDF determination in statistical language

<u>Inverse problem</u>

Given a set of data D, determine $p(f|D)$ in the space of functions $f : [0,1] \to \mathbb{R}$.

<u>Solution: parametric regression</u>

Approximate $p(f|D)$ with its projection in the space of parameters $p(\boldsymbol{\theta}|D)$

$$xf_i(x, Q_0^2) = A_{f_i}\, x^{a_{f_i}}\, (1-x)^{b_{f_i}}\, \mathscr{F}(x, \{c_{f_i}\})$$

Determine $p(\boldsymbol{\theta}|D) \propto p(D|\boldsymbol{\theta})p(\boldsymbol{\theta})$ as MAP $\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|D)$

$$\chi^2 = \sum_{i,j}^{N_{\rm dat}} [T_i[\boldsymbol{\theta}] - D_i](\mathrm{cov}^{-1})_{ij}[T_j[\boldsymbol{\theta}] - D_j]$$

Use a prescription to compute expectation values and uncertainties of observables

$$E[\mathcal{O}] = \int \mathcal{D}f \mathcal{P}(f|D)\mathcal{O}(f) \qquad V[\mathcal{O}] = \int \mathcal{D}f \mathcal{P}(f|D)[\mathcal{O}(f) - E[\mathcal{O}]]^2$$

Monte Carlo: $\mathcal{P}(f|D) \longrightarrow \{f_k\}$

$E[\mathcal{O}] \approx \frac{1}{N}\sum_k \mathcal{O}(f_k)$

$V[\mathcal{O}] \approx \frac{1}{N}\sum_k [\mathcal{O}(f_k) - E[\mathcal{O}]]^2$

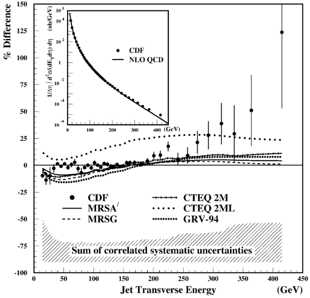
Maximum likelihood: $\mathcal{P}(f|D) \longrightarrow f_0$

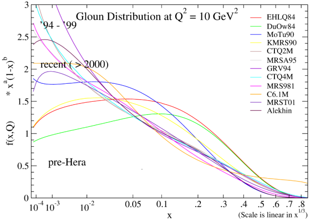
$E[\mathcal{O}] \approx \mathcal{O}(f_0)$

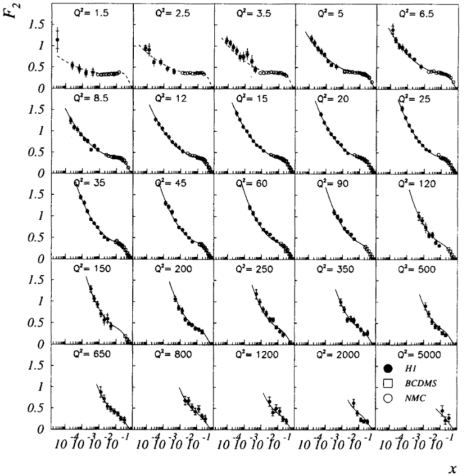
$V[\mathcal{O}] \approx$ Hessian, $\Delta\chi^2$envelope, ...

Interplay between DATA, THEORY, and METHODOLOGY

Why is the methodology important?



