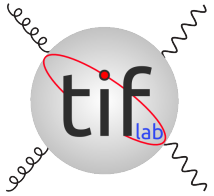
PDF DETERMINATION AS MACHINE LEARNING

STEFANO FORTE
UNIVERSITÀ DI MILANO & INFN

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA



DEEP-LEARNING ERA OF PARTICLE THEORY

MAINZ, JULY 5, 2022

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 740006

SUMMARY

- THE STATE OF THE ART
  - PDFs AND DATA
  - UNCERTAINTIES: DATA AND EXTRAPOLATION
- PDF UNCERTAINTIES
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  - METHODOLOGY AND THEORY BIAS
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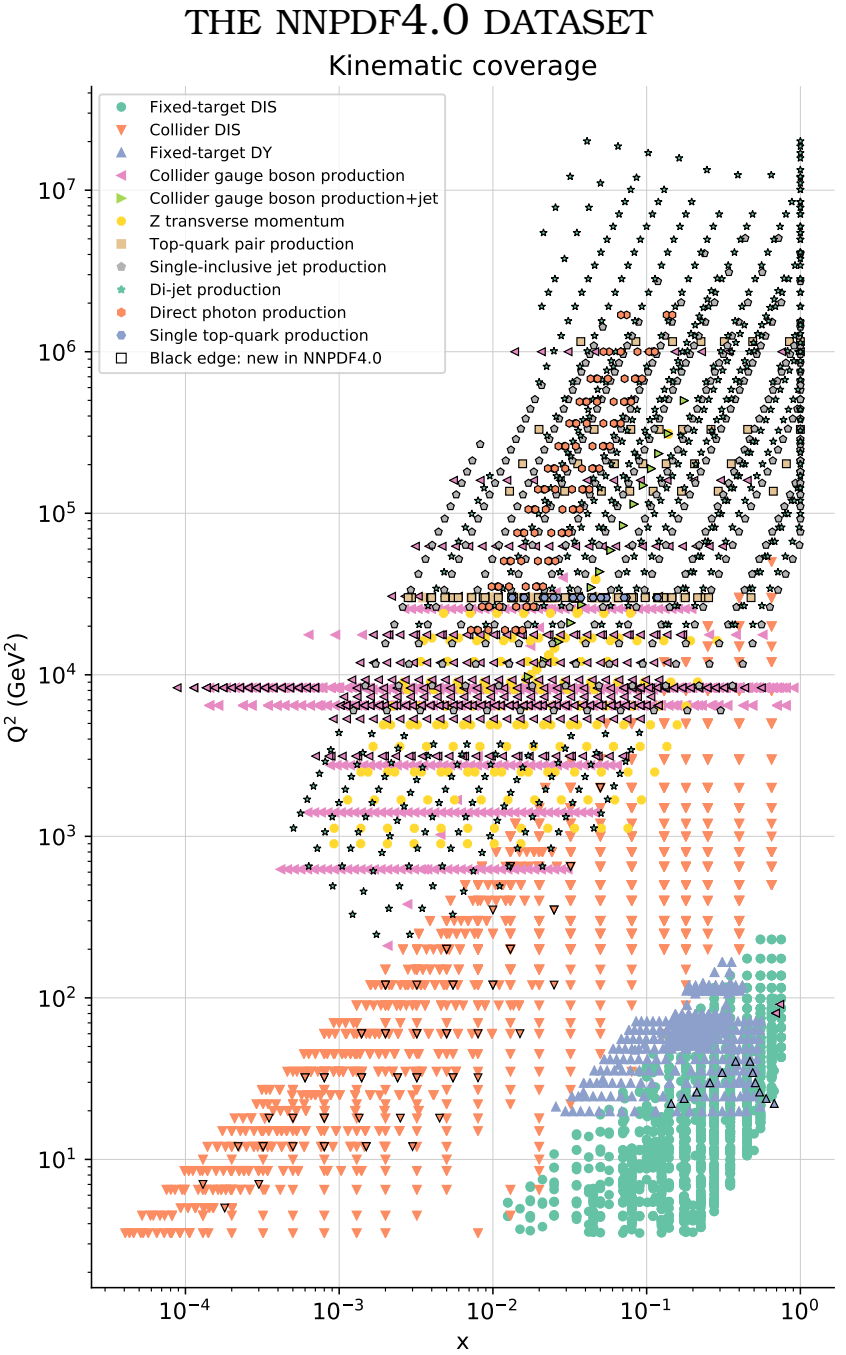
  - GAN OPTIMIZATION
- FUTURE DEVELOPMENTS
  - FEATURE SCALING
  - OVERLEARNING METRICS

PDFs: THE STATE OF THE ART

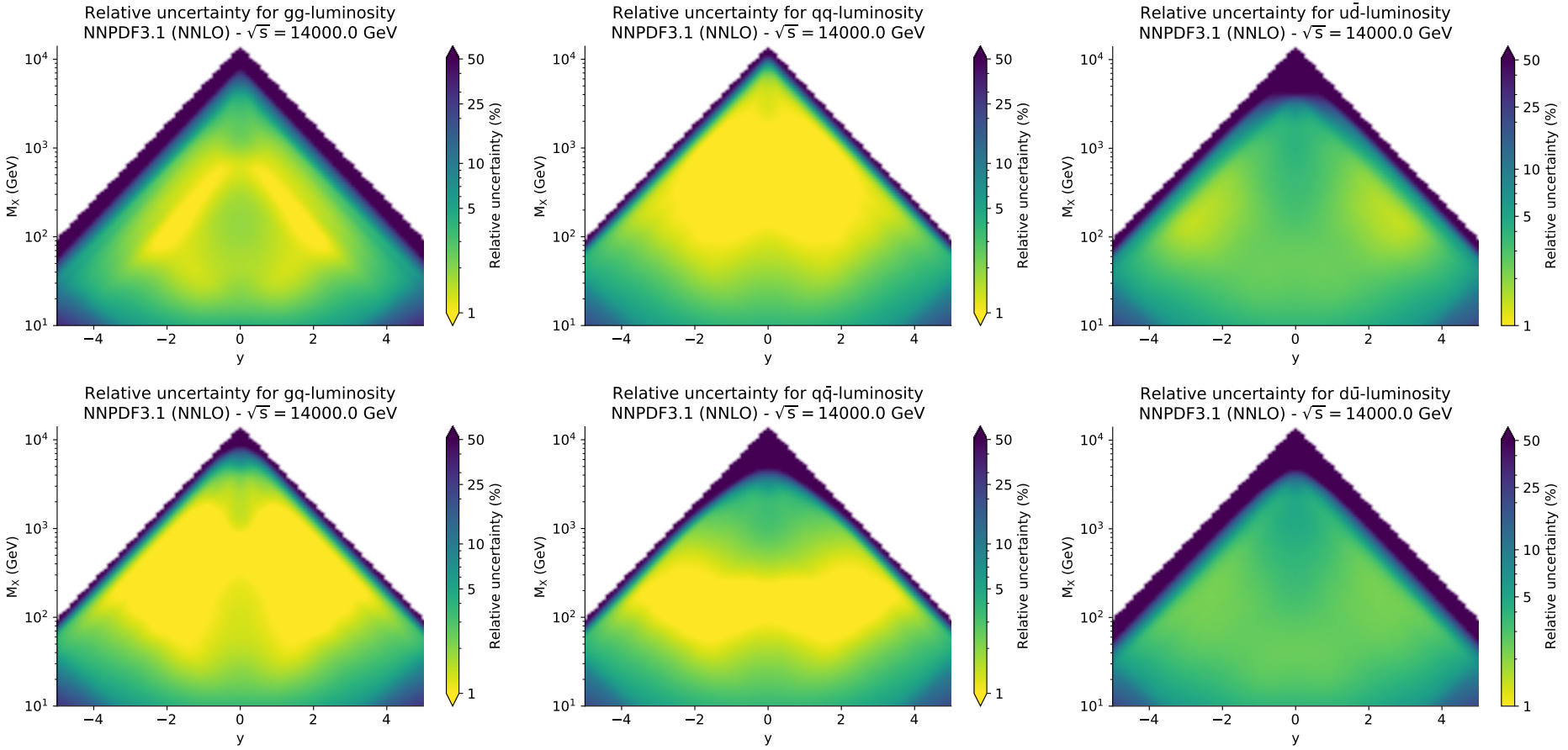
PDFs AND DATA

- LHC CROSS SECTION:
  - $\sigma = \sum_{ij} \hat{\sigma}_{ij} \otimes f_i^{(1)} \otimes f_j^{(2)}$
  - $\hat{\sigma}_{ij}$ PARTONIC CROSS SECTION, INCOMING PARTONS i, j
  - $f_i^{(j)}(x, Q^2)$ PDF FOR PARTON OF SPECIES i IN j-TH INCOMING PROTON
  - $\otimes$ CONVOLUTION OVER x
  - PDF DEPENDS ON Q^2 AND x, OTHER KINEMATIC VARIABLES IN $\hat{\sigma}$
- PARTONIC CROSS SECTION COMPUTED PERTURBATIVELY
- PDFs DETERMINED COMPARING σ TO DATA
  - ABOUT 4600 DATAPOINTS
  - LEPTOPRODUCTION & HADROPRODUCTION, COLLIDER & FIXED-TARGET



UNCERTAINTIES: RECENT (NNPDF3.1, 2017)

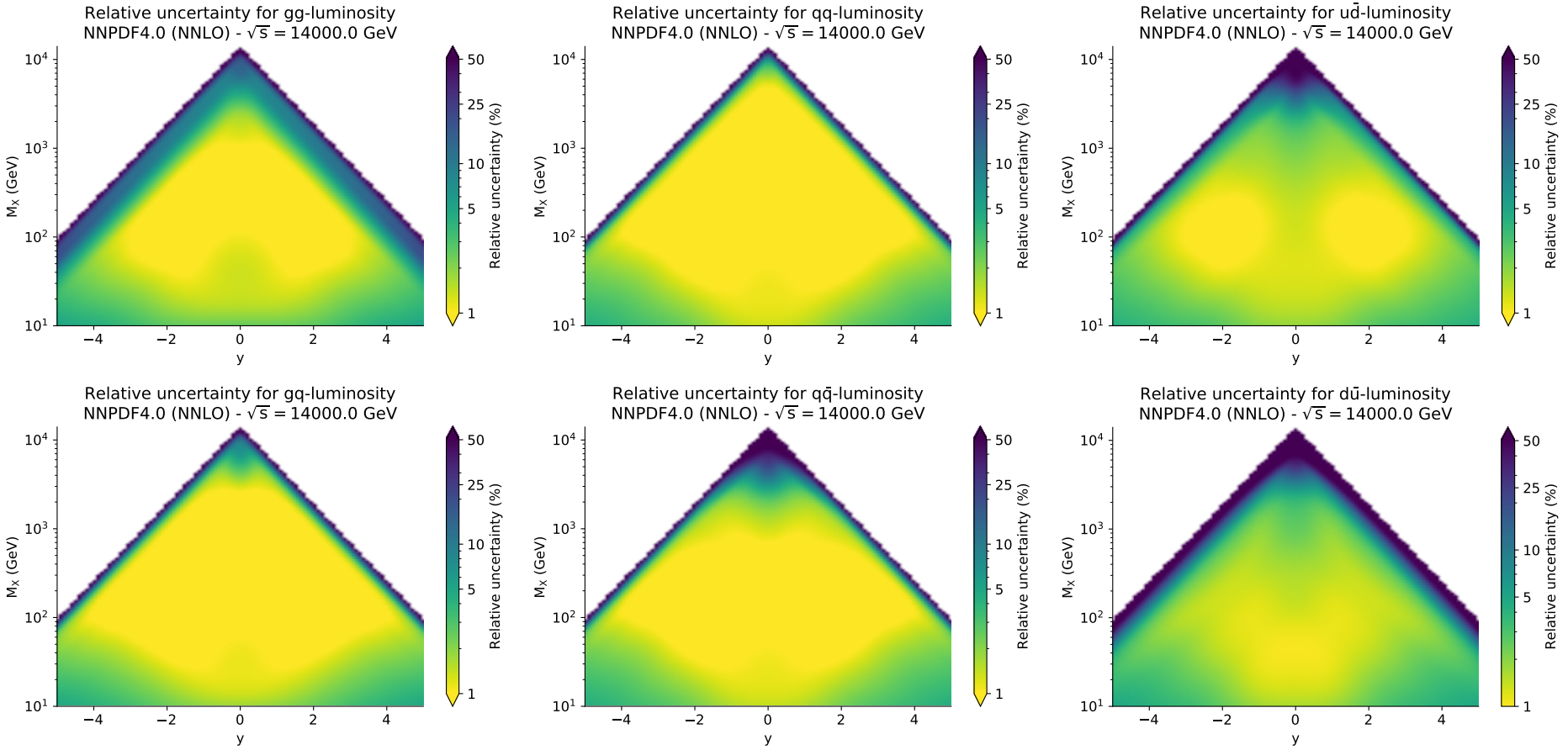
GLUON SINGLET FLAVORS



- TYPICAL UNCERTAINTIES IN DATA REGION: SINGLET $\sim 3\%$, NONSINGLET $\sim 5\%$
- DATA REGION: $10^2 \lesssim M_X \lesssim 10^3$ TeV, $-2 \lesssim y \lesssim 2$

UNCERTAINTIES: STATE OF THE ART (NNPDF4.0, 2021)

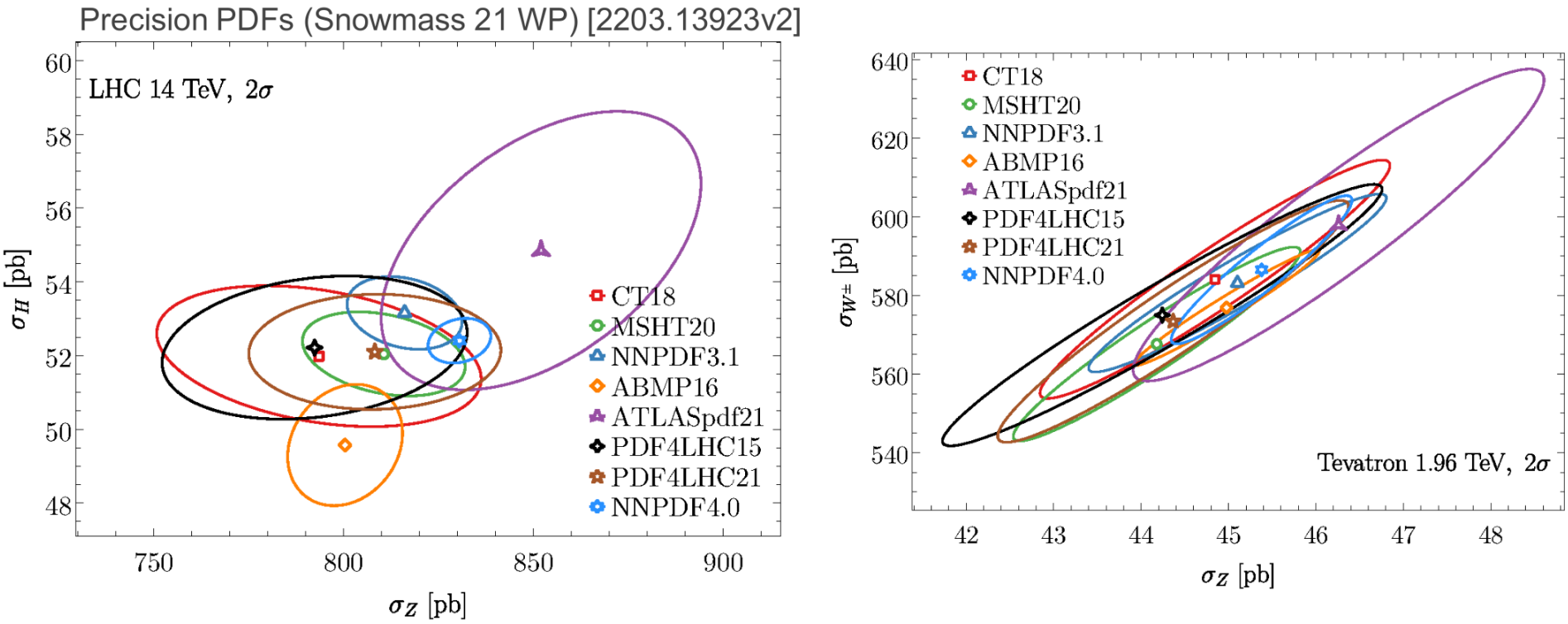
GLUON SINGLET FLAVORS



- TYPICAL UNCERTAINTIES IN DATA REGION: SINGLET $\sim 1\%$, NONSINGLET $\sim 2-3\%$
- DATA REGION: $10 \lesssim M_X \lesssim 3 \cdot 10^3$ TEV, $-4 \lesssim y \lesssim 4$

