PDFs WITH 1% ACCURACY

STEFANO FORTE
UNIVERSITÀ DI MILANO & INFN

IRN TERASCALE MEETING

LPC-CLERMONT, NOV. 22, 2021

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

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THE NNPDF COLLABORATION

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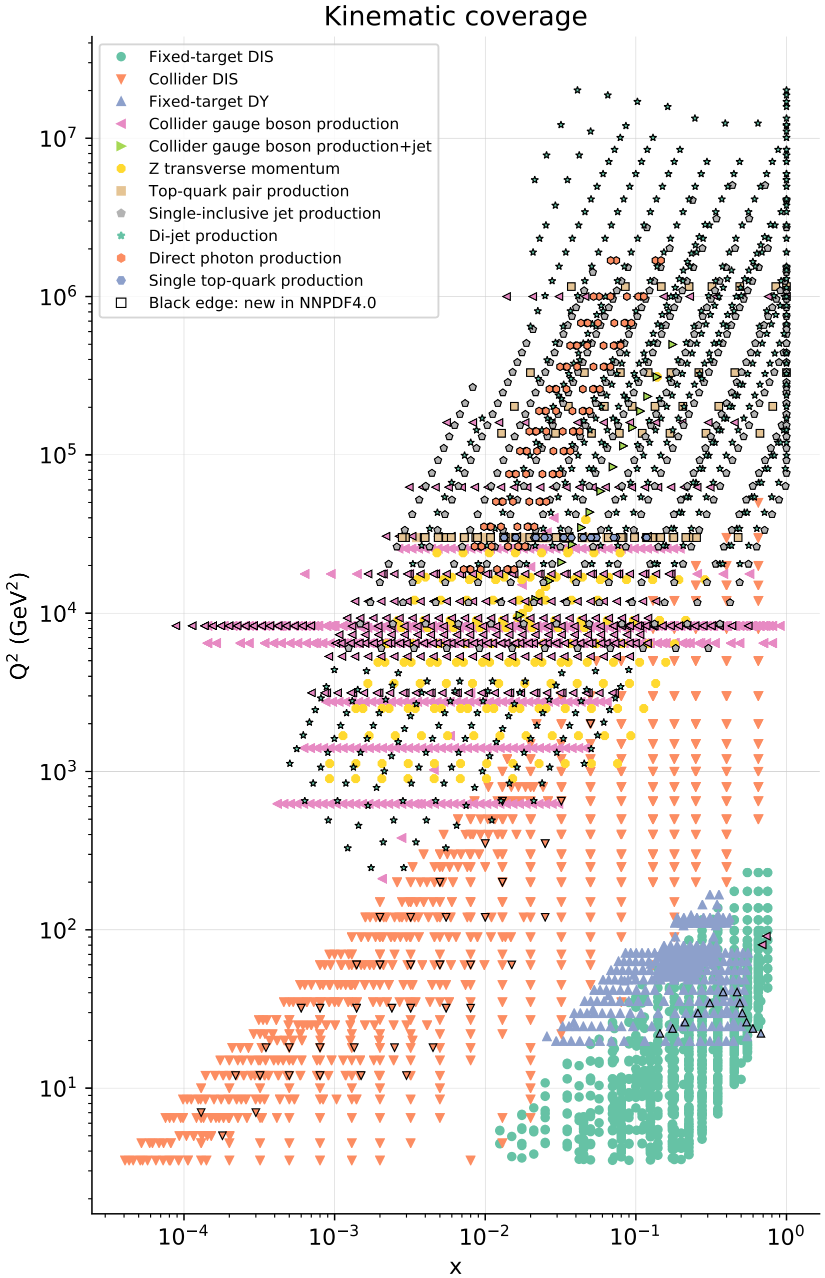
SUMMARY

NNPDF4.0

- DATA
- THEORY
- METHODOLOGY
- DATASET SELECTION
- UNCERTAINTIES
- VALIDATION
- STABILITY
- DELIVERY

DATA

DATA



- ABOUT 50 NEW DATASETS & 400 EXTRA DATAPOINTS
- FULL DIS AND FT DY DATASET
  - AS IN NNPDF3.1: FINAL HERA, NMC, BCDMS, CHORUS, NUTEV
  - NOW ALSO NOMAD NEUTRINO
  - SEAQUEST DY
- FULL 7 TEV AND 8 TEV DATASET & EXTENSIVE USE OF 13 TEV DATA:
  - W, Z PRODUCTION: RAPIDITY DISTRIBUTIONS, ASYMMETRIES, Z p_T DISTRIBUTIONS
  - TOP PAIR PRODUCTION: ALL AVAILABLE DISTRIBUTIONS
  - SINGLE-INCLUSIVE JETS
- SEVERAL NEW PROCESSES:
  - PROMPT PHOTON
  - SINGLE TOP
  - DIJETS
  - HERA JETS

TYPICAL PDF DETERMINATION: $\sim 10^{10}$ PREDICTIONS NEEDED

LHC DATA

LHCb

Data set	NNPDF4.0	NNPDF3.1	ABMP16	CT18	MSHT20
LHCb Z 940 pb	✓	✓	✗	✗	✓
LHCb $Z \to ee$ 2 fb	✓	✓	✓	✓	✓
LHCb $W, Z \to \mu$ 7 TeV	✓	✓	✓	✓	✓
LHCb $W, Z \to \mu$ 8 TeV	✓	✓	✓	✓	✓
LHCb $Z \to \mu\mu, ee$ 13 TeV	✓	✗	✗	✗	✗

ATLAS

Data set	NNPDF4.0	NNPDF3.1	ABMP16	CT18	MSHT20
ATLAS W, Z 7 TeV (2010)	✓	✓	✓	✓	✓
ATLAS W, Z 7 TeV (2011)	✓	✓	✗	✓	✓
ATLAS low-mass DY 7 TeV	✓	✓	✗	✗	✗
ATLAS high-mass DY 7 TeV	✓	✓	✗	✗	✓
ATLAS W 8 TeV	✓	✗	✗	✗	✓
ATLAS DY 2D 8 TeV	✓	✗	✗	✗	✓
ATLAS high-mass DY 2D 8 TeV	✓	✗	✗	✗	✓
ATLAS $\sigma_{W,Z}$ 13 TeV	✓	✗	✓	✗	✗
ATLAS W^++jet 8 TeV	✓	✗	✗	✗	✓
ATLAS Z p_T 8 TeV	✓	✓	✗	✓	✓
ATLAS $\sigma_{tt}^{\rm tot}$ 7, 8 TeV	✓	✓	✓	✗	✗
ATLAS $\sigma_{tt}^{\rm tot}$ 13 TeV	✓	✓	✓	✗	✗
ATLAS $t\bar{t}$ lepton+jets 8 TeV	✓	✓	✗	✓	✓
ATLAS $t\bar{t}$ dilepton 8 TeV	✓	✗	✗	✗	✓
ATLAS single-inclusive jets 7 TeV, R=0.6	✗	✓	✗	✓	✓
ATLAS single-inclusive jets 8 TeV, R=0.6	✓	✗	✗	✗	✗
ATLAS dijets 7 TeV, R=0.6	✓	✗	✗	✗	✗
ATLAS direct photon production 13 TeV	✓	✗	✗	✗	✗
ATLAS single top R_t 7, 8, 13 TeV	✓	✗	✓	✗	✗
ATLAS single top diff. 7, 8 TeV	✓	✗	✗	✗	✗
ATLAS single top diff. 8 TeV	✓	✗	✗	✗	✗

- CUTOFF DATE AROUND 06/2020
- DIJETS NOW INCLUDED ALONG WITH JETS
  CANNOT INCLUDE SIMULTANEOUSLY FROM SAME UNDERLYING DATASET

CMS

Data set	NNPDF4.0	NNPDF3.1	ABMP16	CT18	MSHT20
CMS W electron asymmetry 7 TeV	✓	✓	✗	✓	✓
CMS W muon asymmetry 7 TeV	✓	✓	✓	✓	✗
CMS Drell-Yan 2D 7 TeV	✓	✓	✗	✗	✓
CMS W rapidity 8 TeV	✓	✓	✓	✓	✓
CMS Z p_T 8 TeV	✓	✓	✗	✓	✗
CMS $W + c$ 7 TeV	✓	✓	✗	✗	✓
CMS $W + c$ 13 TeV	✓	✗	✗	✗	✗
CMS single-inclusive jets 2.76 TeV	✗	✓	✗	✗	✓
CMS single-inclusive jets 7 TeV	✗	✓	✗	✓	✓
CMS dijets 7 TeV	✓	✗	✗	✗	✗
CMS single-inclusive jets 8 TeV	✓	✗	✗	✓	✓
CMS 3D dijets 8 TeV	✗	✗	✗	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 5 TeV	✓	✗	✓	✗	✗
CMS $\sigma_{tt}^{\rm tot}$ 7, 8 TeV	✓	✓	✓	✗	✓
CMS $\sigma_{tt}^{\rm tot}$ 13 TeV	✓	✓	✓	✗	✗
CMS $t\bar{t}$ lepton+jets 8 TeV	✓	✓	✗	✗	✓
CMS $t\bar{t}$ 2D dilepton 8 TeV	✓	✗	✗	✓	✓
CMS $t\bar{t}$ lepton+jet 13 TeV	✓	✗	✗	✗	✗
CMS $t\bar{t}$ dilepton 13 TeV	✓	✗	✗	✗	✗
CMS single top $\sigma_t + \sigma_{\bar{t}}$ 7 TeV	✓	✗	✓	✗	✗
CMS single top R_t 8, 13 TeV	✓	✗	✓	✗	✗