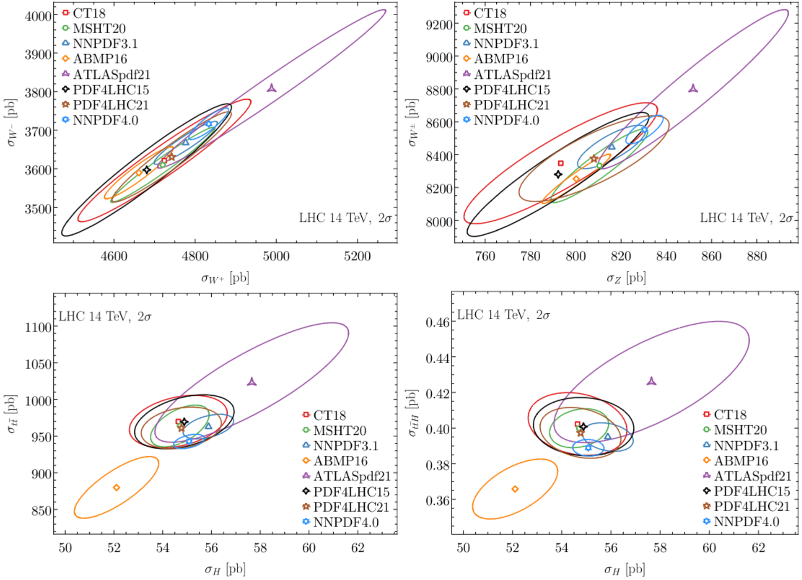




circa 1995: small-x rise of HERA F_2^p and CDF jet discrepancy

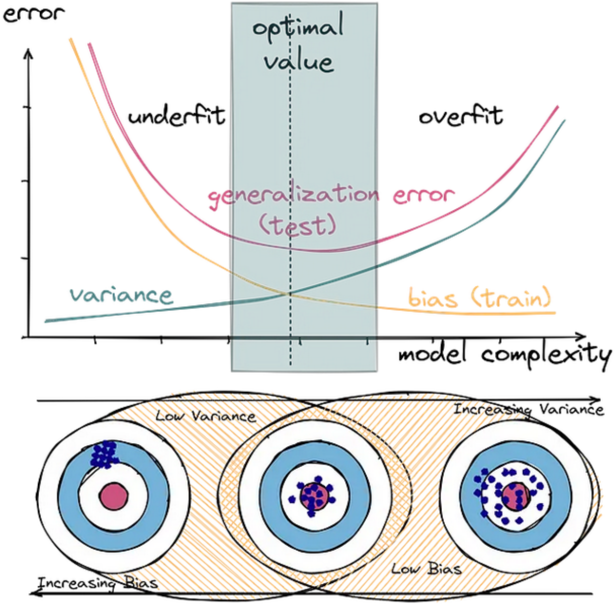
The methodology is crucial if we aim at percent-level accurate PDFs

Making predictions with PDFs



[Acta Phys.Polon.B 53 (2022) 12]

Accuracy vs precision or bias vs variance



A lot of progress in the last (two) years

A Markov Chain Monte Carlo determination of Proton PDF uncertainties at NNLO

Peter Risse [a,*] **Nasim Derakhshanian** [b] **Tomas Ježo** [a] **Karol Kovařík** [a] **and Aleksander Kusina** [b]
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Learning PDFs through Interpretable Latent Representations in Mellin Space

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(Dated: June 21, 2024)

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Bayesian inference with Gaussian processes for the determination of parton distribution functions

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A generalized statistical model for fits to parton distributions

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A critical study of the Monte Carlo replica method

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Explainable AI classification for parton density theory

Brandon Kriesten[a] **Jonathan Gomprecht**[a,b] **and T.J. Hobbs**[a]
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[EPJ C84 (2024) 716; JHEP 11 (2024) 007; JHEP 12 (2024) 064; arXiv:2312.02278; arXiv:2406.01664; arXiv:2407.12377]

NNPDF4.0: a machine learning methodology

uncertainty representation

Monte Carlo sampling of experimental uncertainties
what is the statistical meaning of uncertainties?

parametrisation

neural network(s)
is there a bias due to the parametrisation?

optimisation

(adaptive) gradient descent
is the parameter space explored efficiently?

delivery

GAN enhancement and compression
can the number of replicas be reduced?

uncertainty characterisation and validation

closure tests (what happens if I know in advance the underlying law that I am fitting?)
are interpolation and extrapolation uncertainties statistically faithful?

[EPJC 82 (2022) 428]

The NNPDF code is public, see **https://github.com/NNPDF** [EPJ C81 (2021) 958]