UNCERTAINTIES: STATE OF THE ART (NNPDF4.0, 2021)

Higgs, W, Z production

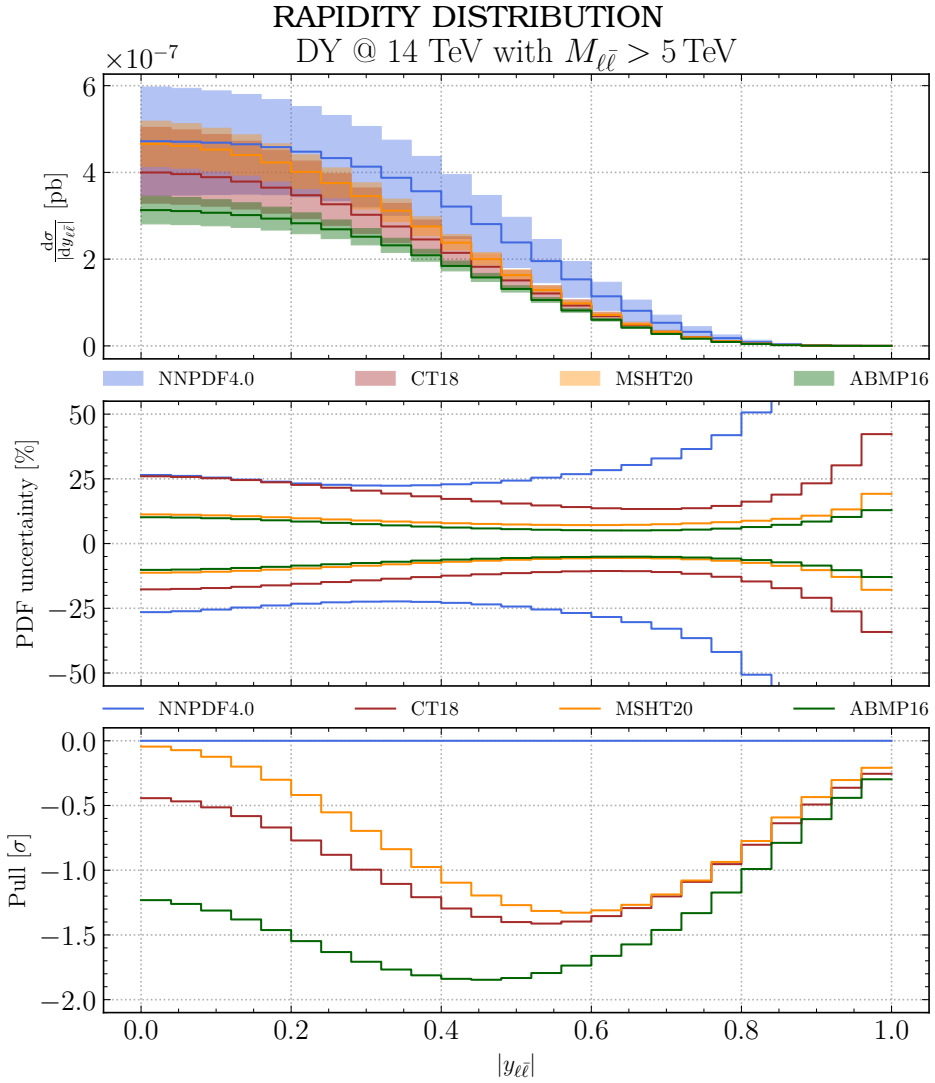


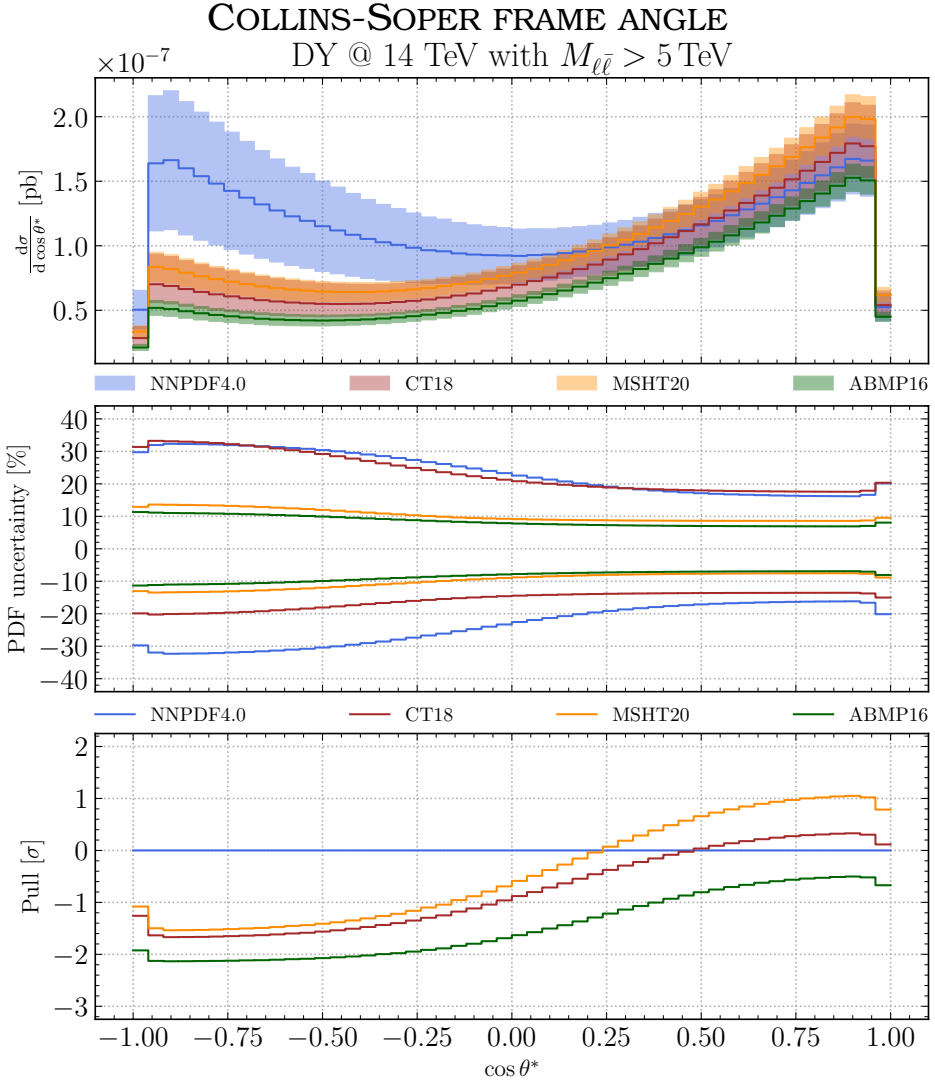
DATA REGION: NNPDF4.0 UNCERTAINTIES $\Rightarrow$ SMALLER THAN OTHER PDF SETS

BACKWARD CONSISTENT WITH NNPDF3.1

UNCERTAINTIES: STATE OF THE ART (NNPDF4.0, 2021)

Z' production





EXTRAPOLATION REGION: NNPDF4.0 UNCERTAINTIES $\Rightarrow$ LARGER THAN OTHER PDF SETS

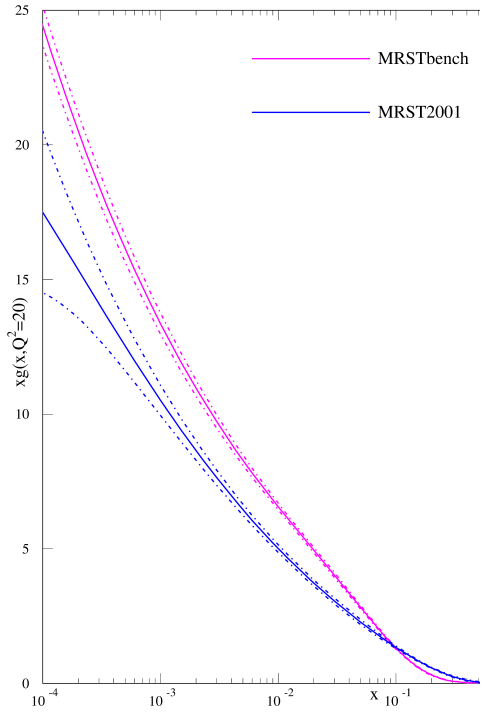
UNBIASED PDF BEHAVIOR

UNCERTAINTY ESTIMATION

THE PDF UNCERTAINTY PROBLEM: THE HERA-LHC BENCHMARK (2005)

- RESTRICTED AND VERY CONSISTENT DATASET USED
- RESULTS COMPARED TO THEN-BEST RESULT FROM FULL DATASET

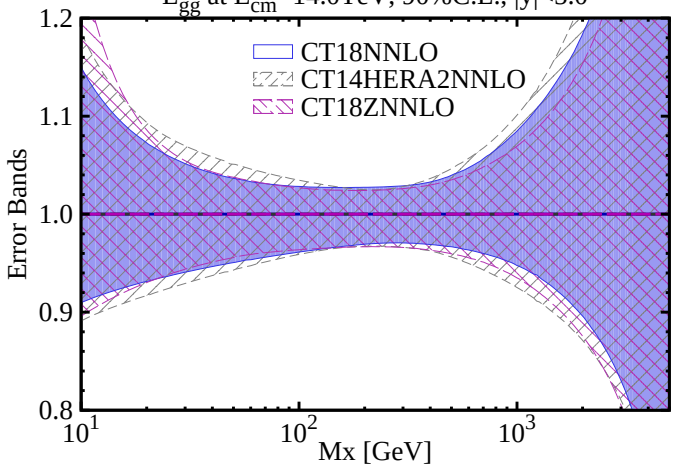
BENCHMARK VS DEFAULT GLUON



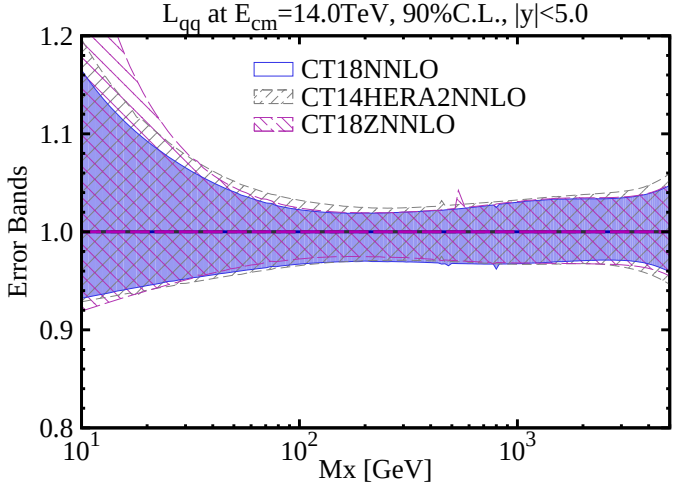
"...the partons extracted using a very limited data set are completely incompatible, even allowing for the uncertainties, with those obtained from a global fit with an identical treatment of errors...The comparison illustrates the problems in determining the true uncertainty on parton distributions." (R.Thorne, HERALHC, 2005)

THE PDF UNCERTAINTY PROBLEM:
UNCERTAINTY REDUCTION?
CT18 VS. CT14: PARTON LUMINOSITY UNCERTAINTIES

GLUON-GLUON



QUARK-QUARK



MORE DATA $\Rightarrow$ BIGGER UNCERTAINTIES (?!)

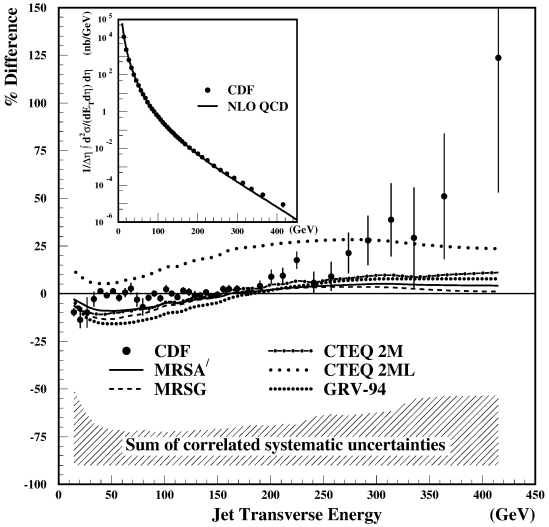
PARTON PARAMETRIZATIONS

- CTEQ5 2002: $xg(x,Q_0^2) = A_0 x^{A_1}(1-x)^{A_2}(1+A_3 x^{A_4})$
- MRST-HERALHC 2005: $xg(x,Q_0^2) = A_g x^{\delta_g}(1-x)^{\eta_g}(1+\epsilon_g x^{0.5}+\gamma_g x) + A_{g'} x^{\delta_{g'}}(1-x)^{\eta_{g'}}$
- CT18: $g(x,Q=Q_0) = x^{a_1-1}(1-x)^{a2}\left[a_3(1-y)^3 + a_4 3y(1-y)^2 + a_5 3y^2(1-y) + y^3\right]$; $y=\sqrt{x}$; $a_5 = (3+2a_1)/3$.

BIAS?

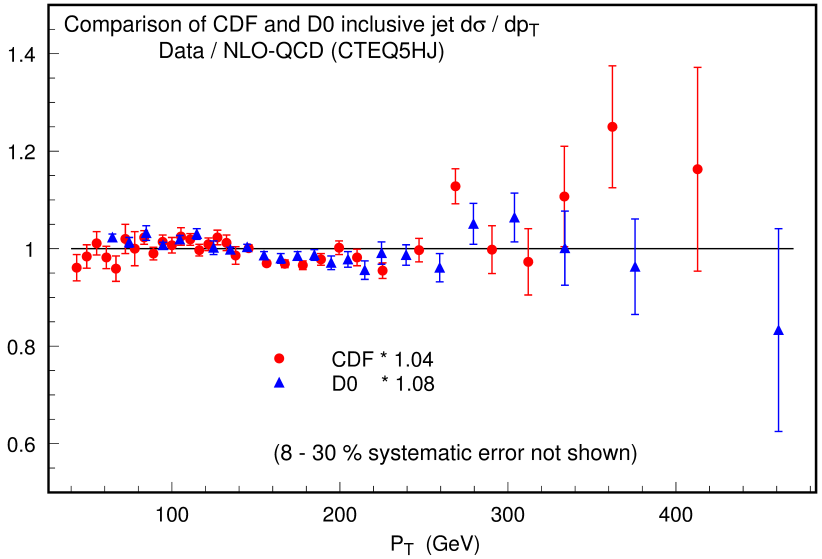
PDF UNCERTAINTIES AND NEW PHYSICS

- DISCREPANCY BETWEEN QCD CALCULATION AND CDF JET DATA (1995)
- EVIDENCE FOR QUARK COMPOSITENESS?
- RESULT STRONGLY DEPENDS ON GLUON AT $x \gtrsim 0.1$
- PDF MUST VANISH AT $x = 0$, BUT (THEN) NO DATA FOR $x \gtrsim 0.05$!