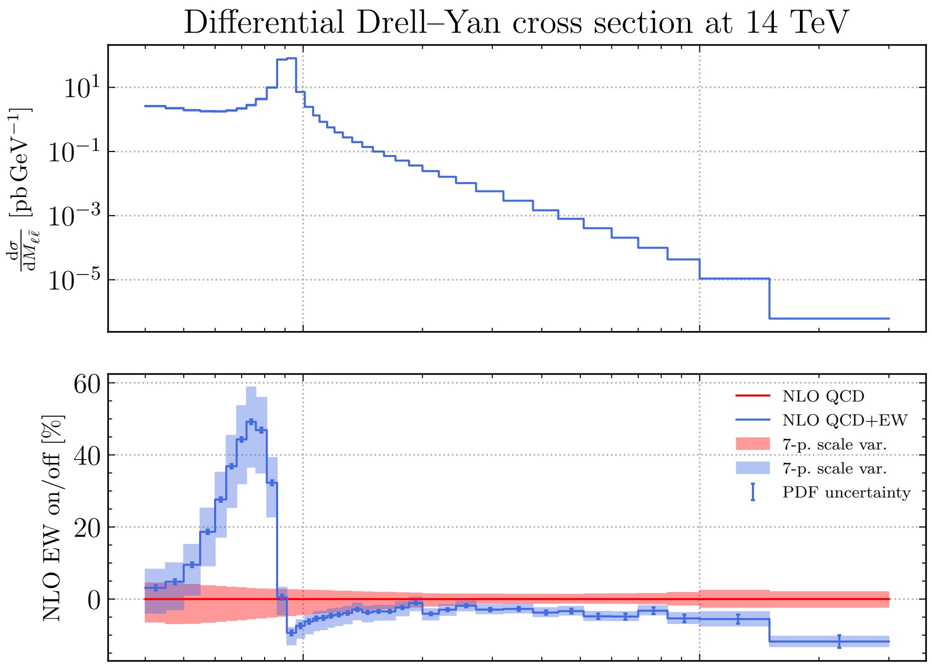
THEORY

ELECTROWEAK CORRECTIONS

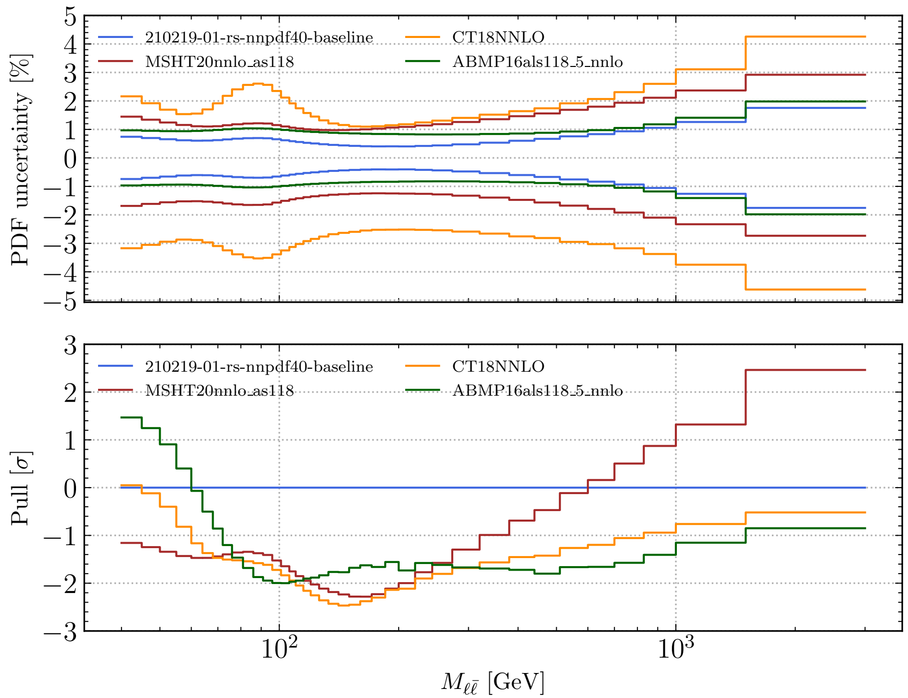
- `PineAPPL` FAST INTERFACE TO `Madgraph5_aMC@NLO` AVAILABLE (Schwan, Carrazza, Nocera, Zaro 2020)
  $\Rightarrow$ FULL NLO EW+QCD POSSIBLE
- DATA W/O FSR & PHOTON-INITIATED SUBTRACTION OFTEN NOT AVAILABLE
- CURRENTLY USED FOR DATASET SELECTION:
  $\Rightarrow$ DISCARDED IF EW CORRNS EXCEED THRESHOLD

EXAMPLE: DRELL-YAN AT 14 TEV

QCD+EW VS. QCD



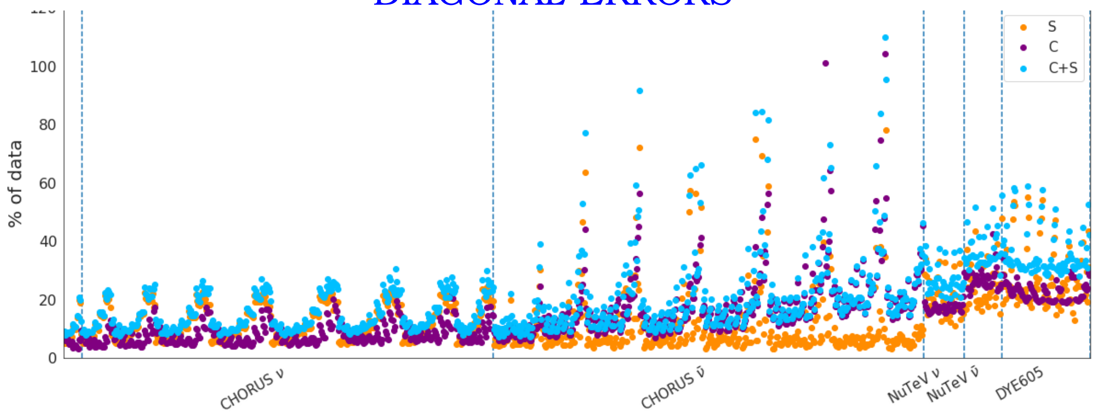
PDF UNCERTAINTIES



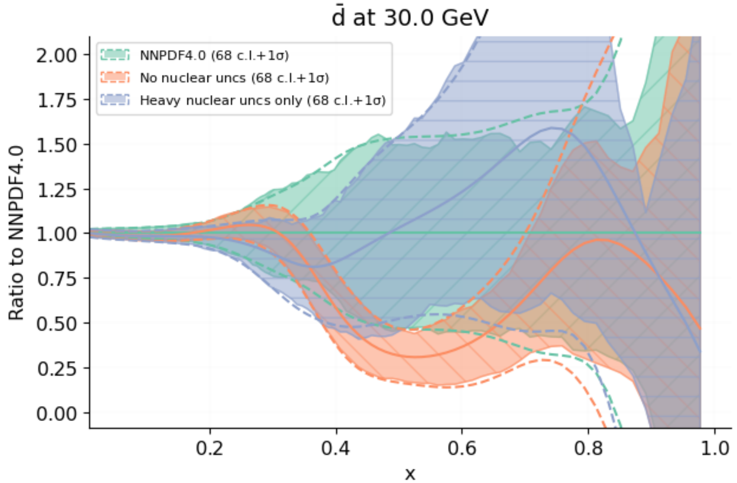
NUCLEAR CORRECTIONS

- INCLUDED AS CONTRIBUTION TO COVARIANCE MATRIX (FULLY CORRELATED) (Ball, Nocera, Pearson, 2019)
- COMPUTED AS SHIFT BETWEEN NUCLEAR & STANDARD PDF
- DEUTERIUM PDF DETERMINED FROM SELF-CONSISTENT NNPDF FIT (Ball, Nocera, Pearson, 2019)
- NUCLEAR PDFS FROM nNNPDF2.0 (Abdul Khalek, Ethier, Rojo, van Weelden, 2020)