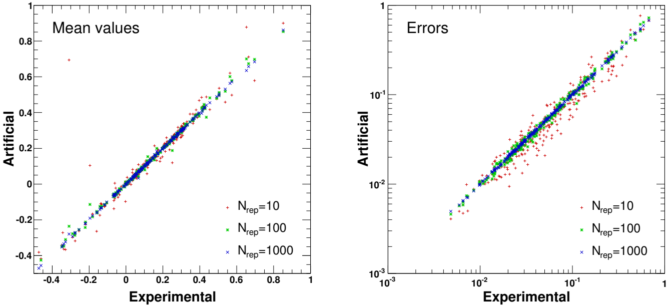
Uncertainty representation

Generate Monte Carlo replicas and perform a fit to each replica

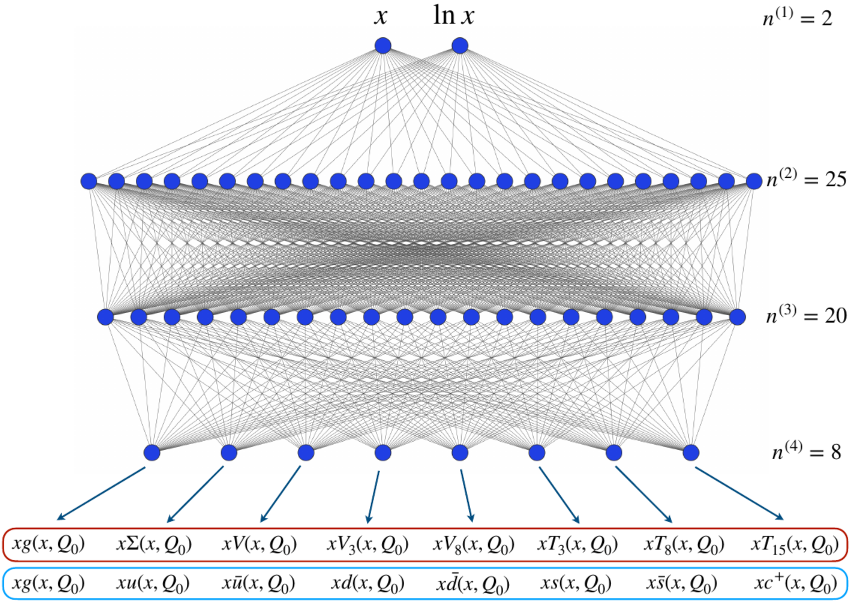
$$\mathcal{O}_i^{(art)(k)} = \mathcal{O}_i^{(exp)} + L_{ij} r_i^{(k)} \quad i,j = 1 \dots N_{\rm dat} \quad k = 1 \dots, N_{\rm rep} \quad {\rm cov} = L \cdot L^T$$

$$\langle \mathcal{O}[f(x,Q^2)] \rangle = \frac{1}{N_{\rm rep}} \sum_{k=1}^{N_{\rm rep}} \mathcal{O}[f^{(k)}(x,Q^2)]$$

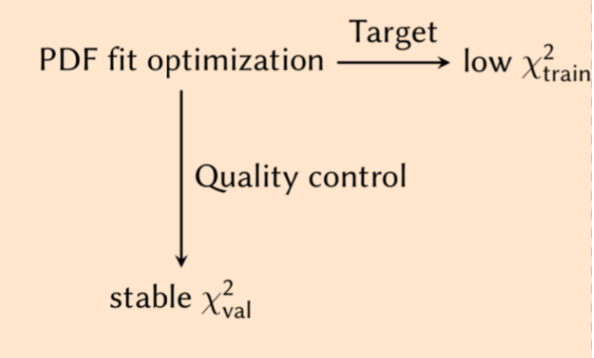
$$\sigma_{\mathcal{O}}[f(x,Q^2)] = \left[\frac{1}{N_{\rm rep}-1} \sum_{k=1}^{N_{\rm rep}} \left(\mathcal{O}[f^{(k)}(x,Q^2)] - \langle \mathcal{O}[f(x,Q^2)] \rangle \right)^2 \right]^{1/2}$$



Parametrisation



Optimisation

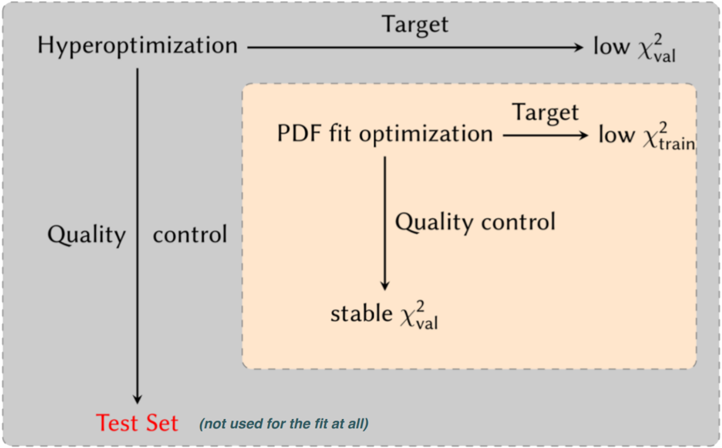


$$\chi^2 = \sum_{i,j}^{N_{\text{dat}}} (T_i[\{\boldsymbol{\theta}\}] - D_i) \left(\text{cov}^{-1}\right)_{ij} (T_j[\{\boldsymbol{\theta}\}] - D_j)$$

$$(\text{cov})_{ij} = \delta_{ij} s_i^2 + \left(\sum_{\alpha}^{N_c} \sigma_{i,\alpha}^{(c)} \sigma_{j,\alpha}^{(c)} + \sum_{\alpha}^{N_{\mathcal{L}}} \sigma_{i,\alpha}^{(\mathcal{L})} \sigma_{j,\alpha}^{(\mathcal{L})} \right) D_i D_j$$