DISCREPANCY REMOVED IF JET DATA USED FOR GLUON DETERMINATION

NEW CTEQ GLUON (1998)

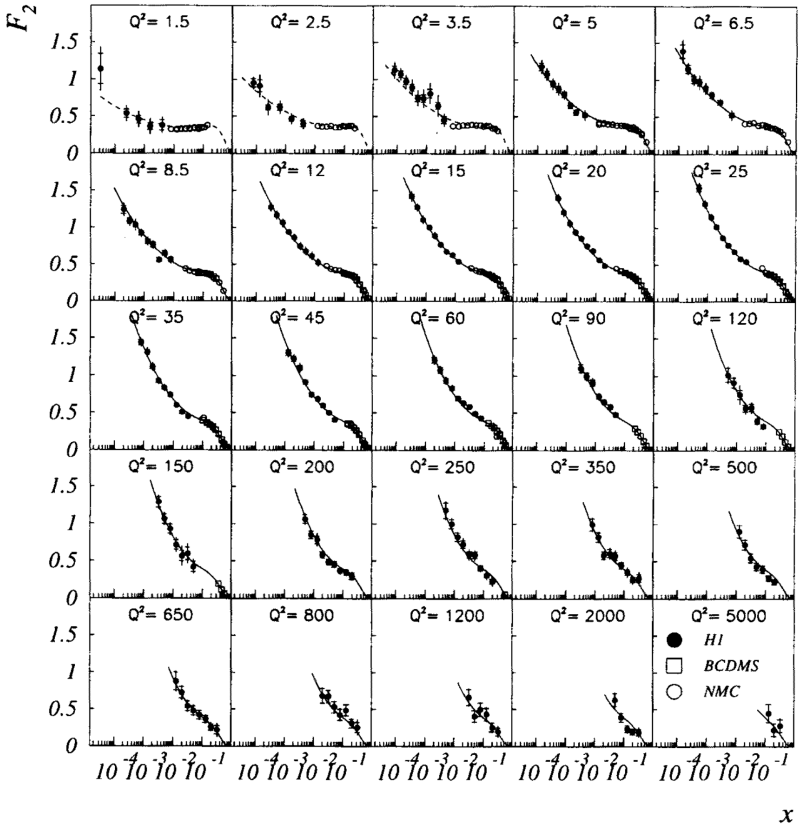


NOW: NO DATA FOR $x \gtrsim 0.5 \Rightarrow$ DISCOVERY (THRESHOLD) REGION!

EXTRAPOLATION AND THEORY BIAS

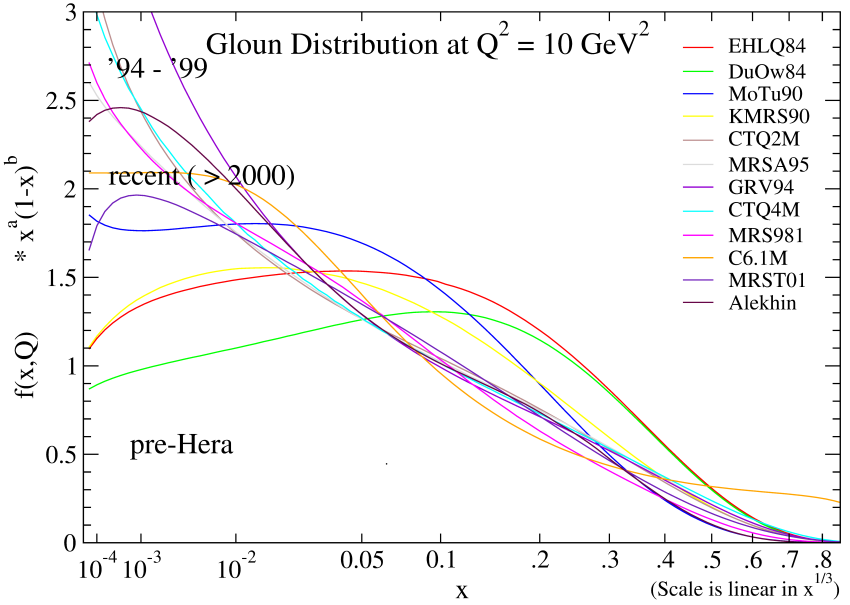
1995: THE RISE OF STRUCTURE FUNCTIONS AT HERA

FIRST HERA DATA VS OLDER DATA



A. de Roeck, Cracow epiphany conf. 1996

HISTORICAL COMPILATION OF GLUON PDFS

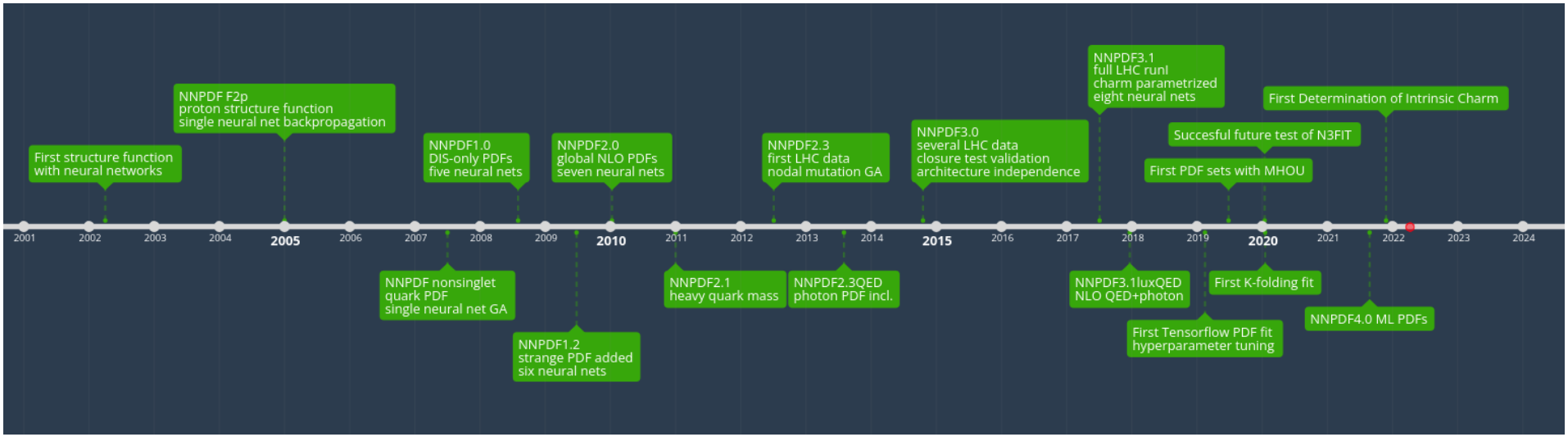


W.K.Tung, DIS 2004

- RISE OF F_2 AT HERA CAME $\Rightarrow$ SURPRIZE
- HINTED BY PRE-HERA DATA; VETOED BY THEORETICAL BIAS

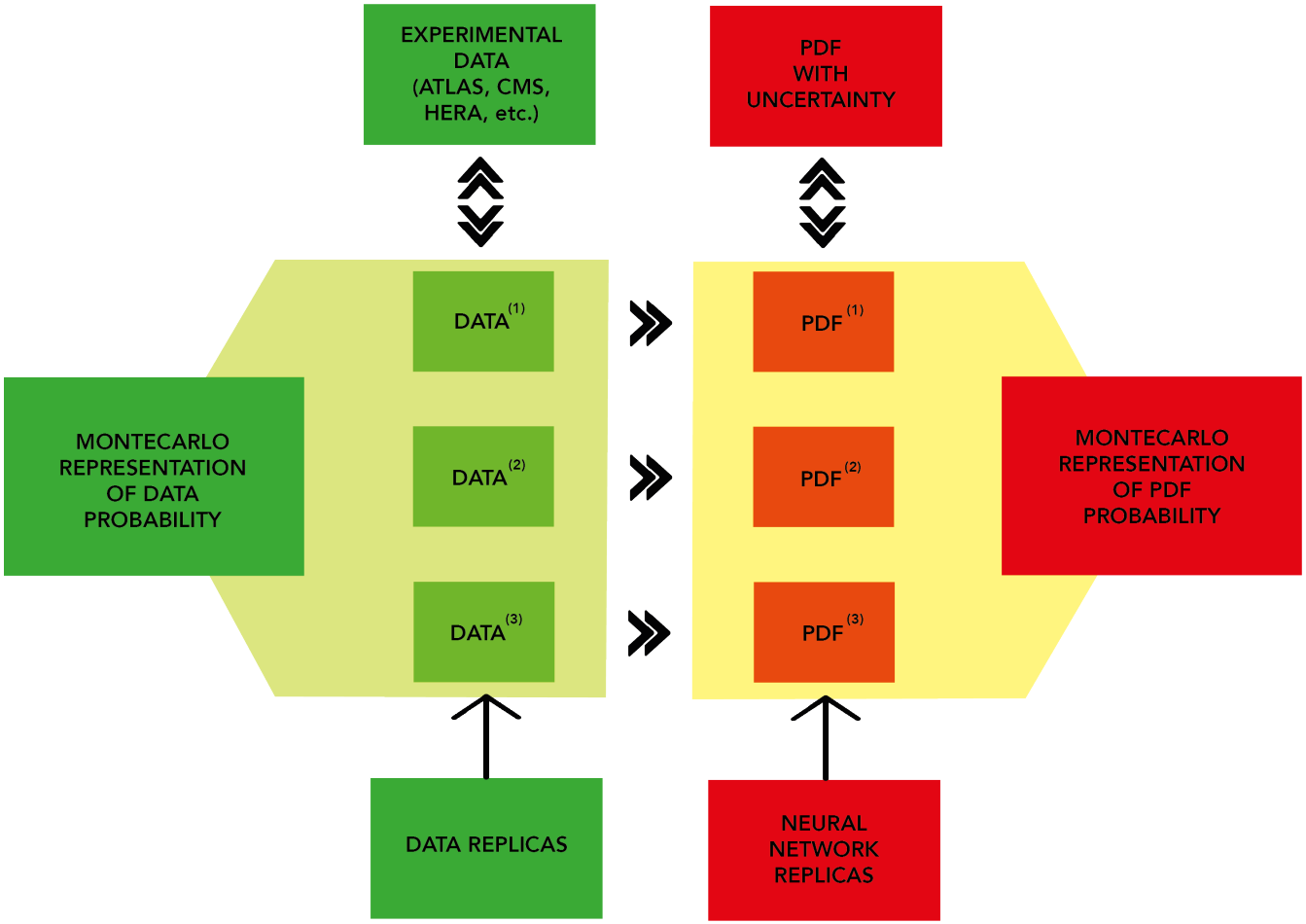
THE NNPDF METHODOLOGY

PROTON STRUCTURE AS AN AI PROBLEM:
NNPDF



THE FUNCTIONAL MONTE CARLO

REPLICA SAMPLE OF FUNCTIONS $\Leftrightarrow$ PROBABILITY DENSITY IN FUNCTION SPACE
KNOWLEDGE OF LIKELIHHOD SHAPE (FUNCTIONAL FORM) NOT NECESSARY

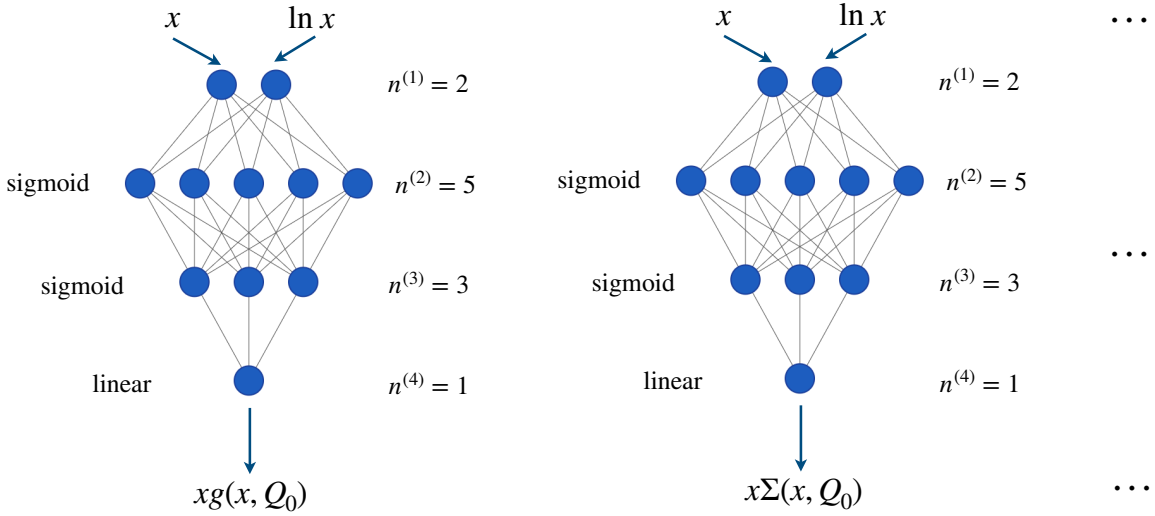


FINAL PDF SET: $f_i^{(a)}(x,\mu)$;
i =up, antiup, down, antidown, strange, antistrange, charm, gluon; $j = 1, 2, \ldots N_{\rm rep}$

OLD NNPDF (UP TP 2021)

NEURAL NETWORKS

$$f_i(x, Q_0^2) = x^{\alpha_i}(1-x)^{\beta_i} NN(x, \ln x)$$



- 37 PARAMETERS $\times$ 8 PDFS
- PREPROCESSING EXPONENTS RANDOMIZED REPLICA PER REPLICA, RANGE DETERMINED SELF-CONSISTENTLY

GENETIC MINIMIZATION

- NODAL MUTATION REPLACED POINT MUTATION
- SINGLE EPOCH WITH NO REWEIGHTING UNLIKE PREVIOUS

OPTIMAL FIT

- CROSS-VALIDATION WITH 50-50 TRAINING & VALIDATION FRACTIONS
- LOOKBACK STOPPING REPLACED THRESHOLD ON DERIVATIVE

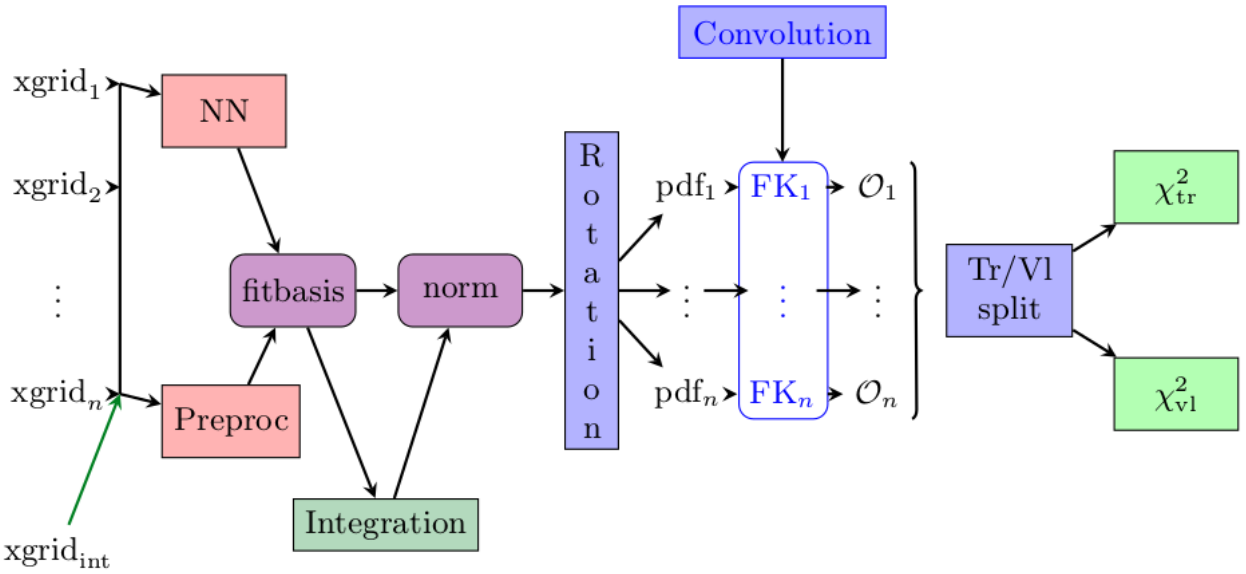
MACHINE LEARNING PDFs

LEARNING THE METHODOLOGY

THE N3FIT PROJECT

HOW DO WE KNOW THAT THE METHODOLOGY IS THE BEST?
"ACCUMULATED WISDOM" INEFFICIENT AND SLOW

CHANGE OF PHILOSOPHY ⇒ DETERMINISTIC MINIMIZATION (GRADIENT DESCENT)
GO FOR THE ABSOLUTE MINIMUM, AND (HYPER)OPTIMIZE



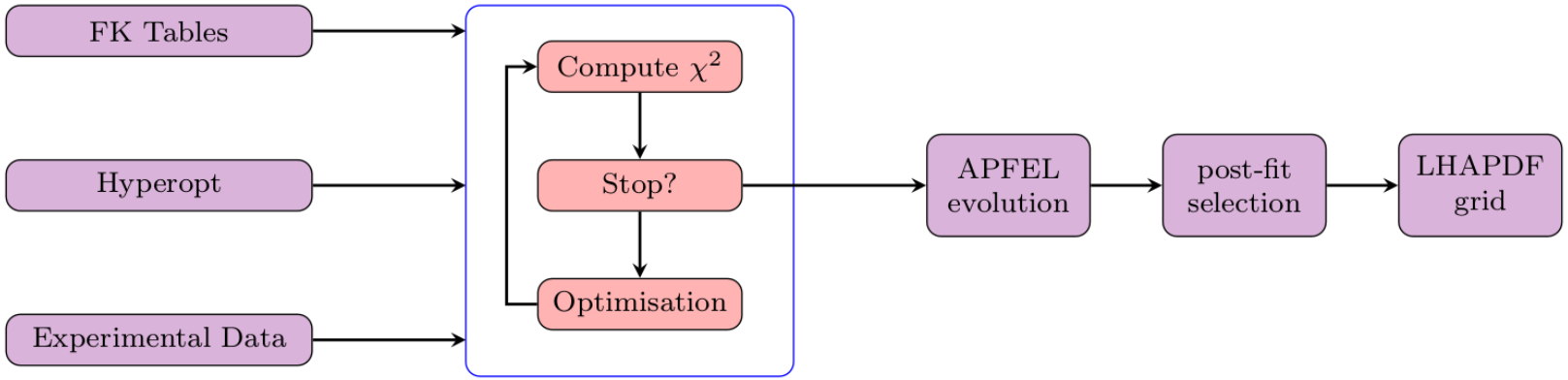
- PYTHON-BASED KERAS + TENSORFLOW FRAMEWORK
- EACH BLOCK INDEPENDENT LAYER
- CAN VARY ALL ASPECTS OF METHODOLOGY