DIAGONAL ERRORS



IMPACT ON PDFS

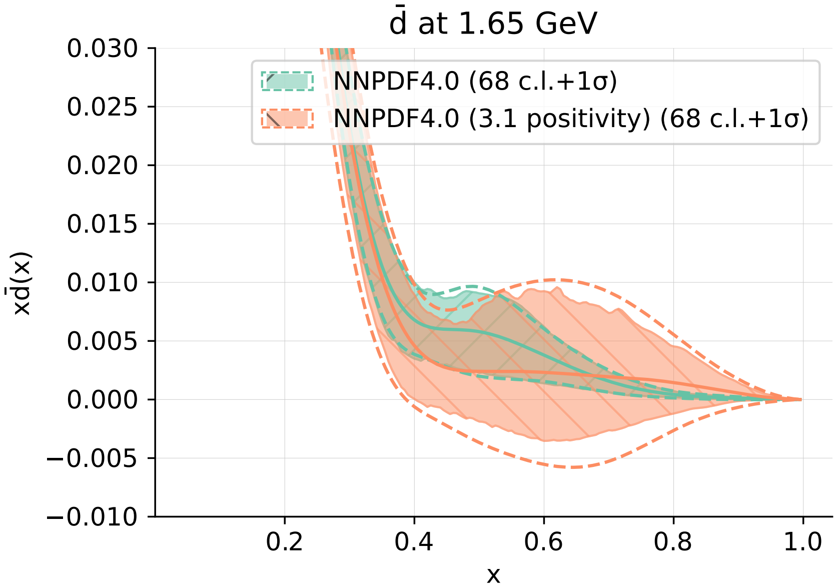


PDF POSITIVITY & INTEGRABILITY

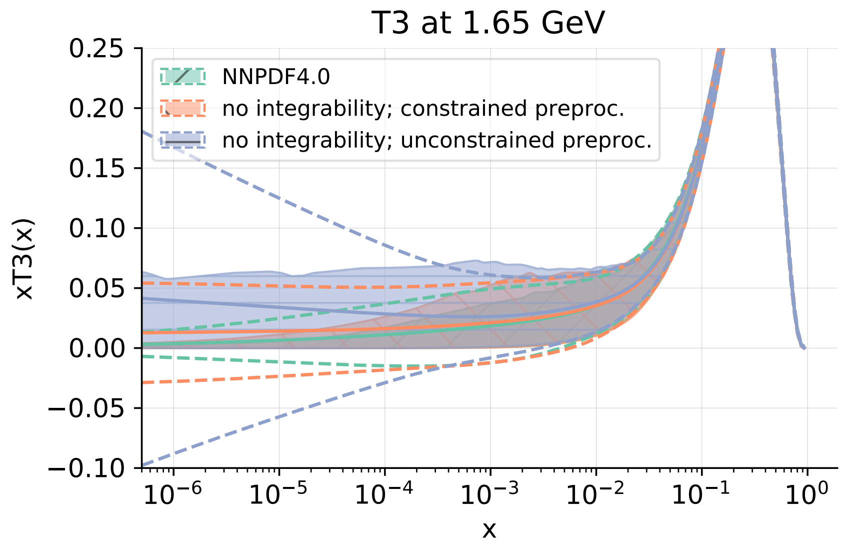
- $\overline{\mathrm{MS}}$ PDFs are non-negative!(Candido, Hekhorn, Forte, 2020)
- PDF positivity imposed (previously: observable positivity)
  $\Rightarrow$ smaller large x uncertainties
- Sea nonsinglet combinations integrable:
  Gottfried $u + \bar{u} - (d + \bar{d})$
  Strangeness $u + \bar{u} + (d + \bar{d}) - 2(s + \bar{s})$
  $\Rightarrow$ smaller small x uncertainties

impact on PDFs

POS.: ANTIDOWN



INTEGR.: GOTTFRIED SR



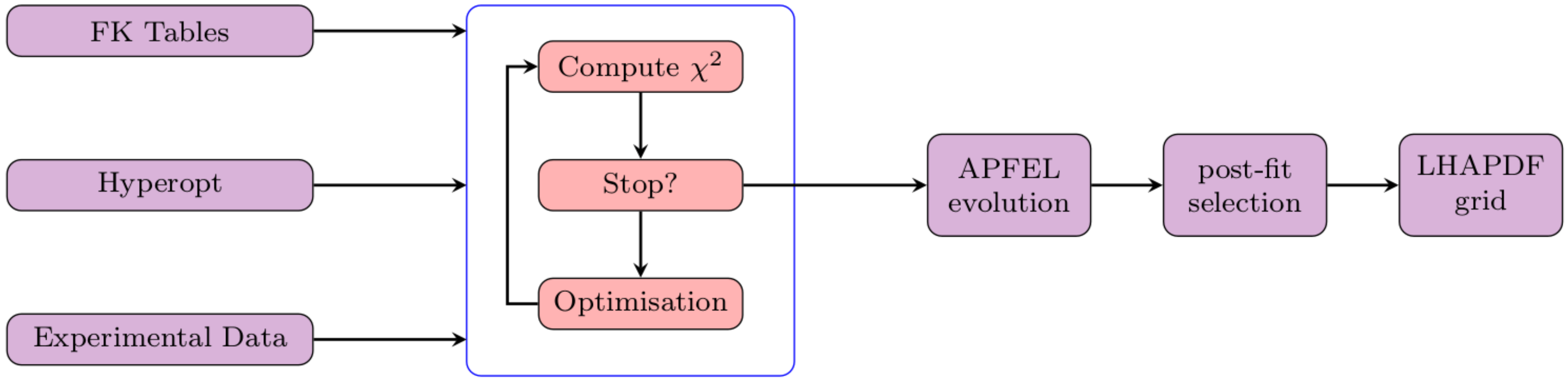
METHODOLOGY

THE NNPDF CODE STRUCTURE

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

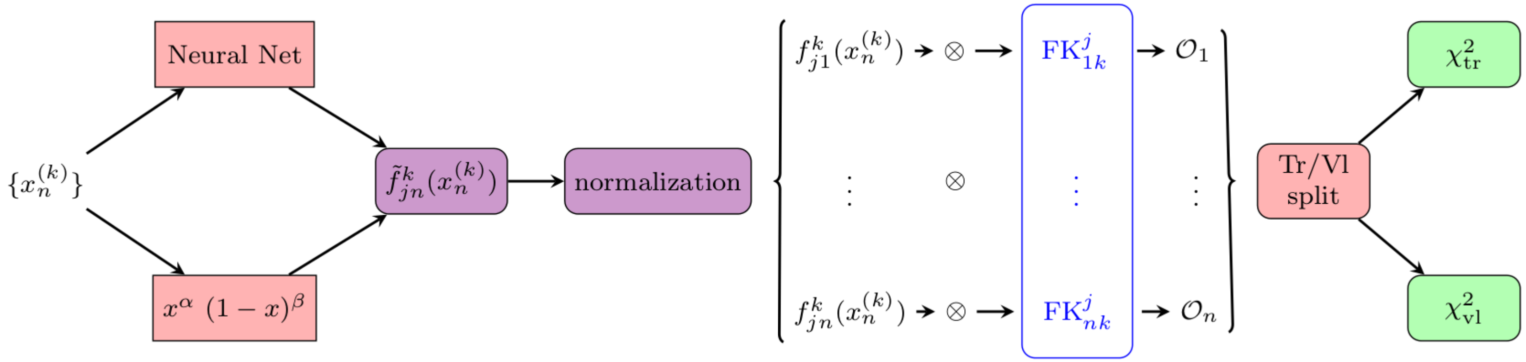
AVERAGE FITTING TIME PER REPLICA AND USE OF RESOURCES
SAME DATASET FOR OLD AND NEW METHODOLOGIES IN CPU AND GPU
CPU: INTEL(R) CORE(TM) I7-4770 AT 3.40GHZ; GPU: NVIDIA TITAN V

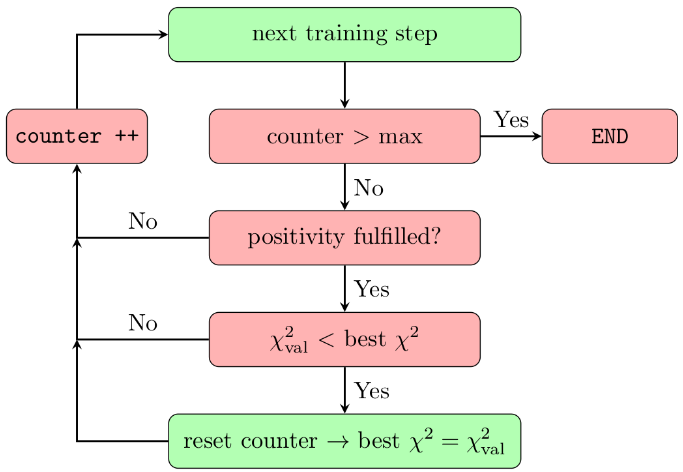
	NNPDF31 CODEBASE	NNPDF40 CODEBASE IN CPU	NNPDF40 CODEBASE IN GPU
TIME	15.2 H.	38 ± 5 MIN.	6.6 MIN.
RAM USE	1.5 GB	6.1 GB	NA



MINIMIZATION AND CROSS-VALIDATION

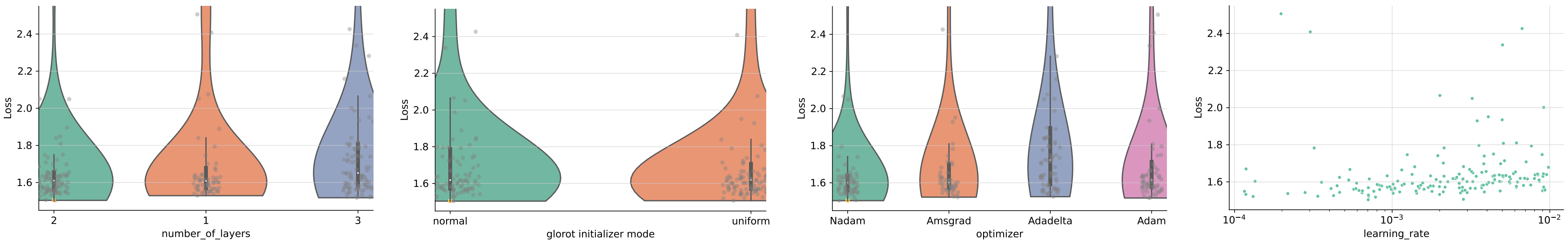
- DATA REPLICAS $\Rightarrow$ PDF REPLICAS
- EACH PDF REPLICA: PREPROCESSED NEURAL NET
- NEURAL NET $\Rightarrow$ OBSERVABLES
- RANDOM TRAINING-VALIDATION SPLIT, χ^2 TO TRAINING DATA REPLICAS MINIMIZED
- TRAINING STOPS IF VALIDATION χ^2 GROWS FOR A WHILE (PATIENCE)
- LOWEST VALIDATION χ^2 $\Rightarrow$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