stochastic gradient descent with backpropagation

Hyperoptimisation: fitting the methodology



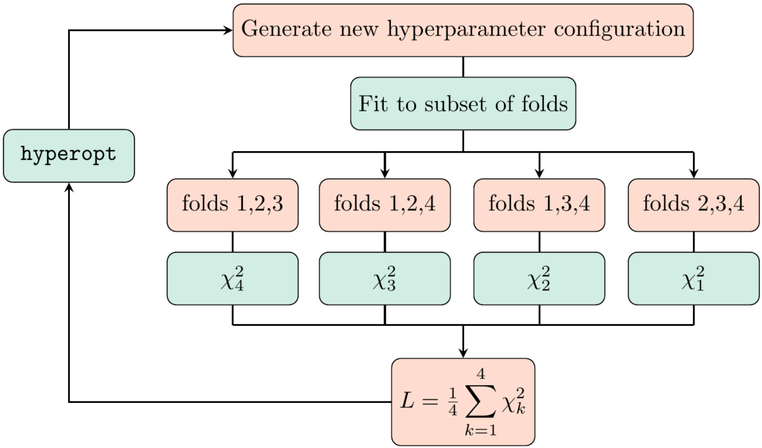
Compare to a Test Set (new set of data previously not used at all)

Who picks the Test Set? Automatic generalisation based on K foldings

Divide the data into n representative sets, fit $n-1$ sets and use the n-th set as test set

Hyperoptimise on mean and standard deviation of $\chi^2_{\text{test},i}$, $i = 1 \ldots n$

Hyperoptimisation: K-folding



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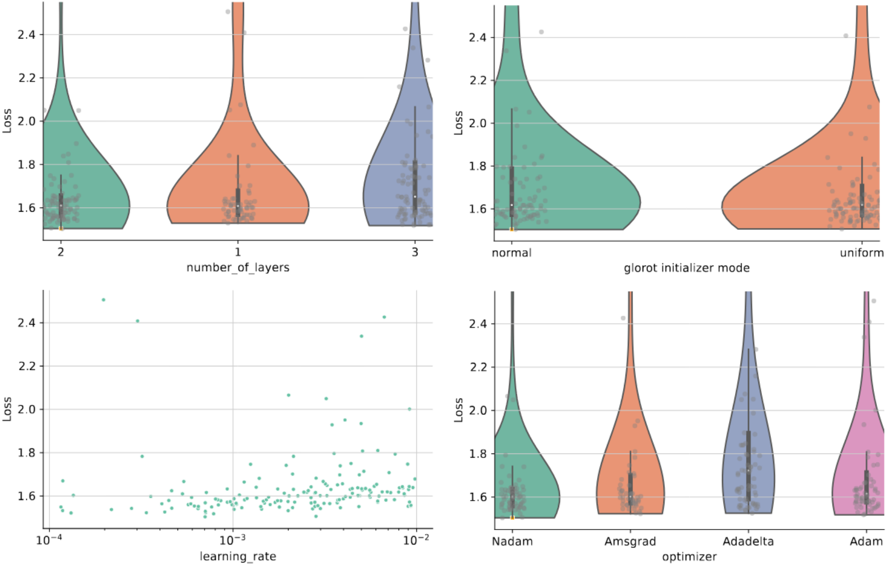
Hyperparameters

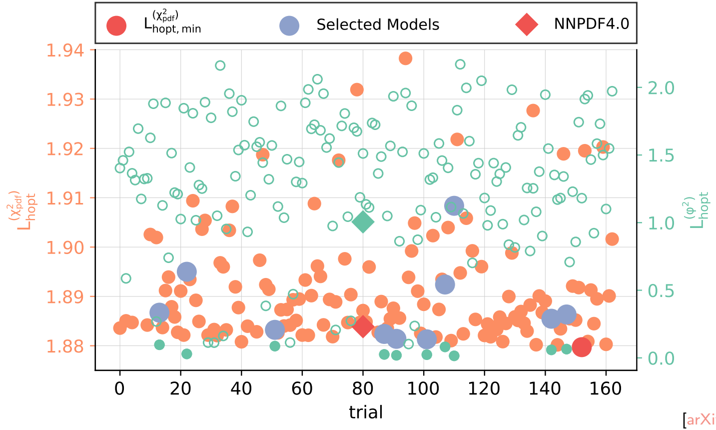


Hyperoptimisation: metrics

$$\varphi^2_{\chi^2} \equiv \left\langle \chi^2 \left[T^{(k)}, D^{(0)} \right] \right\rangle_{\rm rep} - \chi^2 \left[\langle T \rangle_{\rm rep}, D^{(0)} \right] = \frac{1}{n_{\rm dat}} \sum_{i,j}^{n_{\rm dat}} ({\rm cov})^{-1} T_{ij} \qquad L^{(\varphi^2)}_{\rm hopt} = \left(\frac{1}{n_{\rm fold}} \sum_{p}^{n_{\rm fold}} \varphi^{2\,(p)}_{\chi^2} \right)^{-1}$$