THE NNPDF CODE STRUCTURE

- MODULAR PYTHON-BASED CODE
- HIGH DEGREE PARALLELIZATION & HARDWARE ACCELERATION

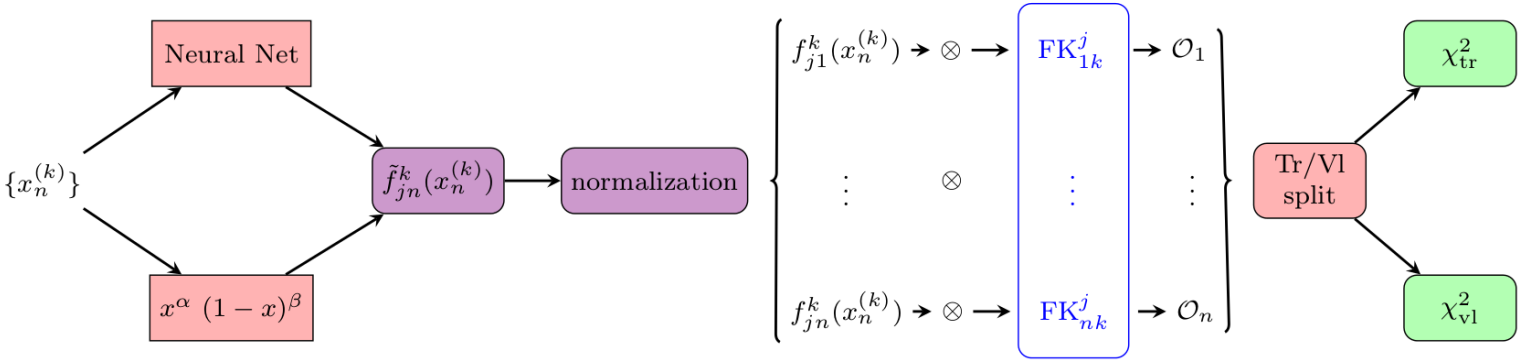
AVERAGE FITTING TIME PER REPLICA AND USE OF RESOURCES
SAME DATASET FOR OLD AND NEW METHODOLOGIES IN CPU AND GPU
CPU: INTEL(R) CORE(TM) I7-4770 AT 3.40GHZ; GPU: NVIDIA TITAN V

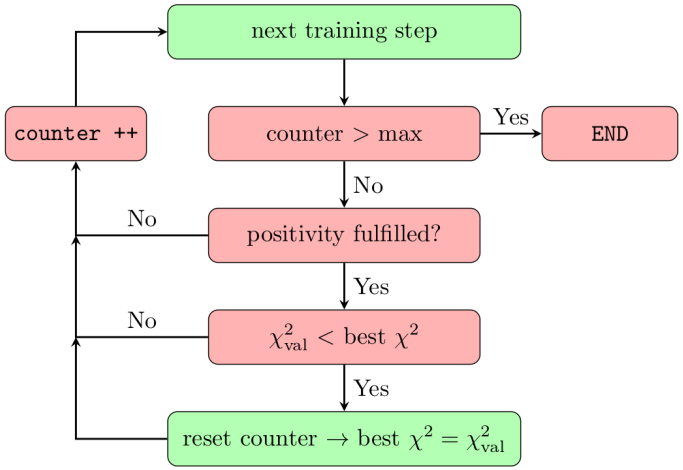
	NNPDF31 CODEBASE	NNPDF40 CODEBASE IN CPU	NNPDF40 CODEBASE IN GPU
TIME	15.2 H.	38 $\pm$ 5 MIN.	6.6 MIN.
RAM USE	1.5 GB	6.1 GB	NA



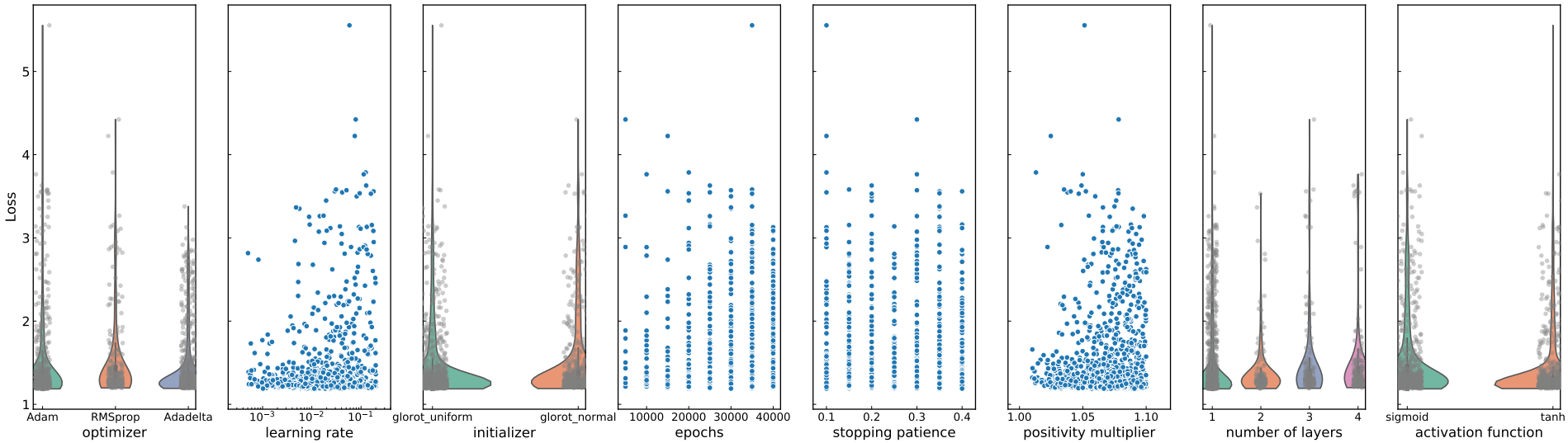
MINIMIZATION AND CROSS-VALIDATION

- DATA REPLICAS $\Rightarrow$ PDF REPLICAS
- EACH PDF REPLICA: PREPROCESSED NEURAL NET
- NEURAL NET $\Rightarrow$ OBSERVABLES
- RANDOM TRAINING-VALIDATION SPLIT, χ^2 TO TRAINING DATA REPLICAS MINIMIZED
- TRAINING STOPS IF VALIDATION χ^2 GROWS FOR A WHILE (PATIENCE)
- LOWEST VALIDATION χ^2 $\Rightarrow$ OPTIMAL FIT





FITTING THE METHODOLOGY
HYPEROPTIMIZATION SCANS



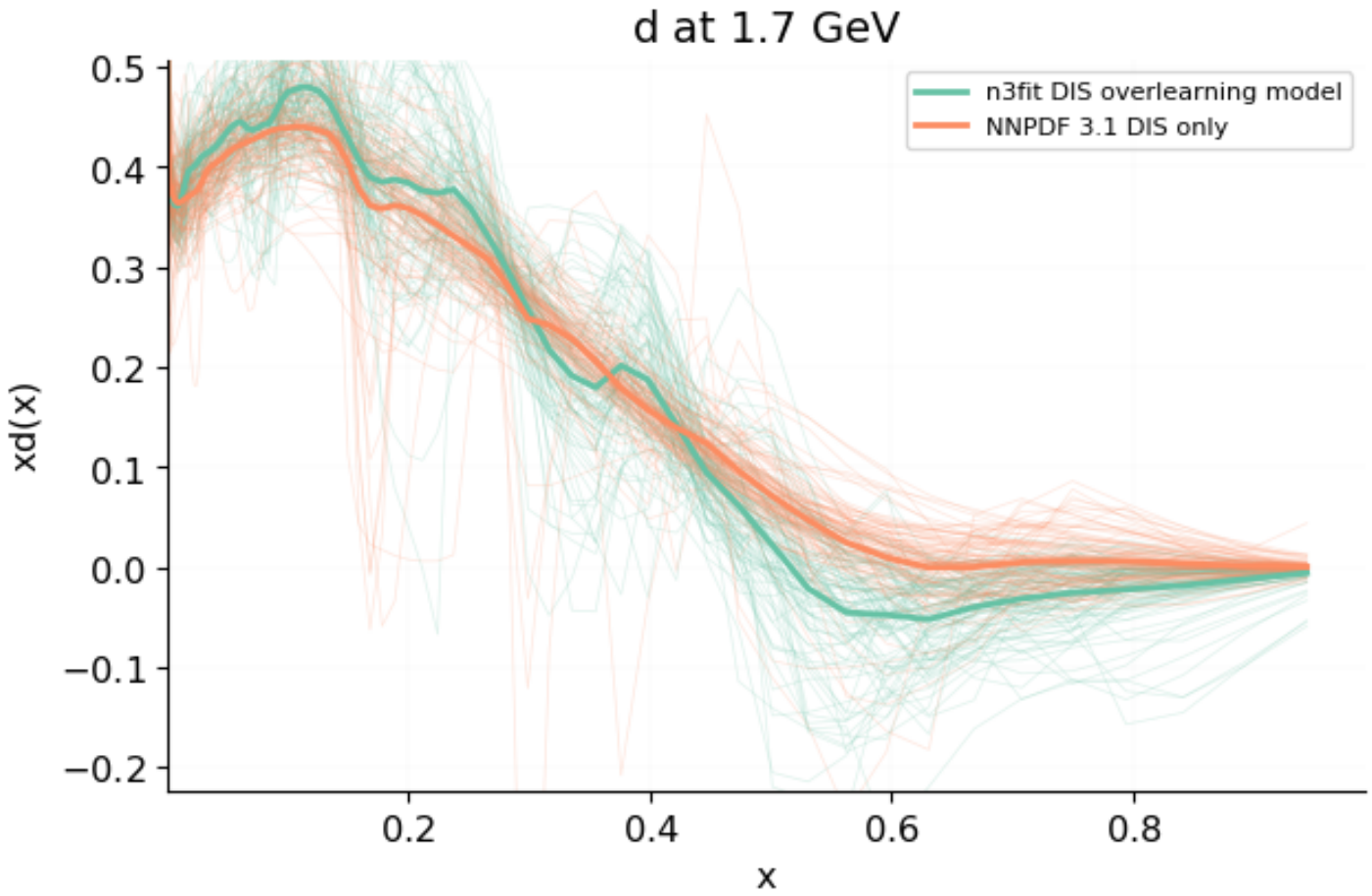
HYPEROPT PARAMETERS

Neural Network	Fit options
Number of layers (*)	Optimizer (*)
Size of each layer	Initial learning rate (*)
Dropout	Maximum number of epochs (*)
Activation functions (*)	Stopping Patience (*)
Initialization functions (*)	Positivity multiplier (*)

- SCAN PARAMETER SPACE
- OPTIMIZE FIGURE OF MERIT: VALIDATION χ^2
- BAYESIAN UPDATING

HYPEROPTIMIZATION: OVERFITTING

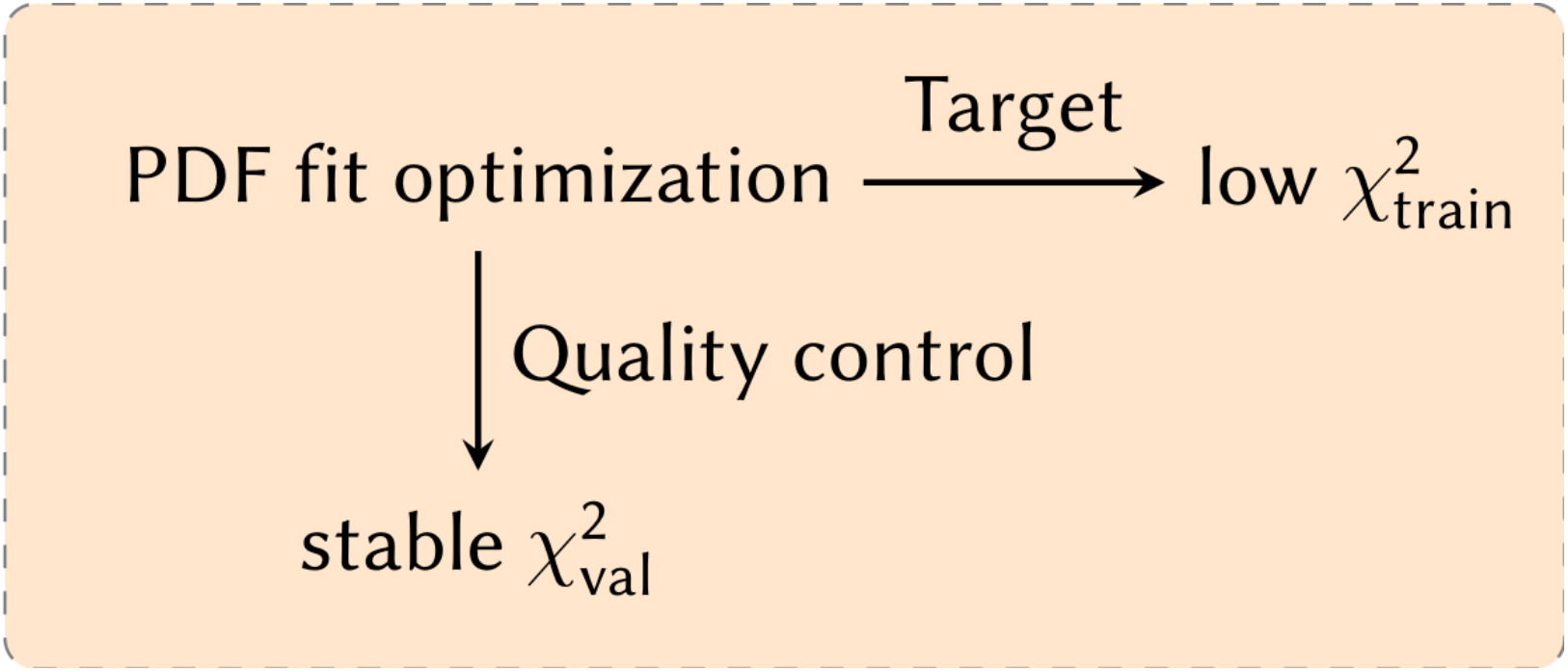
DOWN QUARK: HYPEROPTIMIZED VS. HAND-PICKED



- NOT HYPEROPTIMIZED: WIGGLES: FINITE SIZE $\Rightarrow$ WILL GO AWAY AS $N_{\rm rep}$ GROWS
- N3FIT: WIGGLY PDFS $\Leftrightarrow$ OVERFITTING $\Rightarrow$ WILL NOT GO AWAY ($\chi^2_{\rm train} \ll \chi^2_{\rm valid}$!!)

WHAT HAPPENED?