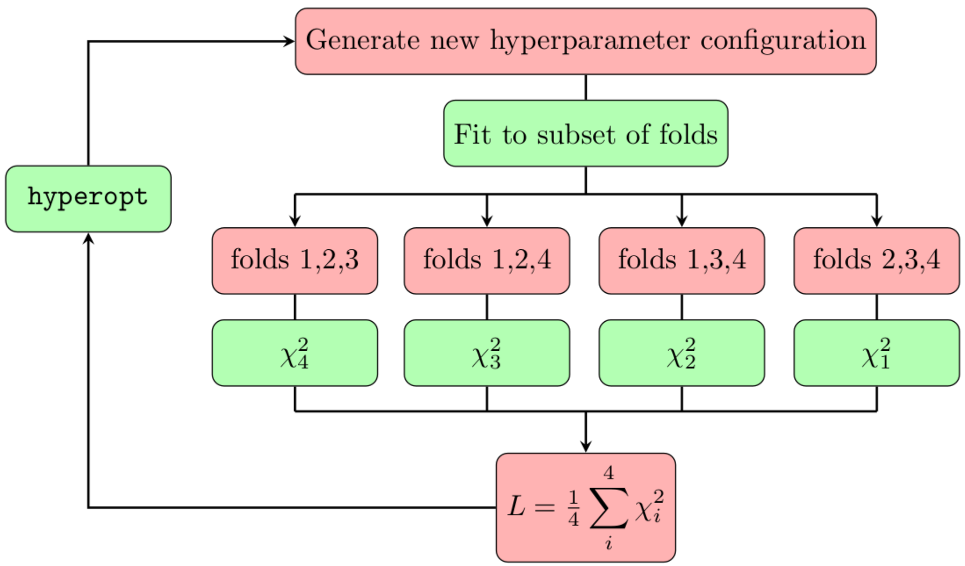


HYPEROPTIMIZATION

- PARAMETRIZATION AND MINIMIZATION PARAMETERS VARIED
- SCAN OF PARAMETER SPACE
- BAYESIAN UPDATING LEADS TO BEST METHODOLOGY



K-FOLDING



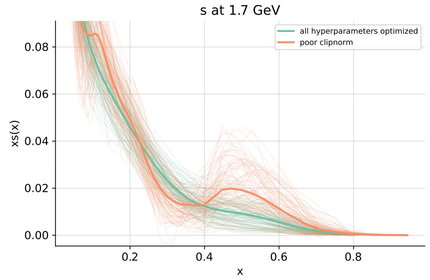
Fold 1		
CHORUS σ^{ν}_{CC}	HERA I+II inc NC e^+p 920 GeV	BCDMS p
LHCb Z 940 pb	ATLAS W, Z 7 TeV 2010	CMS Z p_T 8 TeV (p_T^{ll}, y_{ll})
DY E605 σ^p_{DY}	CMS Drell-Yan 2D 7 TeV 2011	CMS 3D dijets 8 TeV
ATLAS single-$\bar{t}$ y (normalised)	ATLAS single top R_t 7 TeV	CMS $t\bar{t}$ rapidity $y_{t\bar{t}}$
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. $\sigma^{\mathrm{red}}_{b\bar{b}}$
NMC p	NuTeV $\sigma^{\bar{\nu}}_c$	LHCb $Z \to ee$ 2 fb
CMS W asymmetry 840 pb	ATLAS Z p_T 8 TeV (p_T^{ll}, M_{ll})	D0 $W \to \mu\nu$ asymmetry
DY E886 σ^p_{DY}	ATLAS direct photon 13 TeV	ATLAS dijets 7 TeV, R=0.6
ATLAS single antitop y (normalised)	CMS $\sigma^{\mathrm{tot}}_{tt}$	CMS single top $\sigma_t + \sigma_{\bar{t}}$ 7 TeV

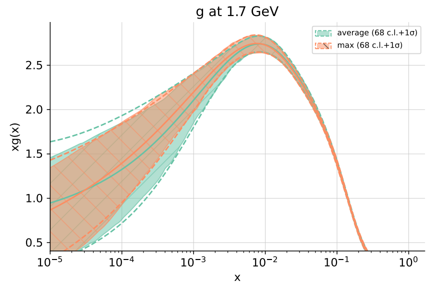
Fold 3		
HERA I+II inc CC e^+p	HERA I+II inc NC e^+p 575 GeV	NMC d/p
NuTeV σ^{ν}_c	LHCb $W, Z \to \mu$ 7 TeV	LHCb $Z \to ee$
ATLAS W, Z 7 TeV 2011 Central selection	ATLAS W^++jet 8 TeV	ATLAS HM DY 7 TeV
CMS W asymmetry 4.7 fb	DYE 866 $\sigma^d_{\mathrm{DY}}/\sigma^p_{\mathrm{DY}}$	CDF Z rapidity (new)
ATLAS $\sigma^{\mathrm{tot}}_{tt}$	ATLAS single top y_t (normalised)	CMS $\sigma^{\mathrm{tot}}_{tt}$ 5 TeV
CMS $t\bar{t}$ double diff. $(m_{t\bar{t}}, y_t)$		

Fold 4		
CHORUS $\sigma^{\bar{\nu}}_{CC}$	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_T^{ll}, 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	

NO K-FOLDING



K-FOLDING VARIATION



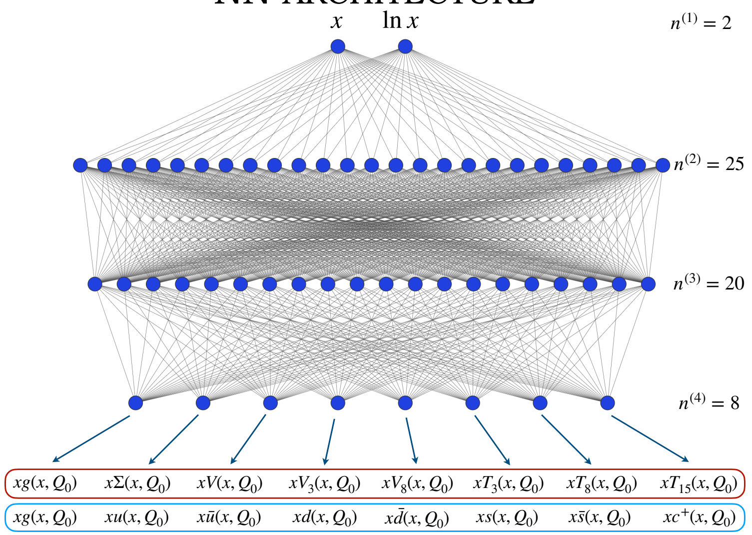
- HYPEROPTIMIZATION $\Rightarrow$ OVERFITTING (χ^2 TOO GOOD)
- CHECK GENERALIZATION POWER: K-FOLDING
  - DIVIDE DATA IN FOLDS
  - EXCLUDE ONE FOLD IN TURN FROM FIT
  - OPTIMIZE ON THE χ^2 OF THE EXCLUDED FOLDS
  - BEST AVERAGE OR BEST WORST

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
- ~ 800 FREE PARAMETERS

DATASET SELECTION

DATA "TENSION"

PROBLEMATIC DATA

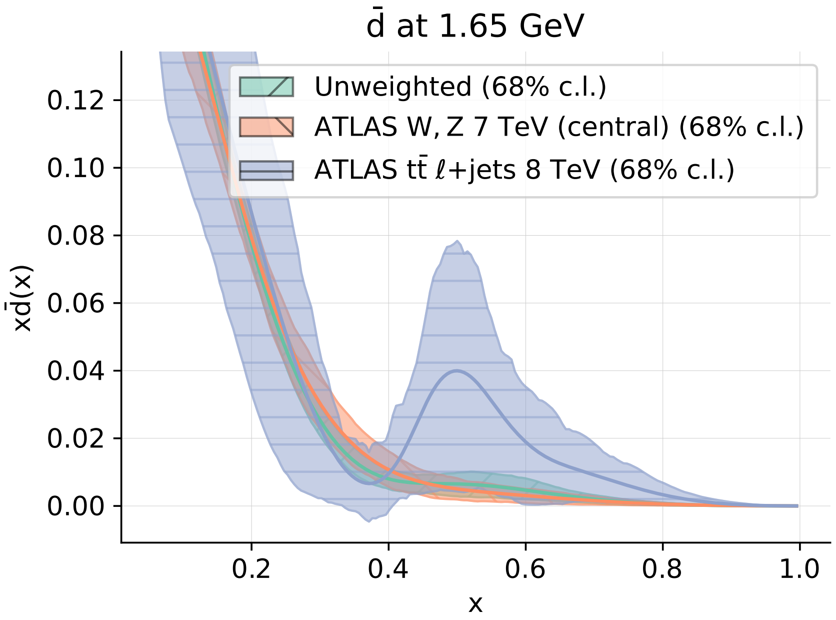
$$\frac{\chi^2-1}{\sigma_{\chi^2}} \gg 1 \Leftrightarrow \text{POOR FIT QUALITY}$$

- MISSING HIGHER-ORDER CORRECTIONS
- NO RESUMMATION WHERE NEEDED
- ILL-CONDITIONED COVARIANCE MATRIX
- EXPERIMENTAL ISSUES

THE WEIGHTED FIT METHOD

- FLAG PROBLEMATIC DATASETS:
  - LARGE χ^2
  - LARGE FROBENIUS NUMBER OF COVMAT (EIGENVALUES TOO SMALL)
- REPEAT GLOBAL FIT WITH LARGE WEIGHT GIVEN TO EACH PROBLEMATIC DATASET IN TURN

INCONSISTENT!