Select hyperparameters leading to best χ^2 and largest PDF errors in non-fitted data

Sample over the acceptable hyperparameters displaying comparable performance



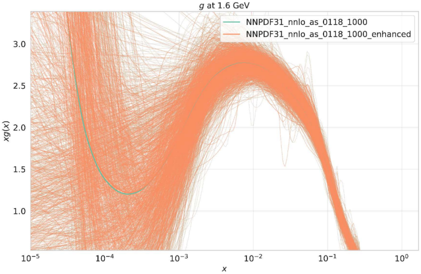
[arXiv:2410.16248]

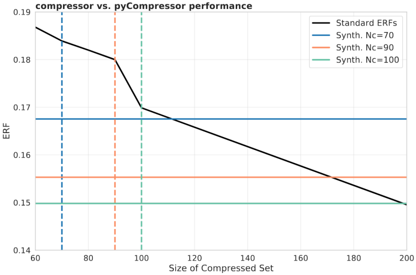
Delivery: compression

Find a subset of replicas that describe the underlying probability distribution as accurately as the original ensemble of replicas

$$\mathrm{ERF} = \frac{1}{N_{\mathrm{EST}}} \sum_k \frac{1}{N_k} \sum_i \left(\frac{C^{(k)}(x_i) - P^{(k)}(x_i)}{P^{(k)}(x_i)} \right)^2$$

Use GANs to enhance the number of replicas before minimising ERF





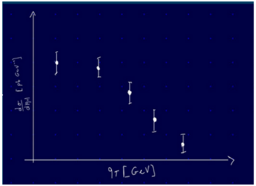
GAN enhancement allows one to achieve the same ERF with fewer replicas

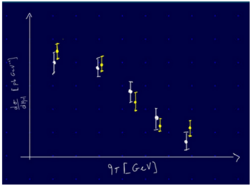
[EPJ C81 (2021) 530]

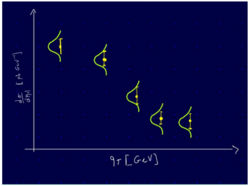
Validation: closure tests

Fit PDFs to pseudodata generated assuming a known underlying law

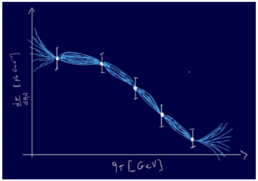
Level 0	Level 1	Level 2
no fluctuations	Gaussian fluctuation	Monte Carlo replicas



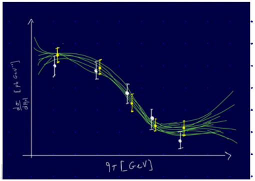




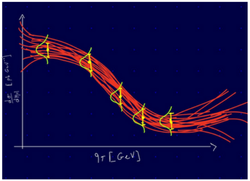
interpolation uncertainty



fuctional uncertainty



data uncertainty



Closure tests at work

Data region: closure tests

Fit PDFs to pseudodata generated assuming a known underlying law

Define bias and variance

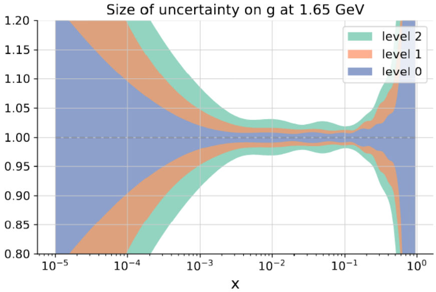
bias difference of central prediction and truth

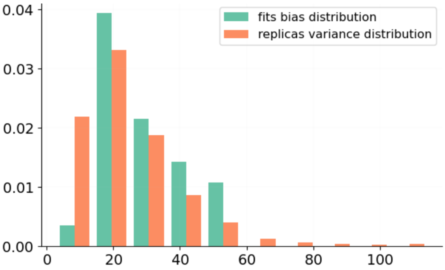
variance uncertainty of replica predictions