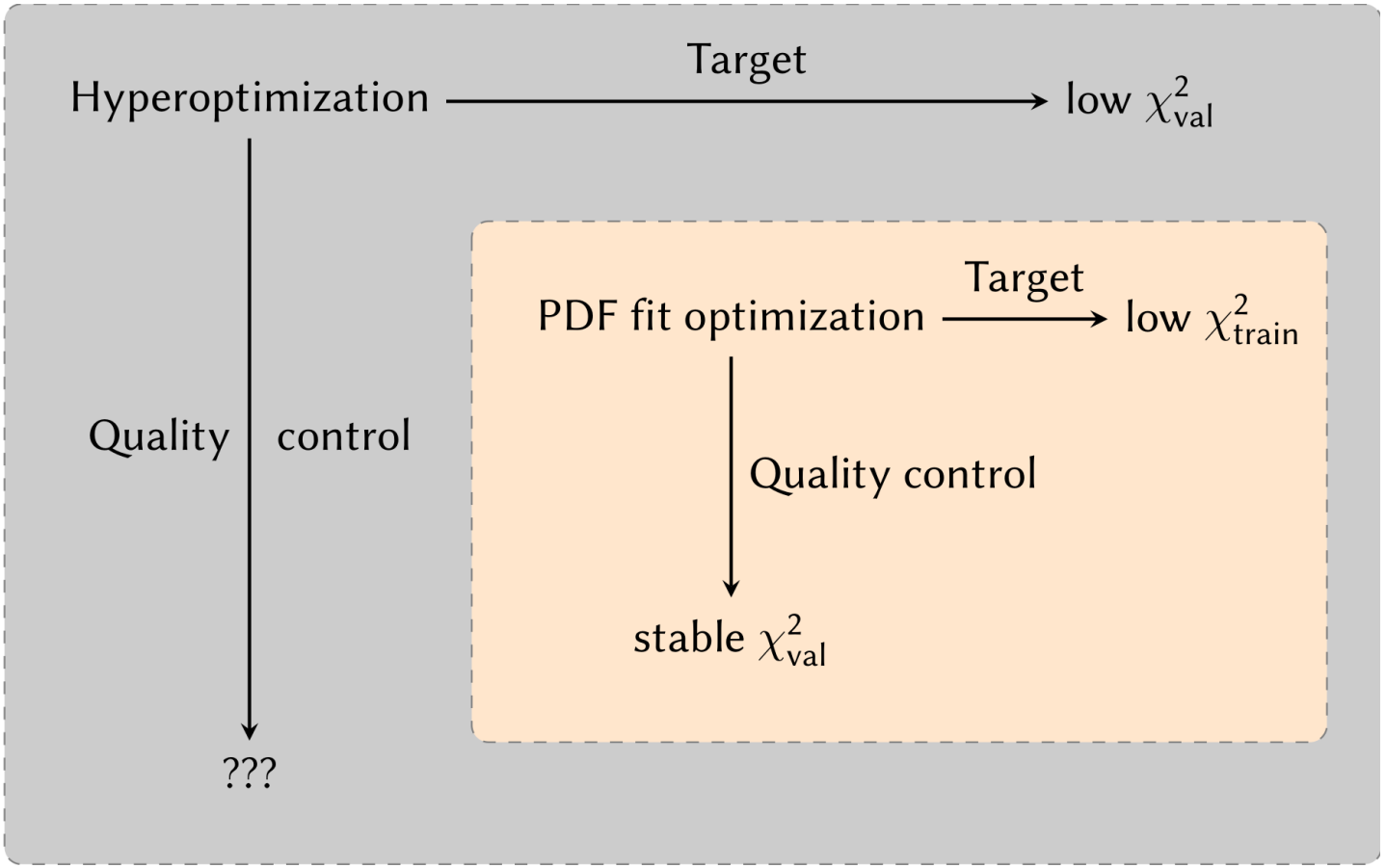
OPTIMIZATION



CROSS-VALIDATION SELECTS THE OPTIMAL MINIMUM

WHAT HAPPENED?

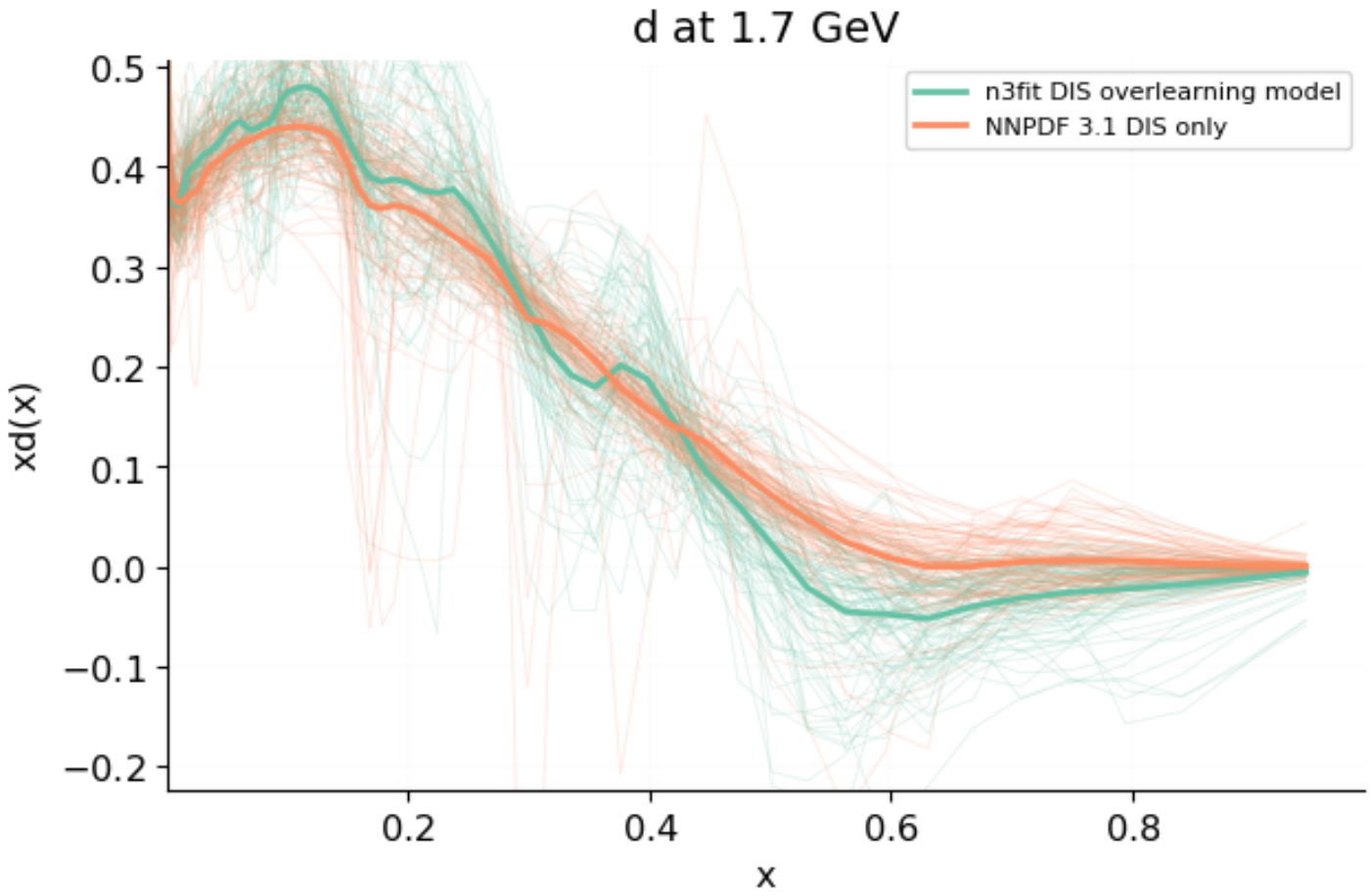
HYPEROPTIMIZATION



WE ARE MISSING A SELECTION CRITERION

HYPEROPTIMIZATION: OVERFITTING

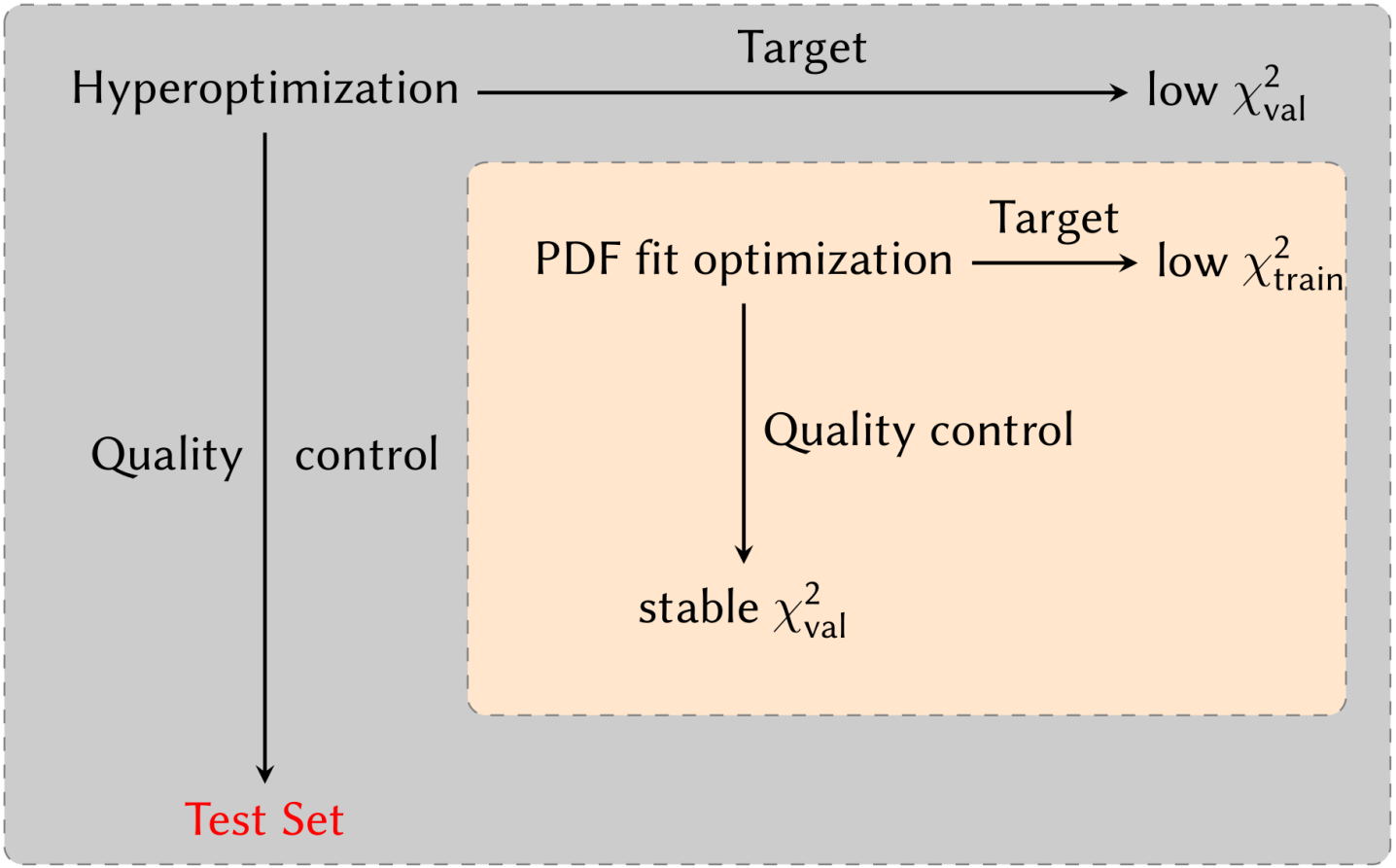
DOWN QUARK: HYPEROPTIMIZED VS. HANDPICKED



- HANDPICKED: WIGGLES: FINITE SIZE $\Rightarrow$ WILL GO AWAY AS $N_{\rm rep}$ GROWS
- N3FIT: WIGGLY PDFS $\Leftrightarrow$ OVERFITTING $\Rightarrow$ WILL NOT GO AWAY ($\chi^2_{\rm train} \ll \chi^2_{\rm valid}$!!)
- CORRELATIONS BETWEEN TRAINING AND VALIDATION DATA

THE SOLUTION

TUNED HYPEROPTIMIZATION



COMPARE TO A A TEST SET (NEW SET OF DATA PREVIOUSLY NOT USED AT AL)
TESTS GENERALIZATION POWER

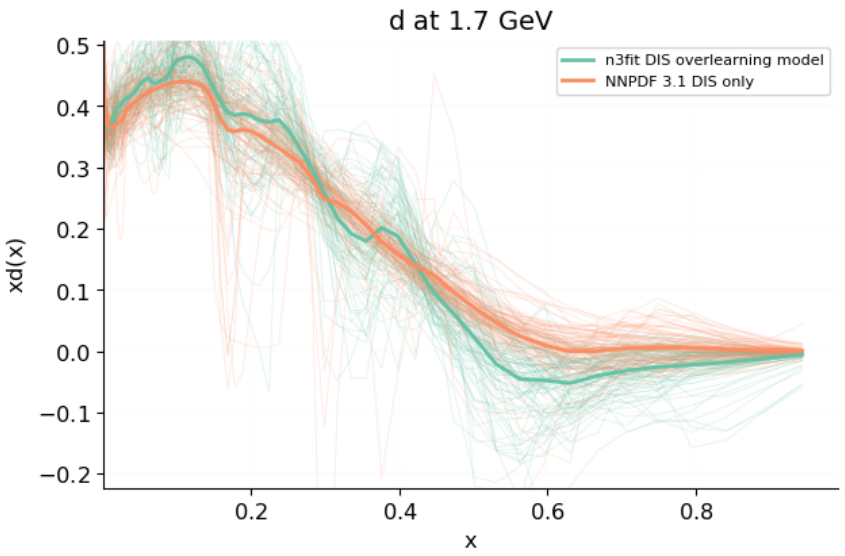
THE TEST SET METHOD

- COMPLETELY UNCORRELATED TEST SET
- OPTIMIZE ON WEIGHTED AVERAGE OF VALIDATION AND TEST
  $\Rightarrow$ NO OVERLEARNING

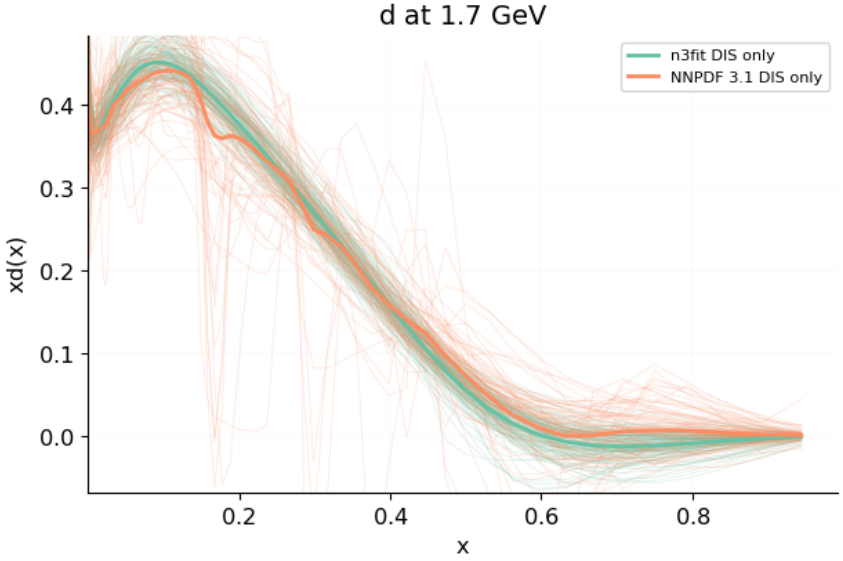
HYPEROPTIMIZED PDFS

DOWN QUARK

OVERFIT VS HANDPICKED



HYPEROPT VS HANDPICKED



- NO OVERFITTING
- COMPARED TO HANDPICKED
  - MUCH GREATER STABILITY $\Rightarrow$ FEWER REPLICAS FOR EQUAL ACCURACY
  - UNCERTAINTIES SOMEWHAT REDUCED