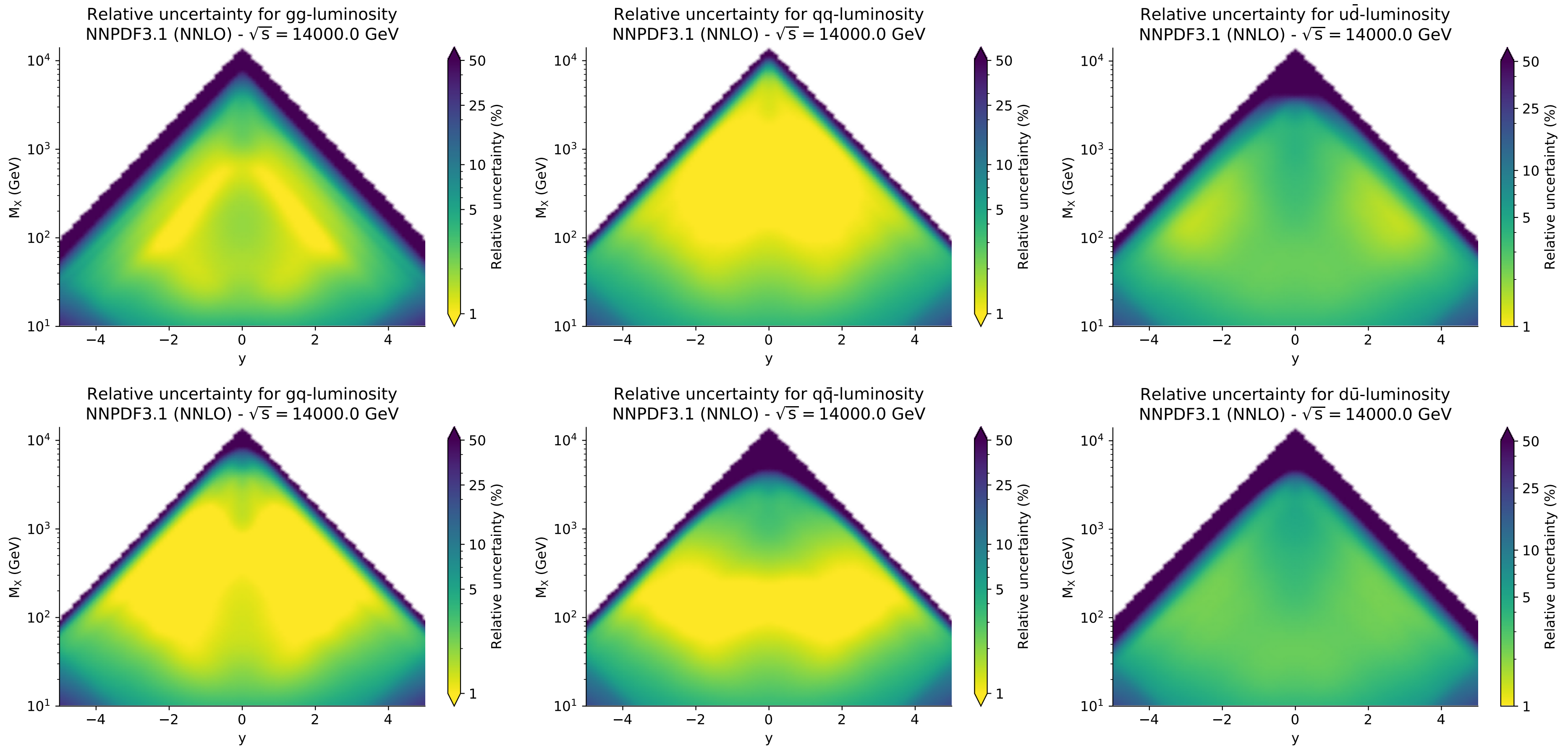


- χ^2 OF DATASET
  - UNCHANGED $\Rightarrow$ INTERNAL INCONSISTENCY
  - DECREASES $\Rightarrow$ TENSION
- GLOBAL χ^2
  - UNCHANGED $\Rightarrow$ CONSISTENT, KEEP
  - INCREASES $\Rightarrow$ INSONSISTENT, DISCARD

UNCERTAINTIES

UNCERTAINTIES: FROM NNPDF3.1...

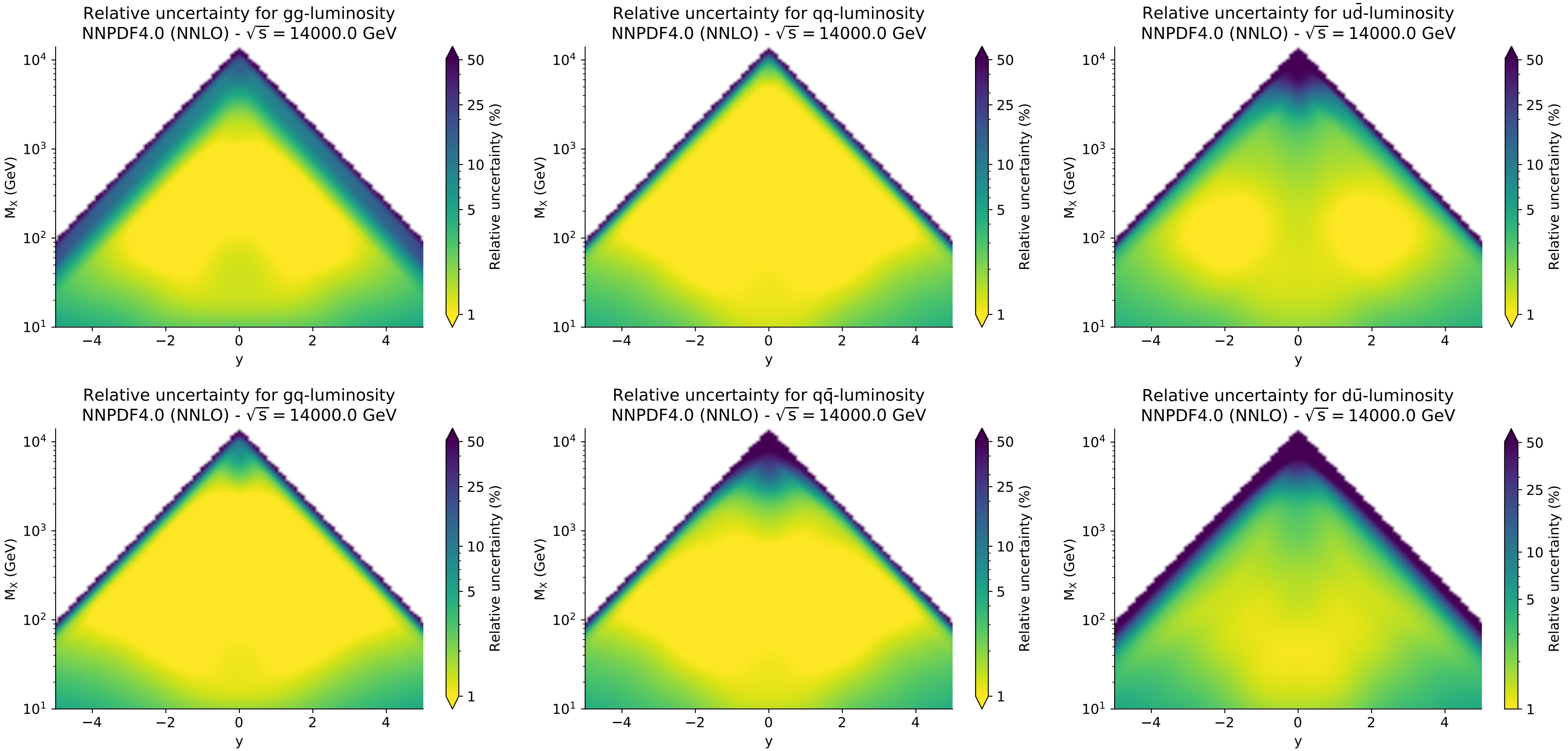
GLUON SINGLET FLAVORS



- 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: ...TO NNPDF4.0

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, $-4 \lesssim y \lesssim 4$