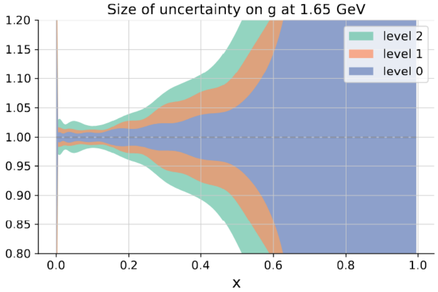
If PDF uncertainty faithful, then

E[bias] = variance

25 fits, 40 replicas each

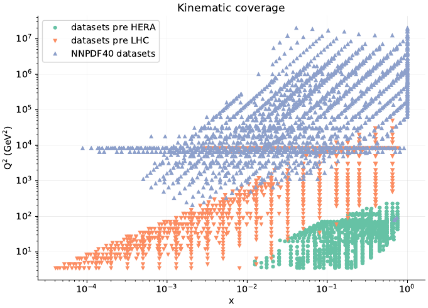


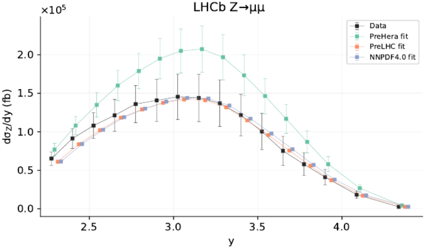




[EPJ C77 (2017) 663; EPJ C82 (2022) 330]

Future tests



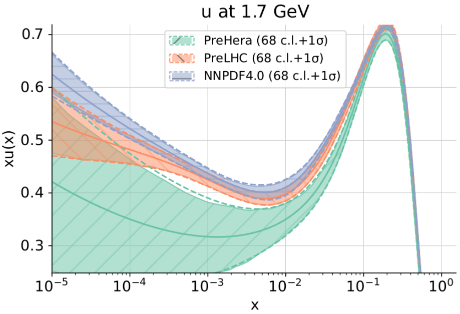


Extrapolation regions: future test

Test PDF uncertainties on data sets
not included in a given PDF fit
that cover unseen kinematic regions

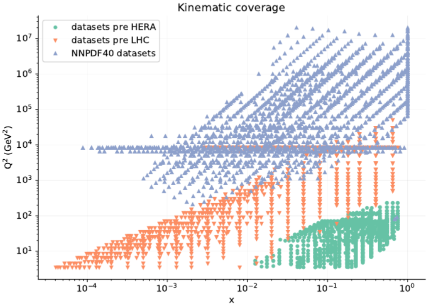
Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA	1.09	1.01	0.90
pre-LHC	1.21	1.20	23.1
NNPDF4.0	1.29	3.30	23.1

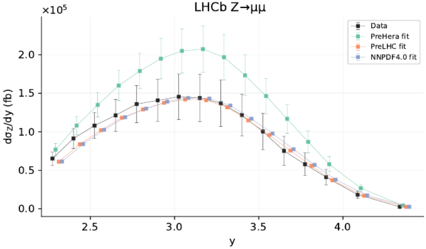
Only exp. cov. matrix



[Acta Phys.Polon. B52 (2021) 243]

Future tests



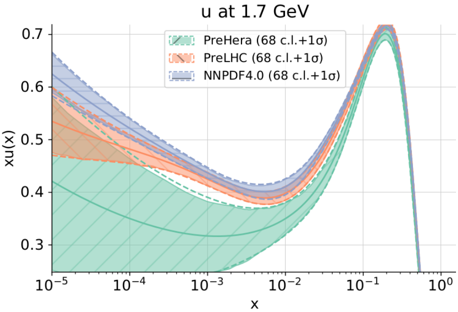


Extrapolation regions: future test

Test PDF uncertainties on data sets
not included in a given PDF fit
that cover unseen kinematic regions

Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA			0.86
pre-LHC		1.17	1.22
NNPDF4.0	1.12	1.30	1.38

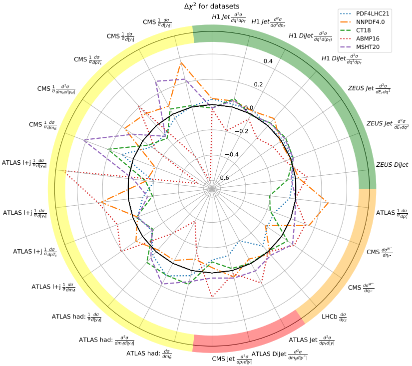
Exp+PDF cov. matrix

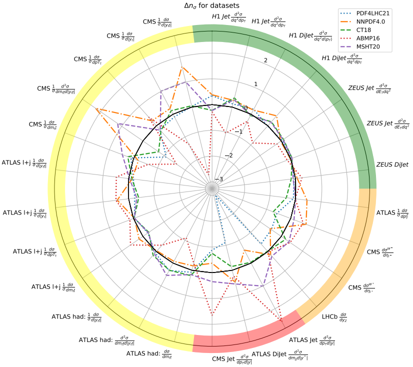


[Acta Phys.Polon. B52 (2021) 243]