K-FOLDING

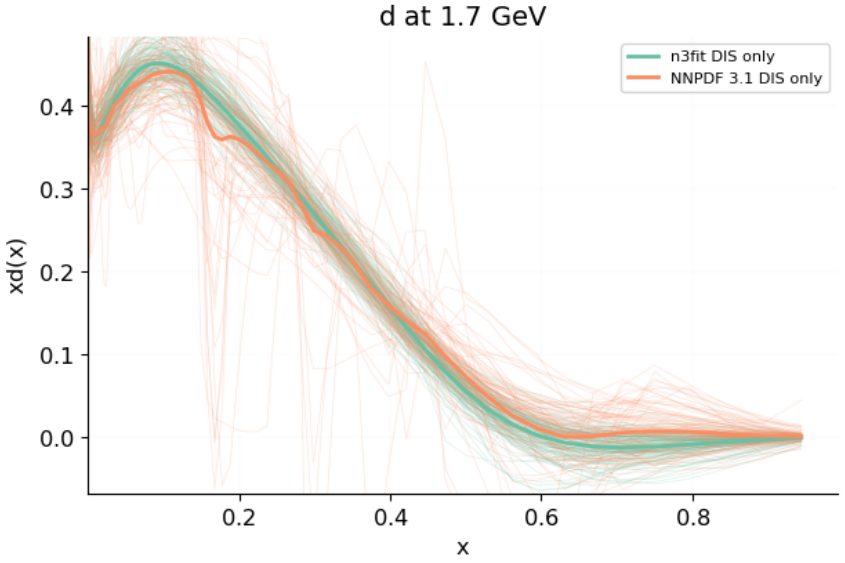
THE BASIC IDEA:

- DIVIDE THE DATA INTO n REPRESENTATIVE SUBSETS
  EACH CONTAINING PROCESS TYPES, KINEMATIC RANGE OF FULL SET
- FIT $n-1$ SETS AND USE n-TH SET AS TEST
  $\Rightarrow$ n VALUES OF $\chi^2_{\text{test, i}}$
- HYPEROPTIMIZE ON NON FITTED $\chi^2_{\text{test, i}}$
  $\rightarrow$ GOOD & STABLE GENERALIZATION

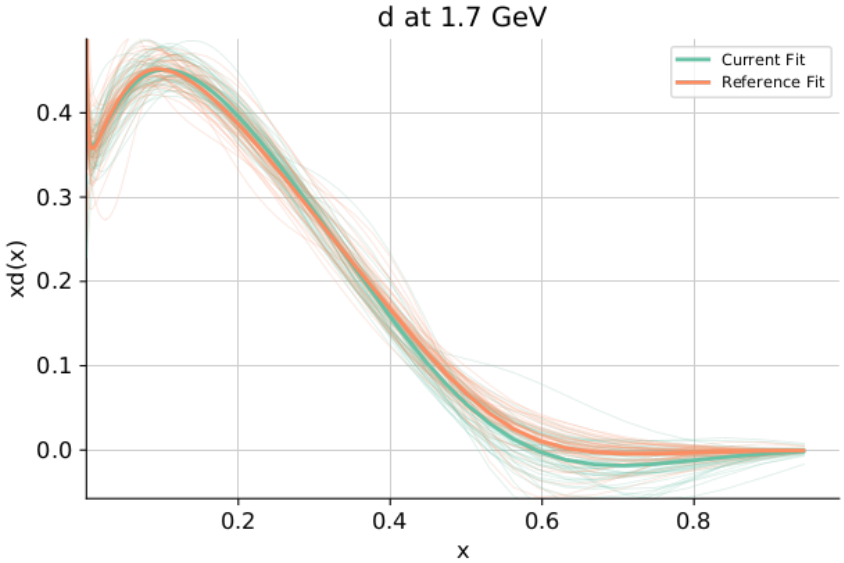
FOLDED PDFS

DOWN QUARK

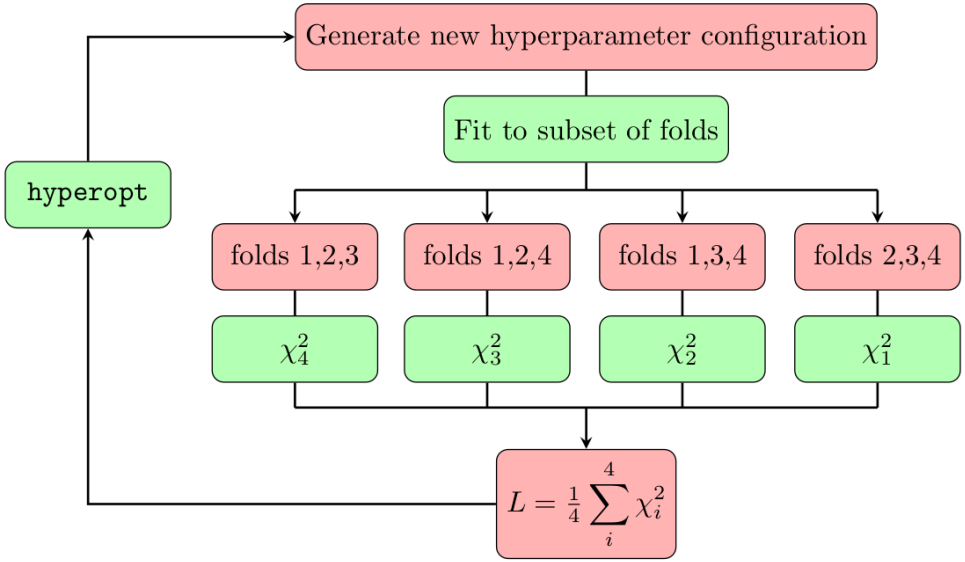
TEST-SET HYPER VS HANDPICKED



K-FOLD HYPER VS. TEST-SEY HYPER



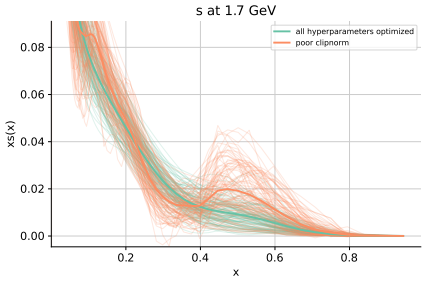
K-FOLDING IMPLEMENTATION



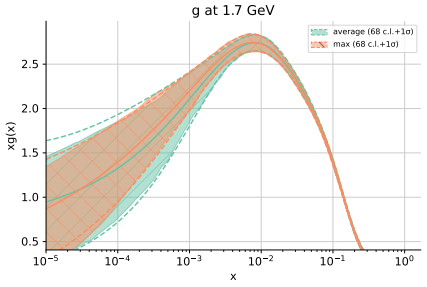
Fold 1		
CHORUS σ^{ν}_{CC}	HERA I+II inc NC e^+p 920 GeV	BCDMS p
LHCb Z 940 pb	ATLAS W,Z 7 TeV 2010	CMS Z p_T 8 TeV (p^{ll}_T, y_{ll})
DY E605 $\sigma^p_{\rm DY}$	CMS Drell-Yan 2D 7 TeV 2011	CMS 3D dijets 8 TeV
ATLAS single-t y (normalised)	ATLAS single top R_t 7 TeV	CMS $t\bar{t}$ rapidity $y_{t\bar{t}}$
CMS single top R_t 8 TeV		
Fold 2		
HERA I+II inc CC e^-p	HERA I+II inc NC e^+p 460 GeV	HERA comb. $\sigma^{\rm red}_{b\bar{b}}$
NMC p	NuTeV σ^{ν}_c	LHCb $Z \to ee$ 2 fb
CMS W asymmetry 840 pb	ATLAS Z p_T 8 TeV (p^{ll}_T, M_{ll})	D0 $W \to \mu\nu$ asymmetry
DY E886 $\sigma^p_{\rm DY}$	ATLAS direct photon 13 TeV	ATLAS dijets 7 TeV, R=0.6
ATLAS single antitop y (normalised)	CMS $\sigma^{\rm tot}_{t\bar{t}}$	CMS single top $\sigma_t + \sigma_{\bar{t}}$ 7 TeV
Fold 3		
HERA I+II inc CC e^+p	HERA I+II inc NC e^+p 575 GeV	NMC d/p
NuTeV σ^{ν}_c	LHCb $W,Z \to \mu$ 7 TeV	LHCb $Z \to ee$
ATLAS W,Z 7 TeV 2011 Central selection	ATLAS W^++jet 8 TeV	ATLAS HM DY 7 TeV
CMS W asymmetry 4.7 fb	DYE 866 $\sigma^d_{\rm DY}/\sigma^p_{\rm DY}$	CDF Z rapidity (new)
ATLAS $\sigma^{\rm tot}_{t\bar{t}}$	ATLAS single top y_t (normalised)	CMS $\sigma^{\rm tot}_{t\bar{t}}$ 5 TeV
CMS $t\bar{t}$ double diff. $(m_{t\bar{t}}, y_t)$		
Fold 4		
CHORUS σ^{p}_{CC}	HERA I+II inc NC e^+p 820 GeV	LHCb $W,Z \to \mu$ 8 TeV
LHCb $Z \to \mu\mu$	ATLAS W,Z 7 TeV 2011 Fwd	ATLAS W^-+jet 8 TeV
ATLAS low-mass DY 2011	ATLAS Z p_T 8 TeV (p^{ll}_T, y_{ll})	CMS W rapidity 8 TeV
D0 Z rapidity	CMS dijets 7 TeV	ATLAS single top y_t (normalised)
ATLAS single top R_t 13 TeV	CMS single top R_t 13 TeV	

- EACH FOLD REPRODUCES FEATURES OF FULL DATASET
- DIFFERENT CHOICES POSSIBLE FOR LOSS (NON-FITTED)
  - BEST WORST
  - BEST AVERAGE
- RESULTS STABLE

NO K-FOLDING



K-FOLDING VARIATION

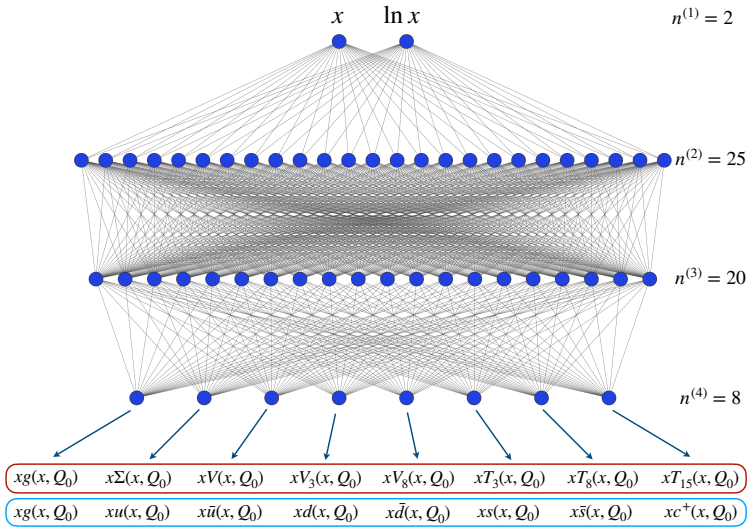


THE ML METHODOLOGY

HYPEROPTIMIZED PARAMETERS

Parameter	NNPDF4.0	L as in Eq. (3.21)	Flavour basis Eq. (3.2)
Architecture	25-20-8	70-50-8	7-26-27-8
Activation function	hyperbolic tangent	hyperbolic tangent	sigmoid
Initializer	`glorot_normal`	`glorot_uniform`	`glorot_normal`
Optimizer	`Nadam`	`Adadelta`	`Nadam`
Clipnorm	6.0×10^{-6}	5.2×10^{-2}	2.3×10^{-5}
Learning rate	2.6×10^{-3}	2.5×10^{-1}	2.6×10^{-3}
Maximum # epochs	17×10^{3}	45×10^{3}	45×10^{3}
Stopping patience	10% of max epochs	12% of max epochs	16% of max epochs
Initial positivity $\Lambda^{(\mathrm{pos})}$	185	106	2
Initial integrability $\Lambda^{(\mathrm{int})}$	10	10	10

NN ARCHITECTURE



- HYPEROPT ADAPTS TO EXTERNAL CHOICES (E.G. PARAMETRIZATION BASIS)
- SIMILAR RESULTS CAN BE OBTAINED WITH RATHER DIFFERENT SETTINGS
- $\sim$ 800 FREE PARAMETERS

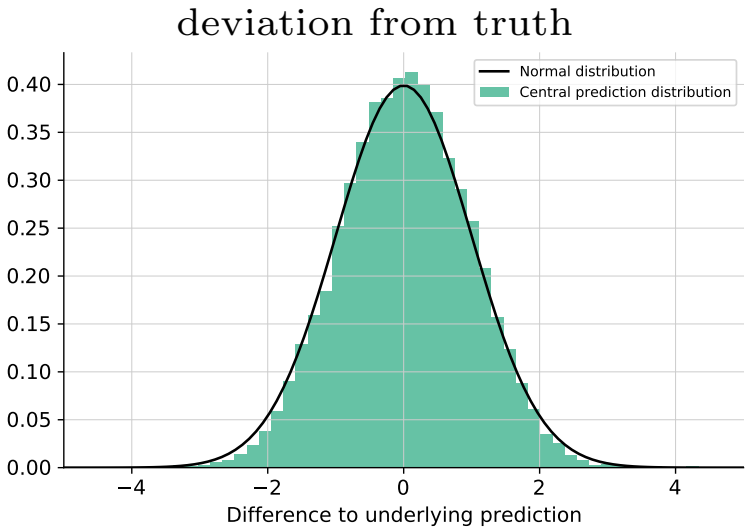
VALIDATION

CLOSURE TESTS

FAITHFUL UNCERTAINTIES IN DATA REGION?

- ASSUME "TRUE" UNDERLYING PDF $\Rightarrow$ E.G. SOME RANDOM PDF REPLICA
- GENERATE DATA DISTRIBUTED ACCORDING TO EXPERIMENTAL COVARIANCE MATRIX
- RUN WHOLE METHDOLOGY ON THESE DATA
- DO STATISTICS ON "RUNS OF THE UNIVERSE", POSSIBLE THANKS TO EFFICIENT METHDOLOGY: COMPARE TO TRUE PDFS, OR TO TRUE VALUES OF OBSERVABLES (NOT FITTED)
  - BIAS/VARIANCE: MEAN SQUARE DEVIATION WR TO TRUTH VS UNCERTAINTY
  - IS TRUTH WITHIN ONE SIGMA 68% OF TIMES?

RESULTS



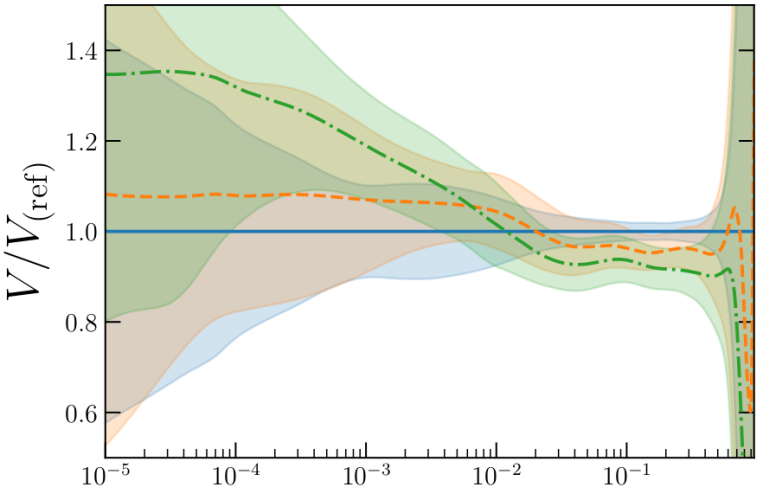
Dataset	$\sqrt{\text{bias/variance}}$	$\xi_{1\sigma}^{(\text{data})}$
DY	0.99 ± 0.08	0.69 ± 0.02
Top-pair	0.75 ± 0.06	0.75 ± 0.03
Jets	1.14 ± 0.05	0.63 ± 0.03
Dijets	0.99 ± 0.07	0.70 ± 0.03
Direct photon	0.71 ± 0.06	0.81 ± 0.03
Single top	0.87 ± 0.07	0.69 ± 0.04
Total	1.03 ± 0.05	0.68 ± 0.02

FUTURE TESTS

FAITHFUL UNCERTAINTIES IN EXTRAPOLATION?