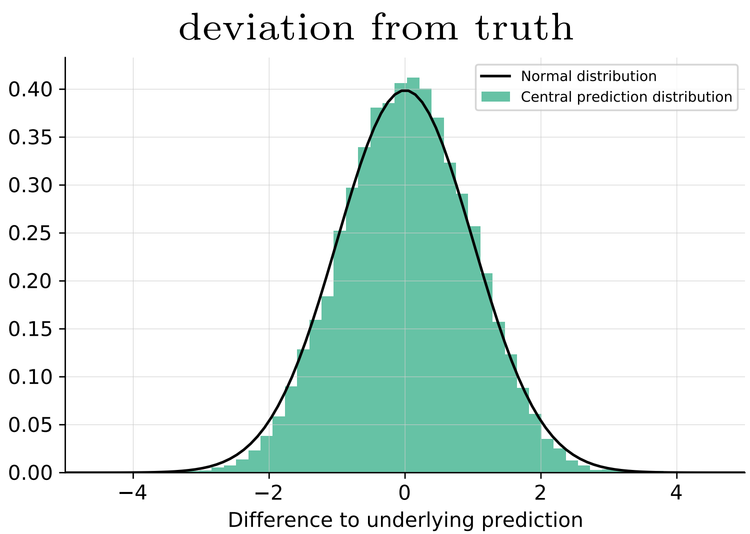
VALIDATION

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



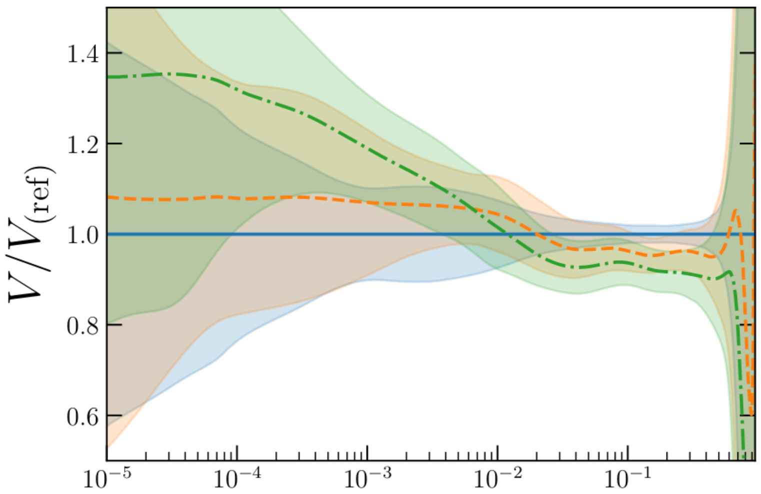
Dataset	$\sqrt{\text{bias/variance}}$	$\xi_{1\sigma}^{(\text{data})}$
DY	0.99 ± 0.08	0.69 ± 0.02
Top-pair	0.75 ± 0.06	0.75 ± 0.03
Jets	1.14 ± 0.05	0.63 ± 0.03
Dijets	0.99 ± 0.07	0.70 ± 0.03
Direct photon	0.71 ± 0.06	0.81 ± 0.03
Single top	0.87 ± 0.07	0.69 ± 0.04
Total	1.03 ± 0.05	0.68 ± 0.02

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.**

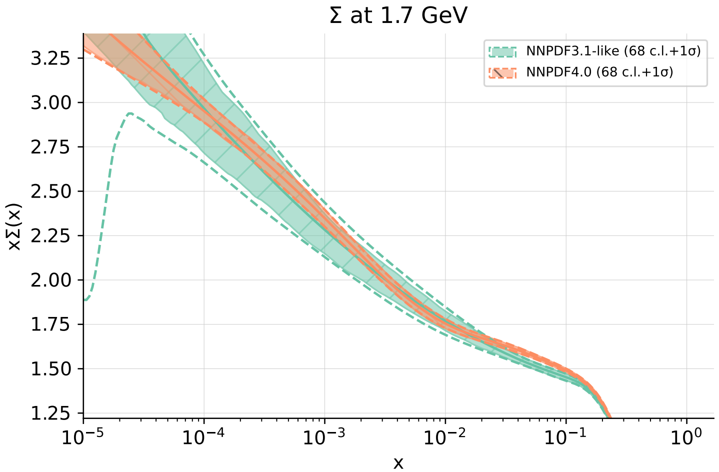
PROCESS	PRE-HERA	PRE-LHC	3.1-LIKE	4.0-GLOB
FT DIS (NC)	1.04	1.17	1.17	1.26
FT DIS (CC)	0.80	0.86	0.88	0.90
FT DY	0.93	1.27	1.43	1.59
HERA	24.01/**1.12**	1.22	1.21	1.21
COLL. DY (TEV.)	5.31/**1.08**	0.96	0.95	1.13
COLL. DY (LHC)	15.50/**1.37**	2.64/**1.54**	1.39	1.54
TOP QUARK	23.35/**1.08**	1.29/**0.86**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

STABILITY

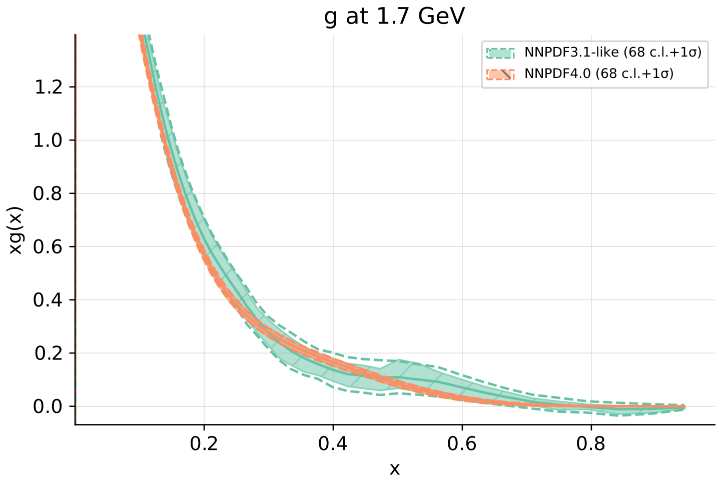
NNPDF4.0 vs. NNPDF3.1

- FULL BACKWARD COMPATIBILITY
- SUBSTANTIAL REDUCTION IN UNCERTAINTY

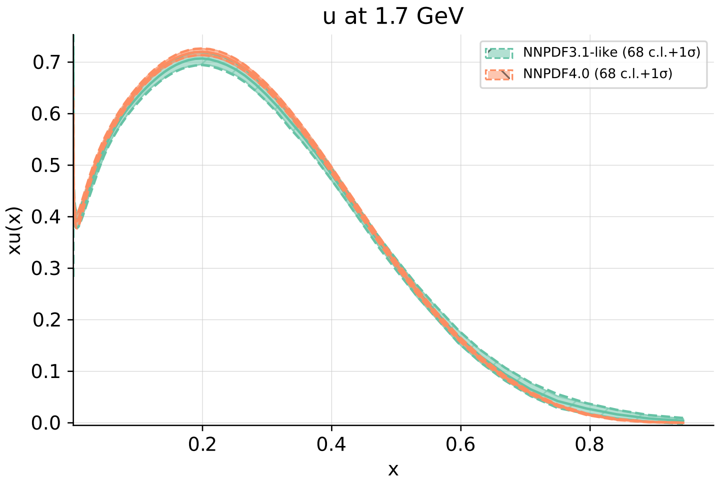
SINGLET



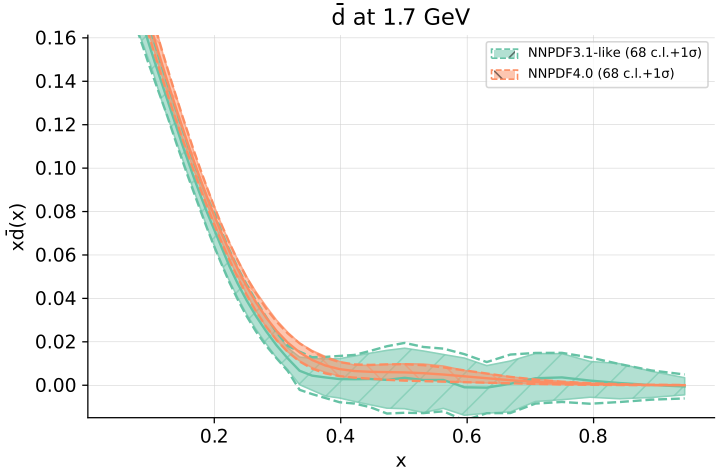
GLUON



UP



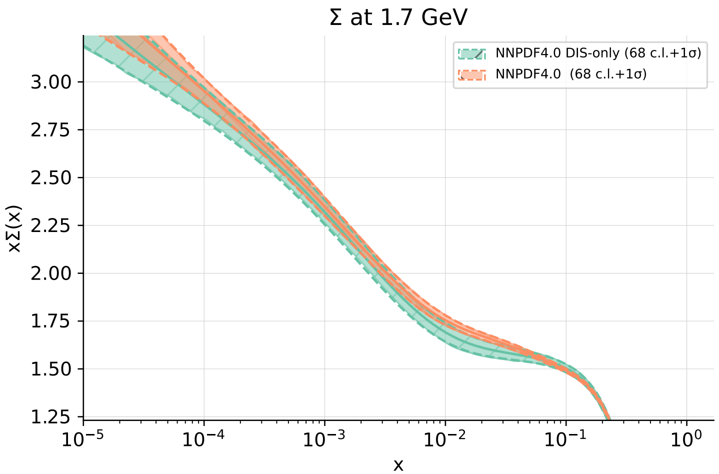
ANTIDOWN



NNPDF4.0 vs DIS-only

- DIS-only fit no longer competitive
- Hadronic data needed for precision

SINGLET



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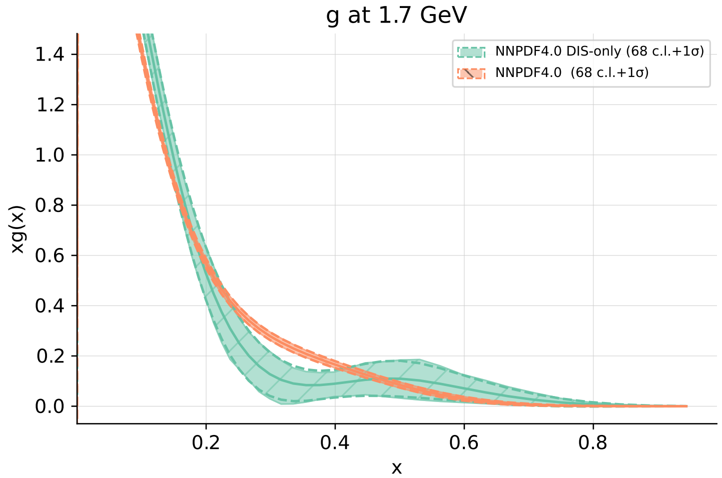