To conclude: are all PDF sets equally accurate?

$$\Delta\chi^{2(i)} = \frac{\chi^{2(i)}_{\rm exp+th} - \left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}}{\left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}} \qquad \Delta n_\sigma^{(i)} = \frac{\chi^{2(i)}_{\rm exp+th} - \left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}}{\sqrt{2/n_{\rm data}}}$$

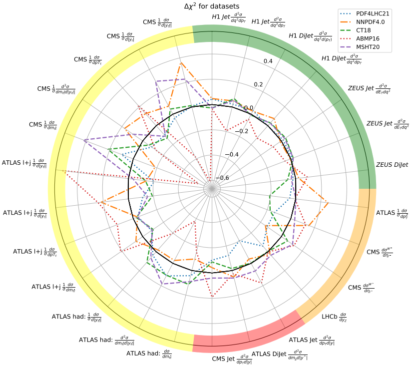


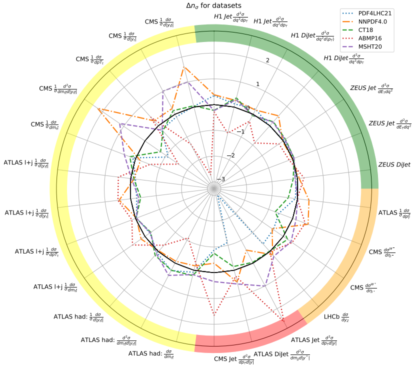


The PDF set obtained with ML is more precise and more accurate than all the others

To conclude: are all PDF sets equally accurate?

$$\Delta\chi^{2(i)} = \frac{\chi^{2(i)}_{\rm exp+th} - \left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}}{\left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}} \qquad \Delta n_\sigma^{(i)} = \frac{\chi^{2(i)}_{\rm exp+th} - \left\langle \chi^2_{\rm exp+th} \right\rangle_{\rm pdfs}}{\sqrt{2/n_{\rm data}}}$$



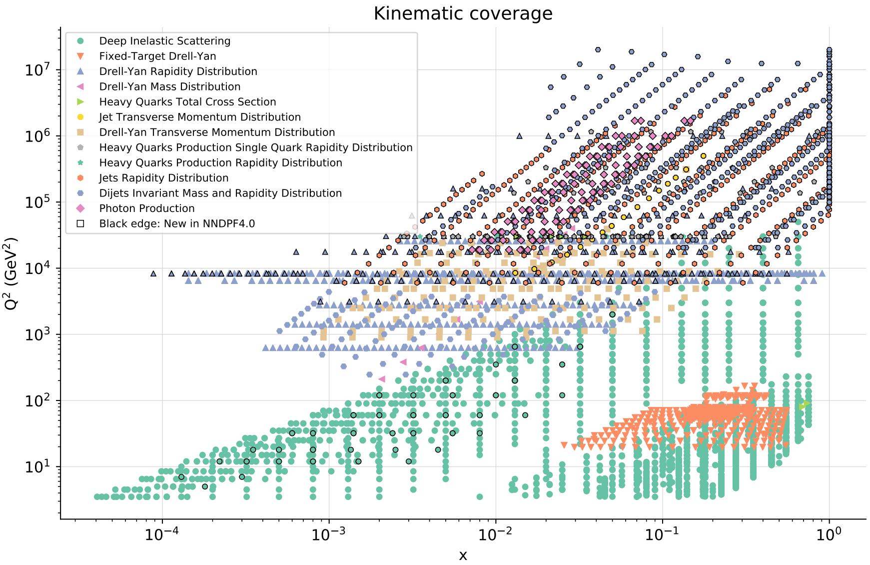


The PDF set obtained with ML is more precise and more accurate than all the others