- DETERMINE PDFs FROM A SUBSET OF CURRENT DATA: "PRE-HERA", "PRE-LHC",...
- COMPUTE χ^2 TO THE FULL CURRENT DATASET:
  - WITHOUT PDF UNCERTAINTIES $\Rightarrow$ IF $\gg 1$, MISSING INFORMATION
  - WITH PDF UNCERTAINTY $\Rightarrow$ IF ~ 1, MISSING INFO REPRODUCED BY UNCERTAINTY

VALENCE: PRE-HERA VS PRE-LHC VS NNPDF4.0



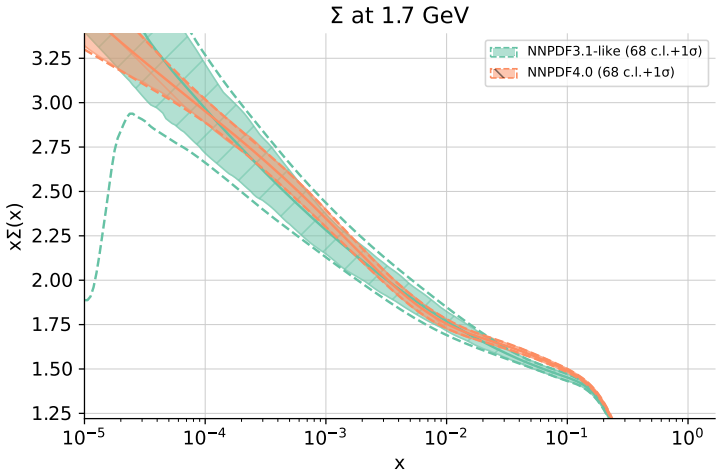
χ^2 WITHOUT/**WITH PDF UNC.**

PROCESS	PRE-HERA	PRE-LHC	3.1-LIKE	4.0-GLOB
FT DIS (NC)	1.04	1.17	1.17	1.26
FT DIS (CC)	0.80	0.86	0.88	0.90
FT DY	0.93	1.27	1.43	1.59
HERA	24.01/**1.12**	1.22	1.21	1.21
COLL. DY (TEV.)	5.31/**1.08**	0.96	0.95	1.13
COLL. DY (LHC)	15.50/**1.37**	2.64/**1.54**	1.39	1.54
TOP QUARK	23.35/**1.08**	1.29/**0.86**	0.82	0.98
JETS	6.18/**1.21**	3.66/**1.29**	2.07/**1.37**	1.26
TOTAL	9.70	1.44	1.22	1.17

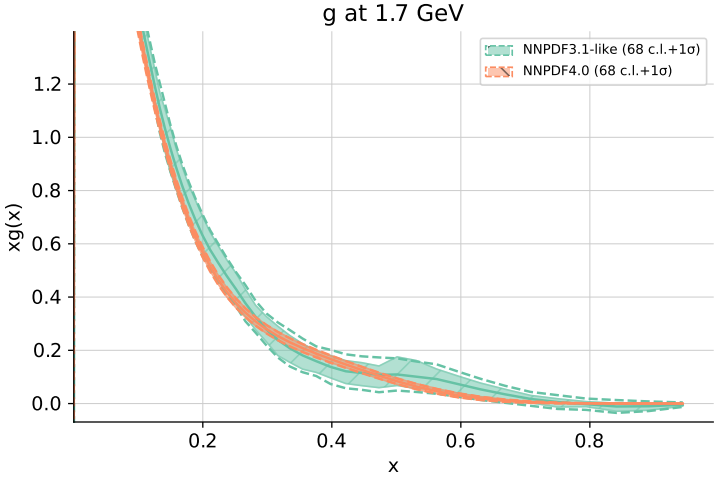
NNPDF4.0 vs. NNPDF3.1

- FULL BACKWARD COMPATIBILITY
- SUBSTANTIAL REDUCTION IN UNCERTAINTY

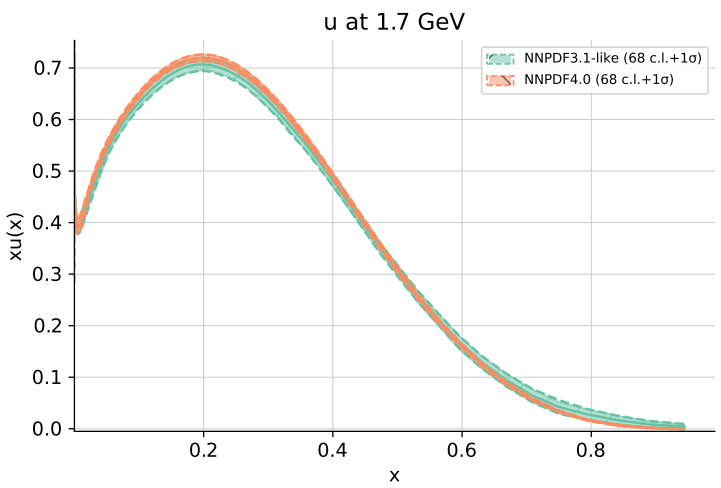
SINGLET



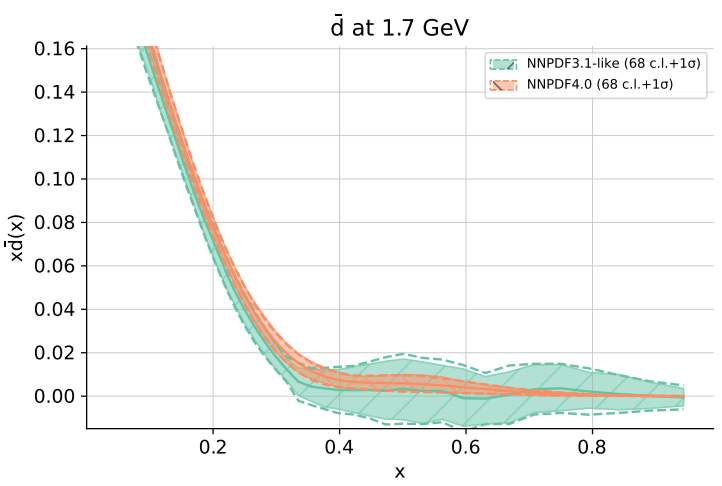
GLUON



UP



ANTIDOWN

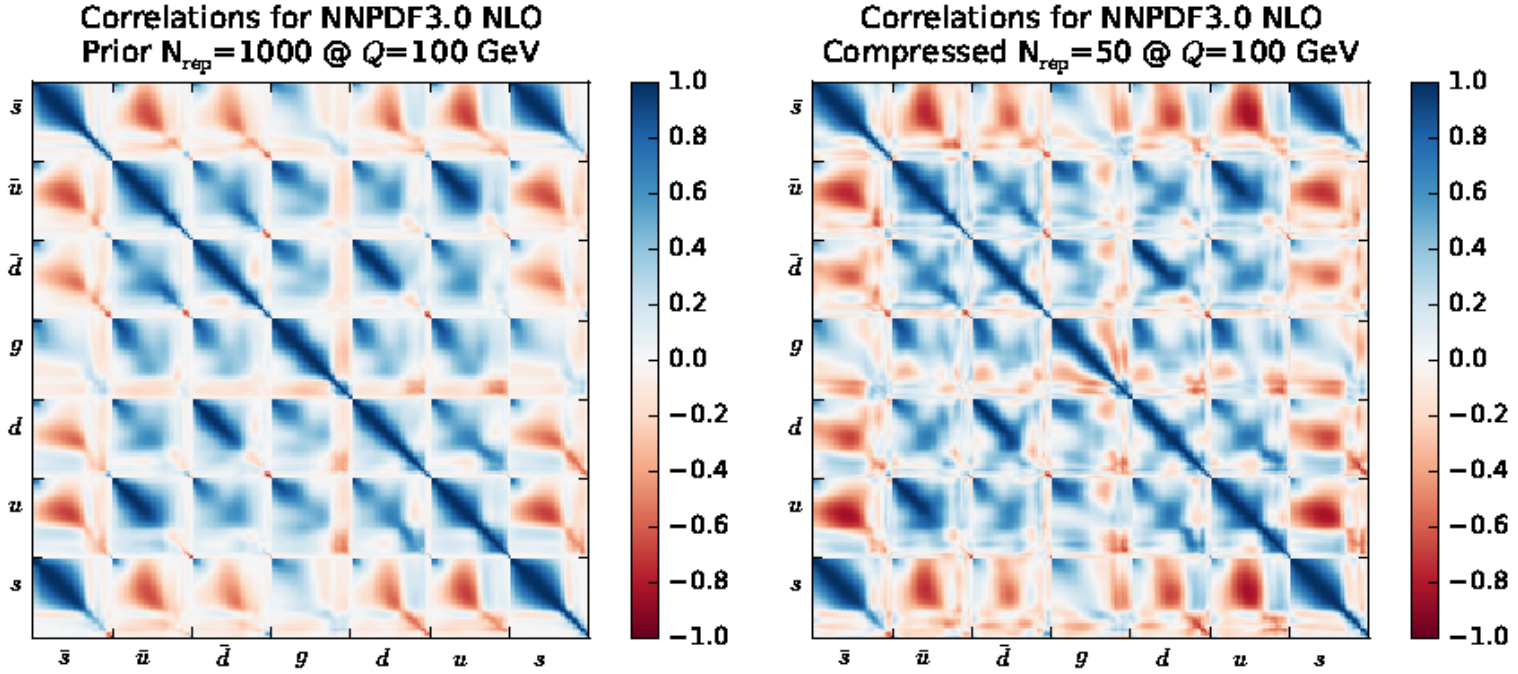


DELIVERY

MONTECARLO COMPRESSION

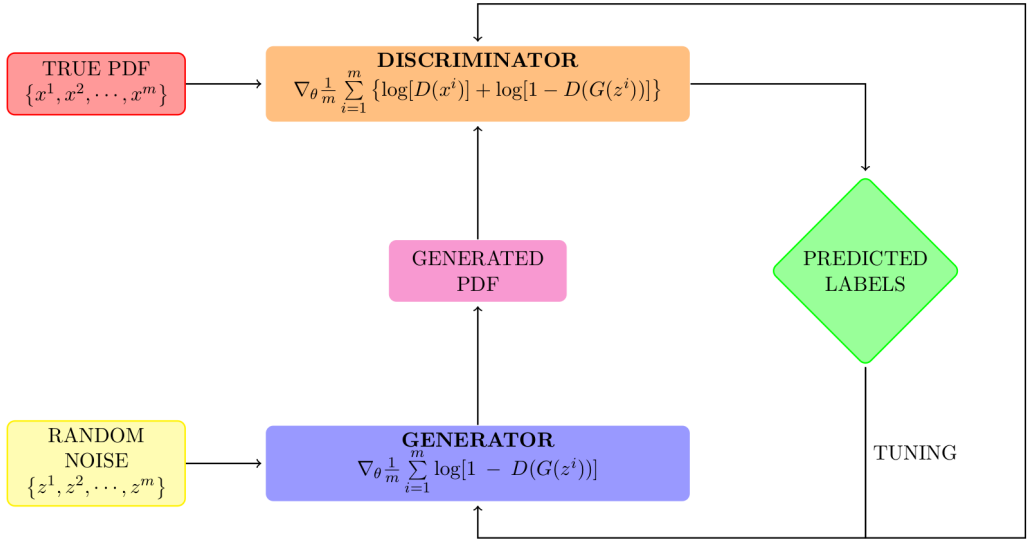
CAN WE REDUCE THE NUMBER OF REPLICAS?

- START WITH LARGE REPLICA SAMPLE
- SELECT BY GENETIC ALGORITHM SUBSET OF REPLICAS $\Rightarrow$ STATISTICAL FEATURES OPTIMIZED TO PRIOR
- MINIMIZE LOSS: DIFFEREMCE OF MOMENTS, KL DIVERGENCE, . . .
- 50 COMPRESSED REPLICA REPRODUCE 1000 REPLICA SET TO PRECENT ACCURACY



GAN ENHANCEMENT

CAN WE FURTHER REDUCE THE NUMBER OF COMPRESSED REPLICAS WITHOUT LOSS OF INFORMATION? GENERATIVE ADVERSARIAL NETWORKS

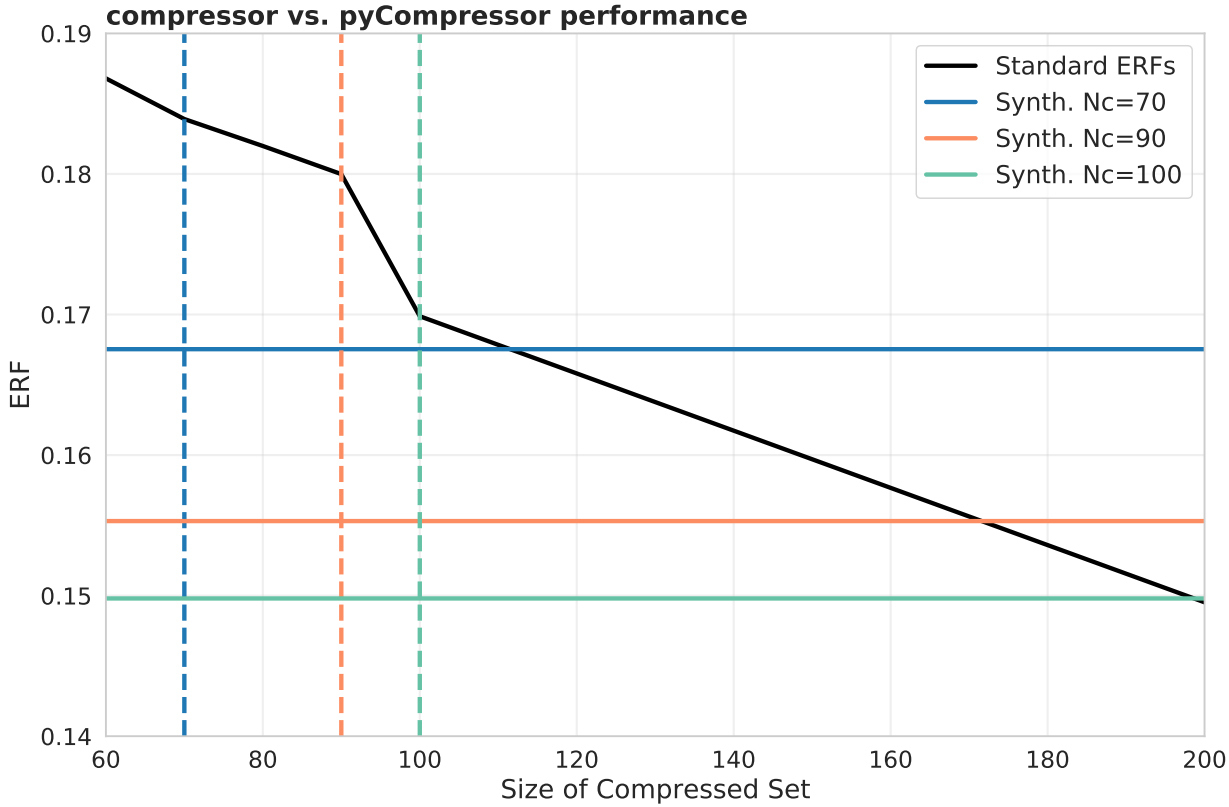


- TRAIN A NETWORK TO SIMULATE THE TRUE DISTRIBUTION (GENERATOR)
- TRAIN A NETWORK TO DISCRIMINATE TRUTH FROM SIMULATION (DISCRIMINATOR)
- TRAIN THE GENERATOR TO TRICK THE DISCRIMINATOR