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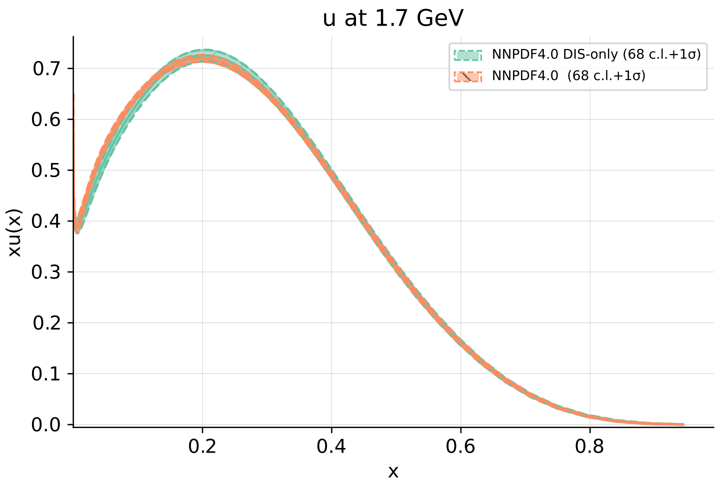

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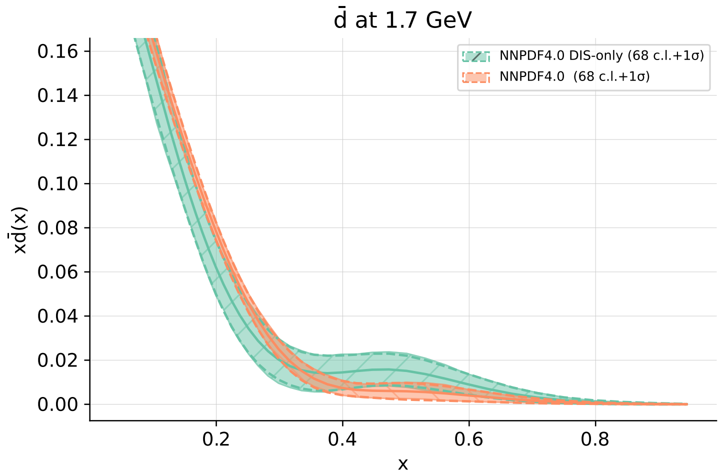
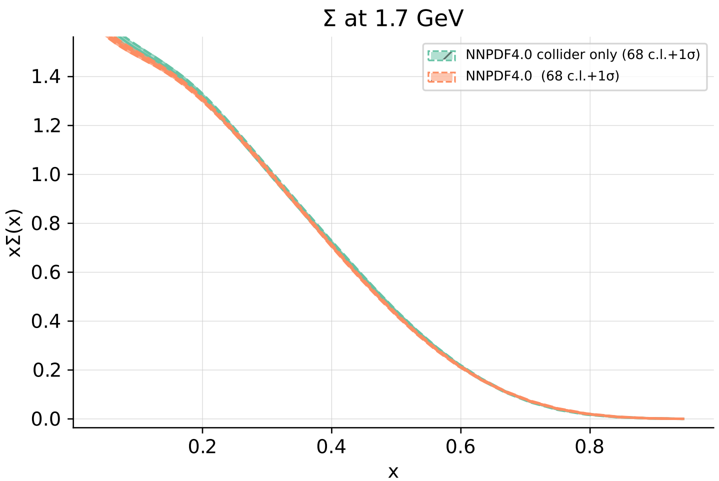


NNPDF4.0 VS COLLIDER ONLY

- COLLIDER ONLY COMPETITIVE!
- ONLY DEUTERIUM FIXED-TARGET DATA STILL RELEVANT

SINGLET



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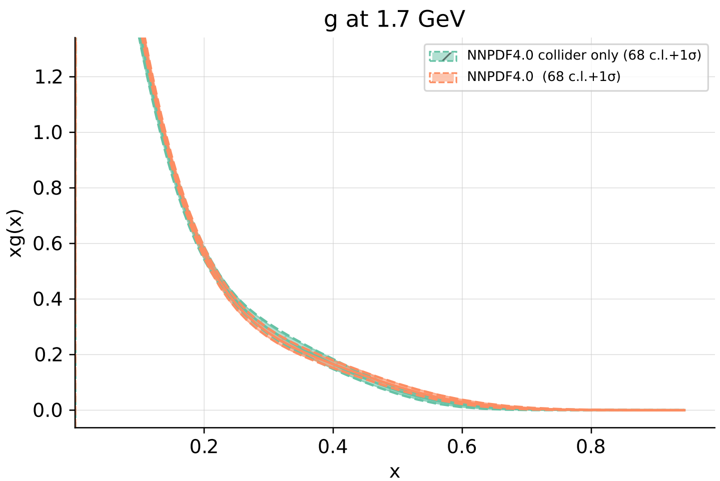

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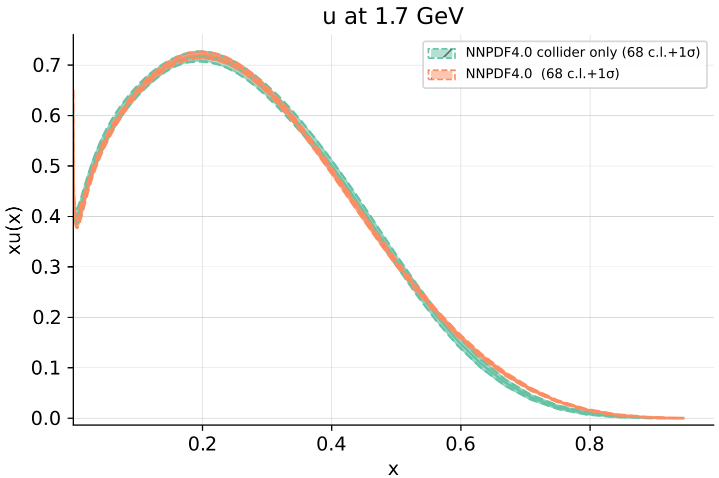

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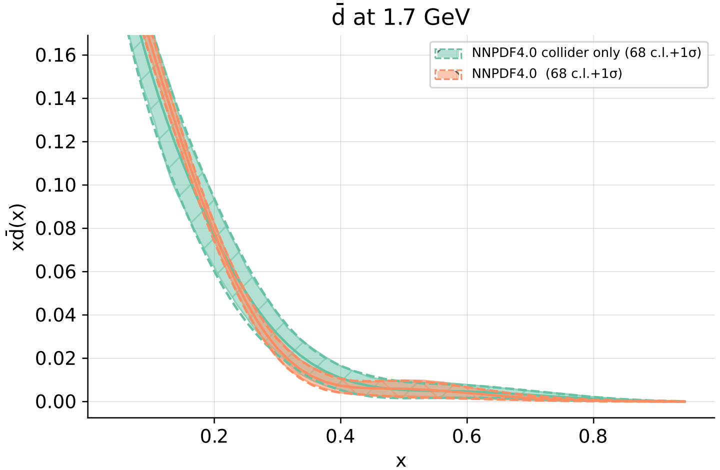


DELIVERY

AN OPEN SOURCE CODE!

- THE FULL NNPDF CODE HAS BEEN MADE PUBLIC!
- INCLUDING HYPEROPTIMIZATION, EVOLUTION, THEORY, FITTING, VISUALIZATION
- FULLY DOCUMENTED CODE

Eur. Phys. J. C (2021) 81:958
https://doi.org/10.1140/epjc/s10052-021-09747-9

THE EUROPEAN PHYSICAL JOURNAL C

Special Article - Tools for Experiment and Theory

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

NNPDF Collaboration

`https:///github.com/NNPDF/nnpdf`
`https://docs.nnpdf.science`

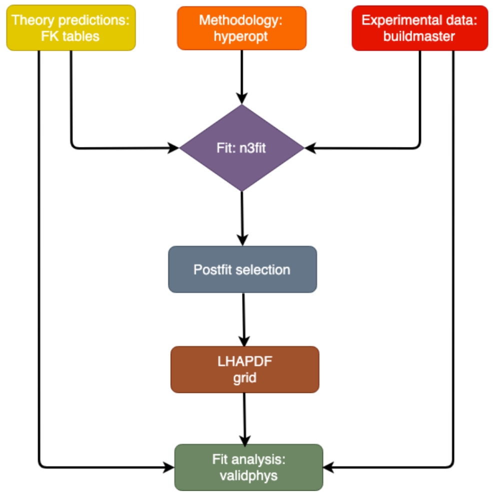


Fig. 2.1. Workflow for an NNPDF fit

OUTLOOK

THE ACCURACY CHALLENGE

- AT 1%, NOT ALL REDUCED DATASETS AGREE
- MUST INCLUDE MISSING HIGHER-ORDER CORRECTION UNCERTAINTIES
- INCLUDE EW CORRECTIONS
- GO BEYOND K-FACTORS
- WEIGHT SMALL DATASETS