Thank you

Extra material

Overview of experimental data

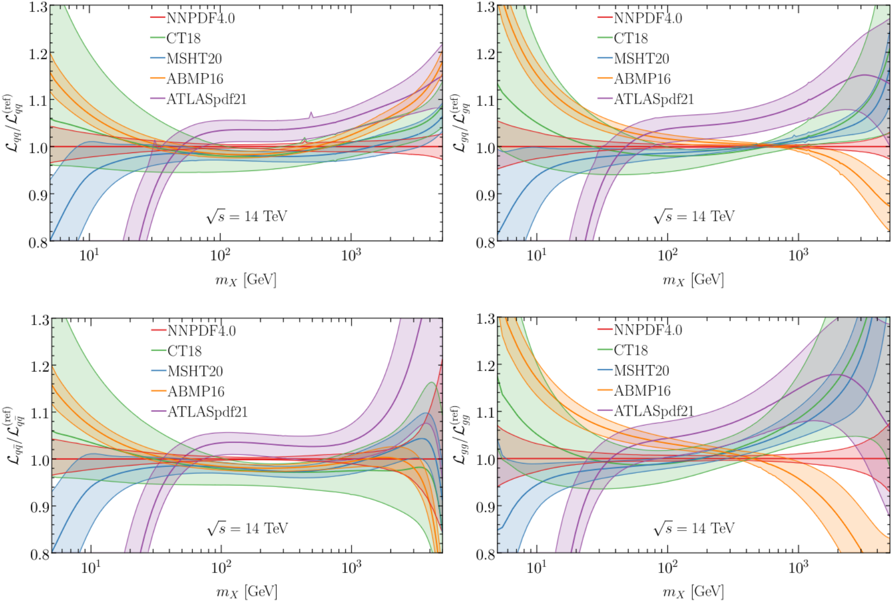


$$N_{\rm dat} = 4618$$

Overview of current PDF determinations

	NNPDF4.0	MSHT20	CT18	HERAPDF2.0	CJ22	ABMP16
Fixed-target DIS	✓	✓	✓	✗	✓	✓
JLAB	✗	✗	✗	✗	✓	✗
HERA I+II	✓	✓	✓	✓	✓	✓
HERA jets	✓	✗	✗	✓	✗	✗
Fixed target DY	✓	✓	✓	✗	✓	✓
Tevatron W, Z	✓	✓	✓	✗	✓	✓
LHC vector boson	✓	✓	✓	✗	✓	✓
LHC $W+c$ $Z+c$	✓	✗	✗	✗	✗	✗
Tevatron jets	✓	✓	✓	✗	✓	✗
LHC jets	✓	✓	✓	✗	✗	✗
LHC top	✓	✓	✗	✗	✗	✓
LHC single t	✓	✗	✗	✗	✗	✗
LHC prompt γ	✓	✗	✗	✗	✗	✗
statistical treatment	Monte Carlo	Hessian $\Delta\chi^2$ dynamical	Hessian $\Delta\chi^2$ dynamical	Hessian $\Delta\chi^2 = 1$	Hessian $\Delta\chi^2 = 1.645$	Hessian $\Delta\chi^2 = 1$
parametrisation	Neural Network	Chebyschev pol.	Bernstein pol.	polynomial	polynomial	polynomial
HQ scheme	FONLL	TR′	ACOT-χ	TR′	ACOT-χ	FFN
accuracy	aN^{3}LO	aN^{3}LO	NNLO	NNLO	NLO	NNLO
latest update	EPJ C82 (2022) 428	EPJ C81 (2021) 341	PRD 103 (2021) 014013	EPJ C82 (2022) 243	PRD 107 (2023) 113005	PRD 96 (2017) 014011

Comparing PDF sets



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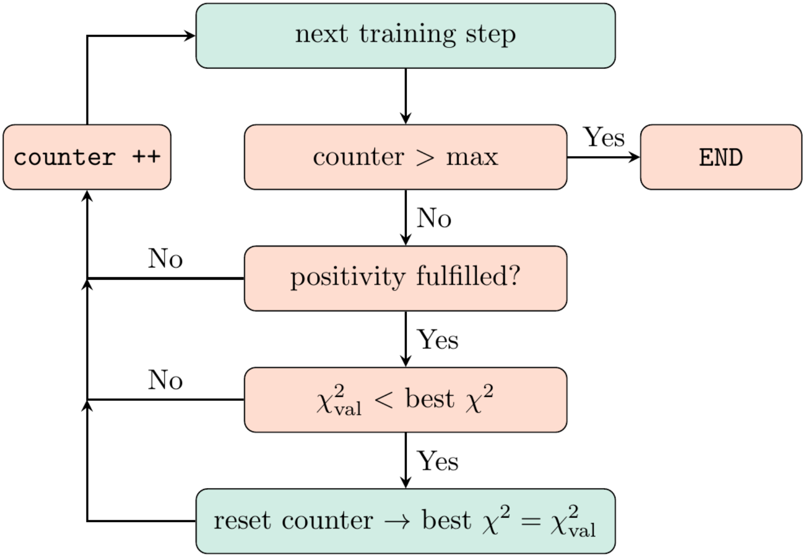
Optimisation



stochastic gradient descent with backpropagation