GAN ENHANCEMENT

- ENHANCE THE STARTING PDF SET BY ADDING GAN-PDFS TO IT
- PERFORM COMPRESSION OF THE ENHANCED SET

PERFORMANCE



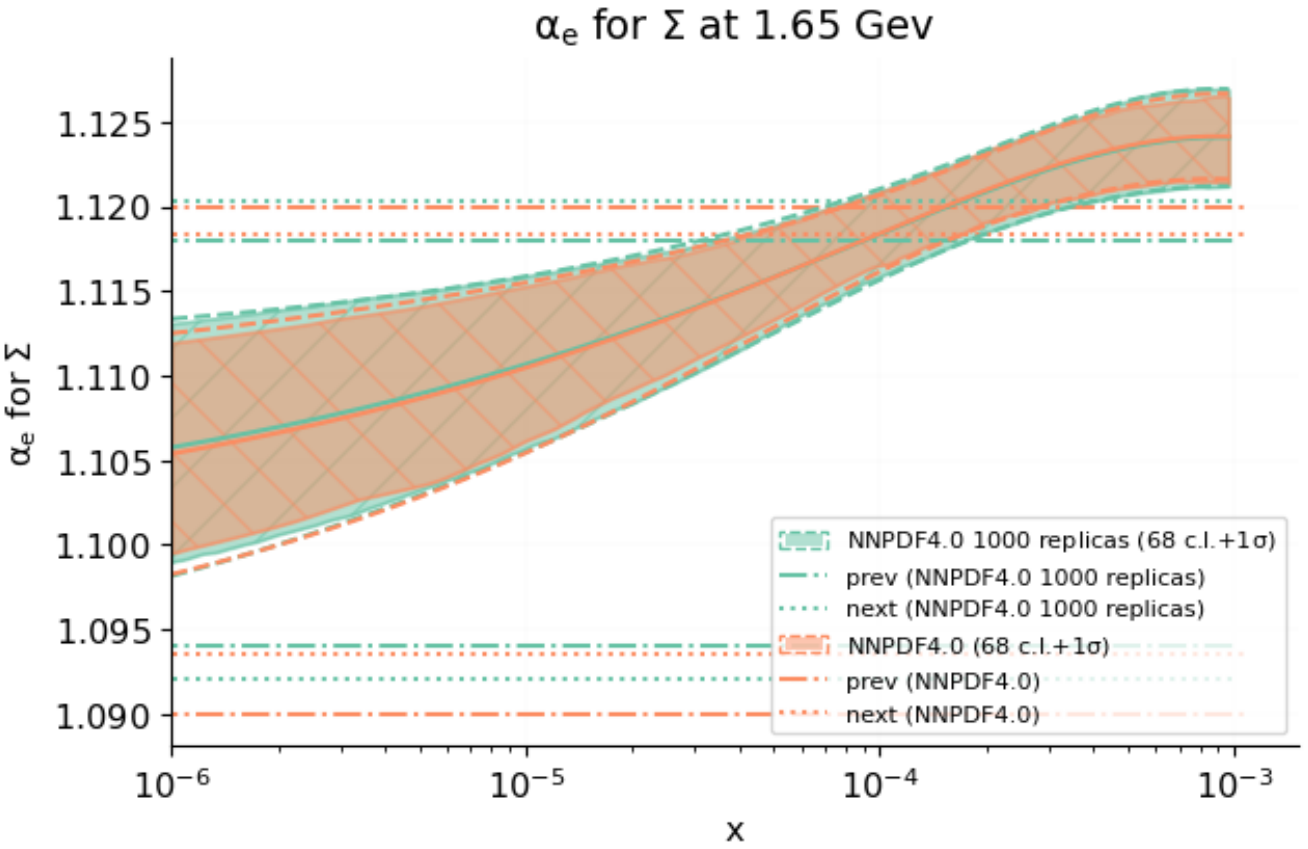
ENHANCED: NUMBER OF REPLICAS CUT IN HALF FOR SAME TARGET ACCURACY

NEW IDEAS

PREPROCESSING

- PDF EQUAL TO PREPROCESSED NN: $f_i = x^{\alpha_i}(1-x)^{\beta}_i NN(i, x, \ln x)$
- PREPROCESSING EXPONENTS α_i, β_i VARIED RANDOMLY REPLICA BY REPLICA
- RANGE OF VARIATION DETERMINED SELF-CONSISTENTLY
- PDF TAKES x, $\ln x$ AS INPUTS

QUARK SINGLET EFFECTIVE α

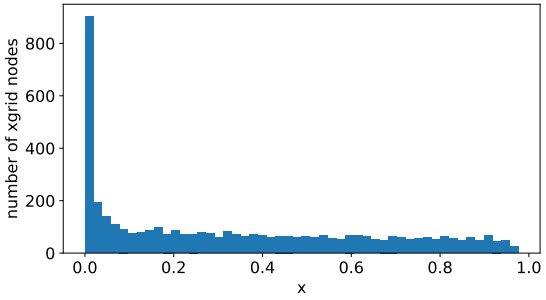


- NEED TO ITERATE FITS
- POSSIBLE SOURCE OF BIAS?

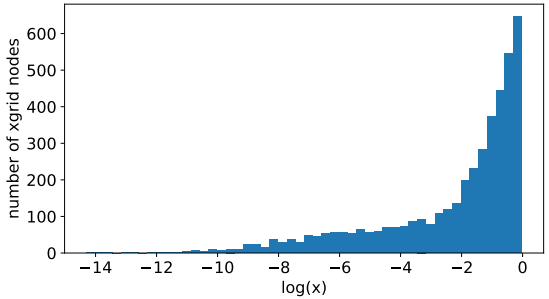
FEATURE SCALING

INPUT NODE DISTRIBUTION

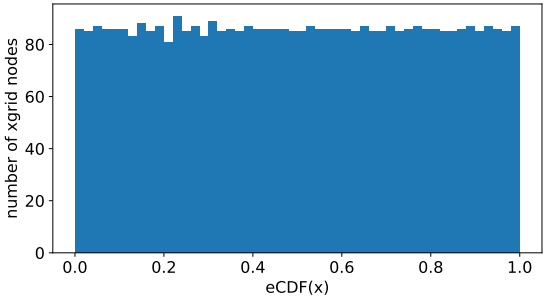
x DISTN



$\ln x$ DISTN



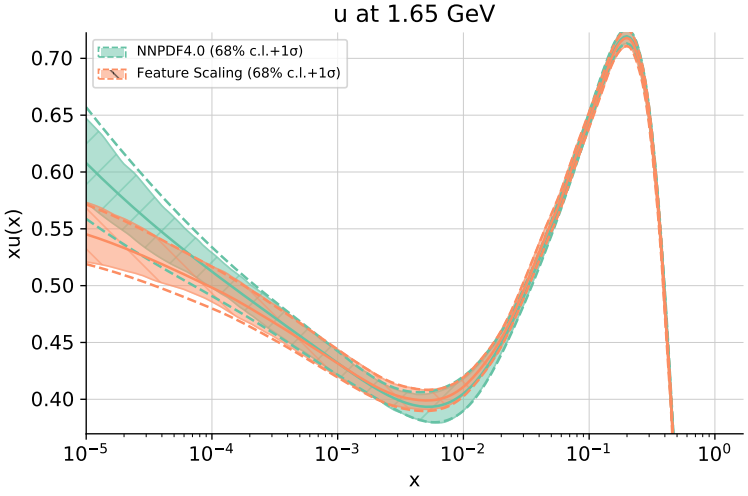
eCDF DISTN



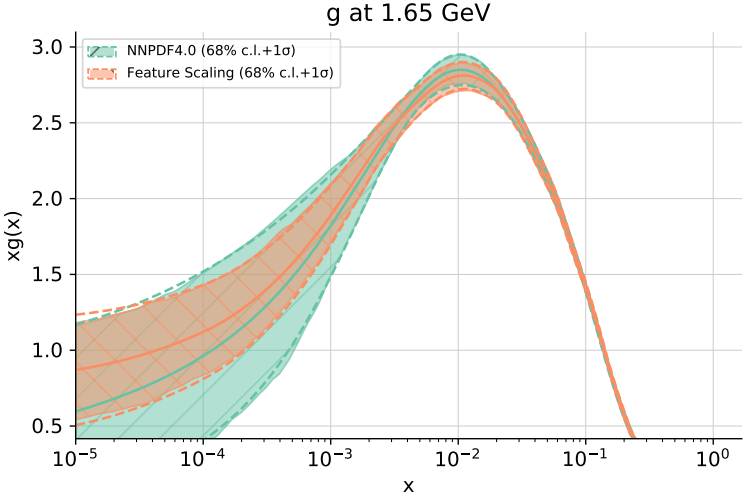
- RESCALE $\Rightarrow$ UNIFORMLY DISTRIBUTED INPUT (eCDF+INTERPOLATION)
- RERUN]BLUE HYPEROPT
- ONLY ONE INPUT NEEDED

STANDARD VS. FEATURE SCALING

UP



GLUON

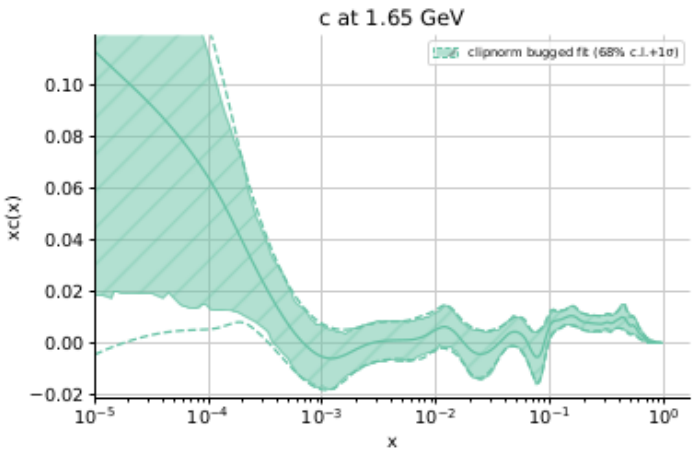


OVERFITTING IN HYPEROPT

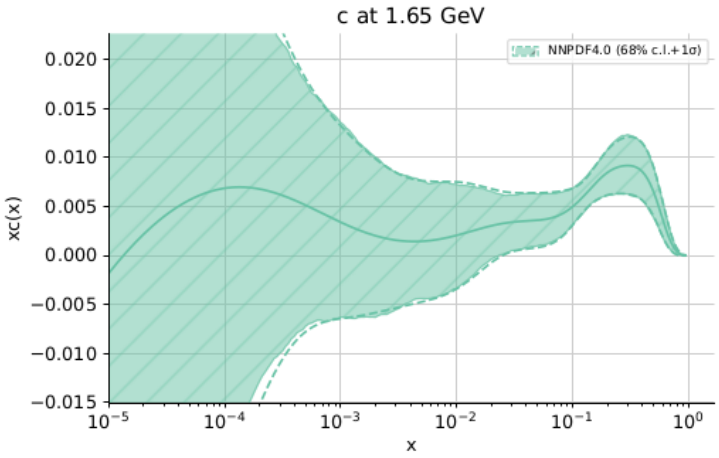
- HYPEROPT $\Rightarrow$ OVERFITTING?
- WHAT IS AN "UNNATURAL" PDF?

CHARM PDF

OVERFIT (NO CLIPNORM)



PROPER FIT (NNPDF4.0)

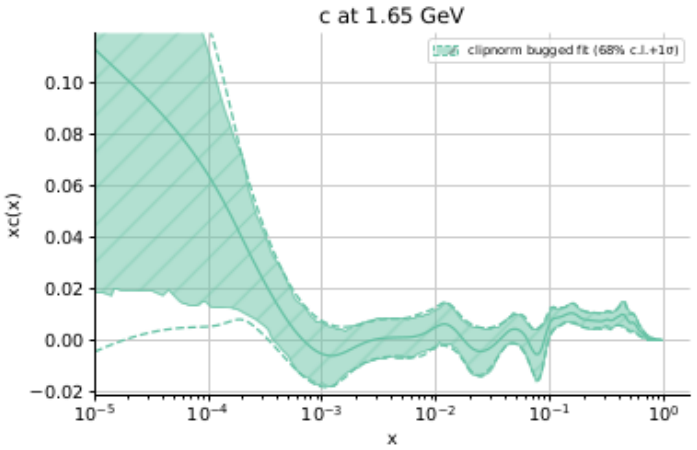


OVERFITTING METRIC

- RECOMPUTE VALIDATION χ^2
  - SAME TRAINING-VALIDATION SPLIT
  - DIFFERENT FLUCTUATED VALIDATION DATA
- COMPUTE AVERAGE χ^2 & DETERMINE DIFFERENCE TO VALIDATION $\mathcal{R}_O = \langle \chi^2_{\rm val} - \chi^2_{\rm val'} \rangle$ (OVERFITNESS)
- NEGATIVE OVERFITNESS $\mathcal{R}_O \Rightarrow$ OVERFIT

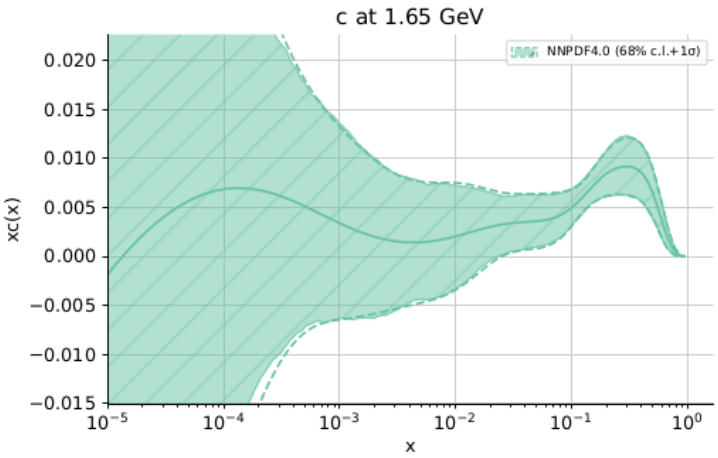
CHARM PDF

OVERFIT (NO CLIPNORM)



$\mathcal{R}_O = -0.024 \pm 0.012$

PROPER FIT (NNPDF4.0)



$\mathcal{R}_O = -0.001 \pm 0.013$

FOOD FOR THOUGHT

- OPTIMIZED FOLDS
- OVERFITTING AND UNDERFITTING METRICS IN HYPEROPT
- HYPEROPT ON FUTURE TESTS
- BEYOND NEURAL NETS

AN OPEN SOURCE CODE!

- THE FULL NNPDF CODE IS PUBLIC!
- INCLUDING HYPEROPTIMIZATION, EVOLUTION, THEORY, FITTING, VISUALIZATION
- FULLY DOCUMENTED CODE
- LINKS TO CODE (GITHUB), DOCUMENENTATION, INSTALLATION BINARY PACKAGES AVAILABLE FROM
  `http://nnpdf.mi.infn.it/nnpdf-open-source-code/`

`https://arxiv.org/abs/2109.02671`

An open-source machine learning framework for global analyses of parton distributions

The NNPDF Collaboration: Richard D. Ball · Stefano Carrazza · Juan Cruz-Martinez · Luigi Del Debbio · Stefano Forte · Tommaso Giani · Shayan Iranipour · Zahari Kassabov · Jose I. Latorre · Emanuele R. Nocera · Rosalyn L. Pearson · Juan Rojo · Roy Stegeman · Christopher Schwan · Maria Ubiali · Cameron Voisey · Michael Wilson

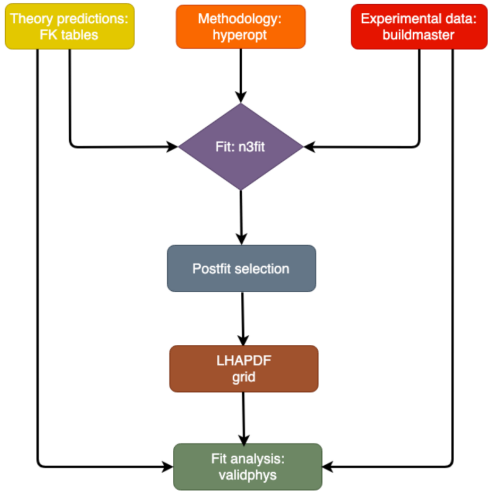


Fig. 2.1. Workflow for an NNPDF fit

THE WORK OF MANY PEOPLE

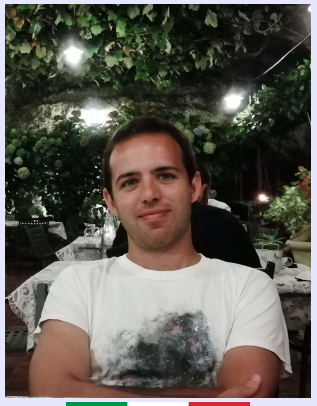
NNPDF collaboration and N^{3}PDF team meeting,
Gargnano, Italy, September 2021

N^{3}PDF

N3PDF
Machine Learning • PDFs • QCD

A. Barontini

A. Candido



S. Carrazza

J. Cruz Martinez

F. Hekhorn

K. Kudashkin

N. Laurenti

T. Rabemananjara

C. Schwan

R. Stegeman