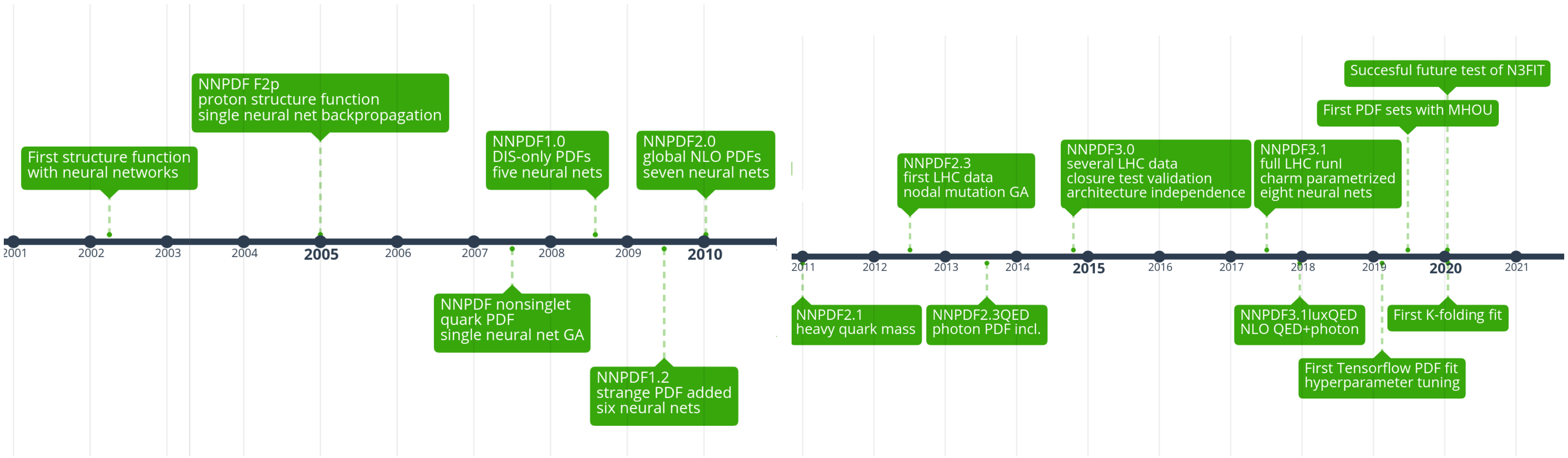
THE ACCURACY CHALLENGE

- AT 1%, NOT ALL REDUCED DATASETS AGREE
- MUST INCLUDE MISSING HIGHER-ORDER CORRECTION UNCERTAINTIES
- INCLUDE EW CORRECTIONS
- GO BEYOND K-FACTORS
- WEIGHT SMALL DATASETS

STAY TUNED FOR NNPDF4.1!!

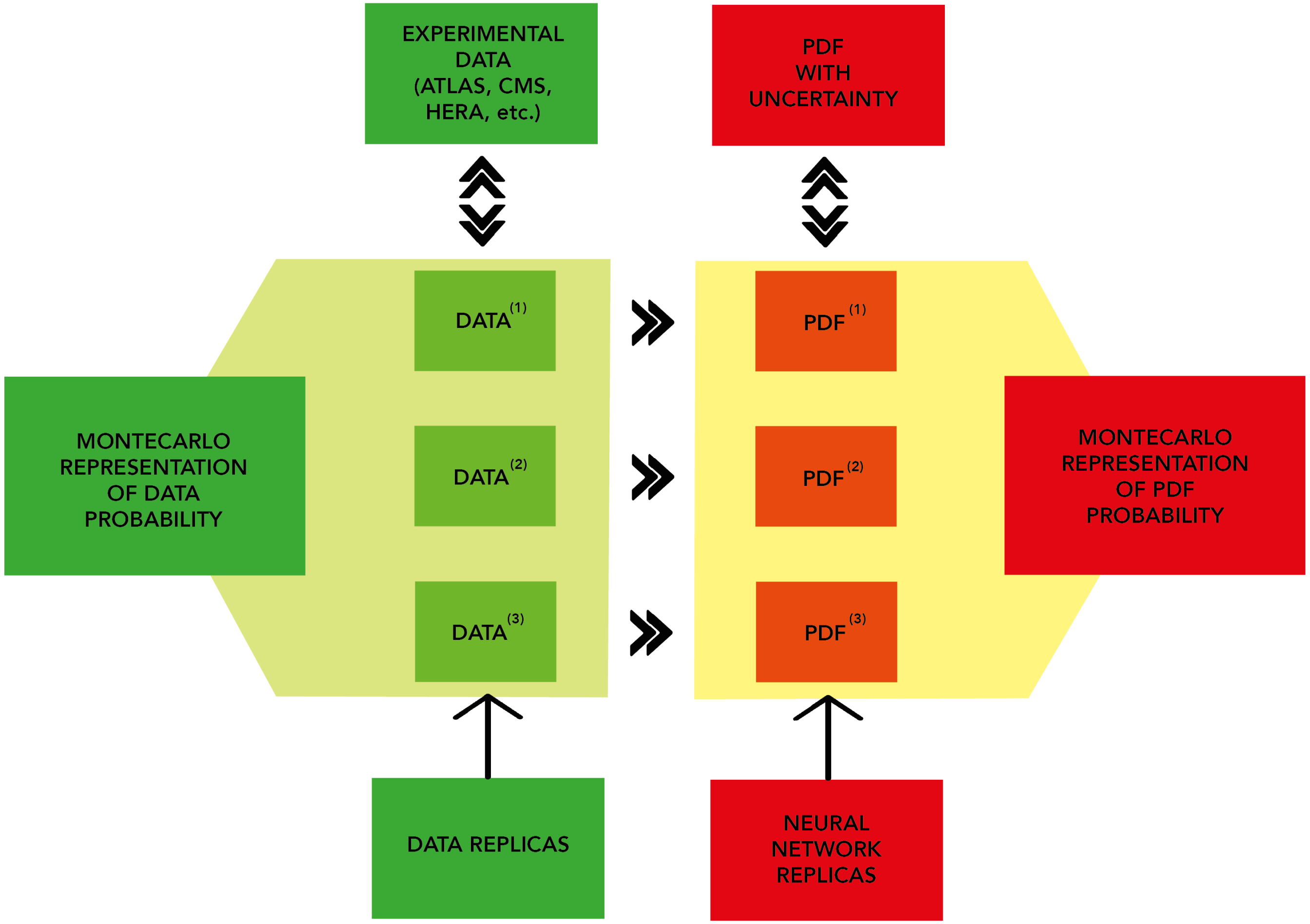
EXTRAS

PROTON STRUCTURE AS AN AI PROBLEM: NNPDF



AI FOR PDFS: THE NNPDF APPROACH
THE FUNCTIONAL MONTE CARLO

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

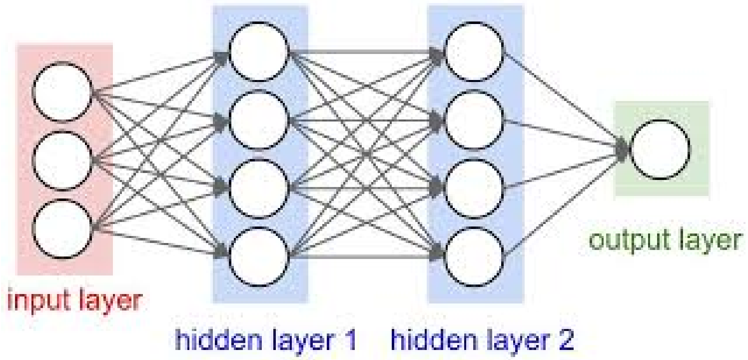


FINAL PDF SET: $f_i^{(a)}(x,\mu)$;
i =up, antiup, down, antidown, strange, antistrange, charm, gluon; $j = 1, 2, \ldots N_{\rm rep}$

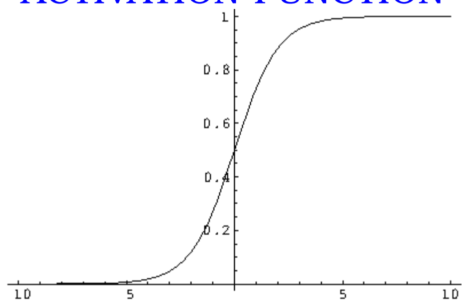
ARTIFICIAL INTELLIGENCE

NEURAL NETWORKS

ARCHITECTURE



ACTIVATION FUNCTION



PARAMETERS

- WEIGHTS ω_{ij}
- THRESHOLDS θ_i

$$F_{\rm out}^{(i)}(\vec{x}_{\rm in}) = F\left(\sum_j \omega_{ij} x_{\rm in}^j - \theta_i\right)$$

SIMPLEST EXAMPLE
1-2-1

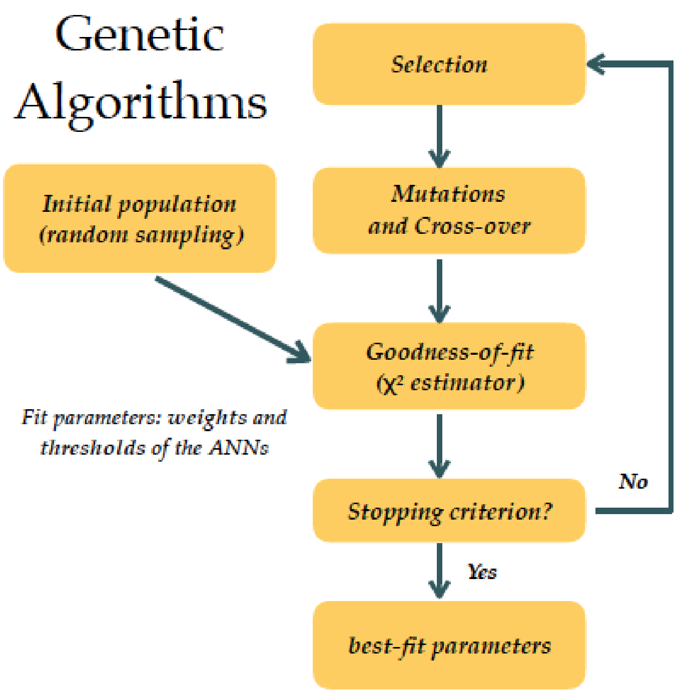
$$f(x) = \frac{1}{1+e^{\theta_1^{(3)} - \frac{\omega_{11}^{(2)}}{1+e^{\theta_1^{(2)} - x\omega_{11}^{(1)}}} - \frac{\omega_{12}^{(2)}}{1+e^{\theta_2^{(2)} - x\omega_{21}^{(1)}}}}}$$

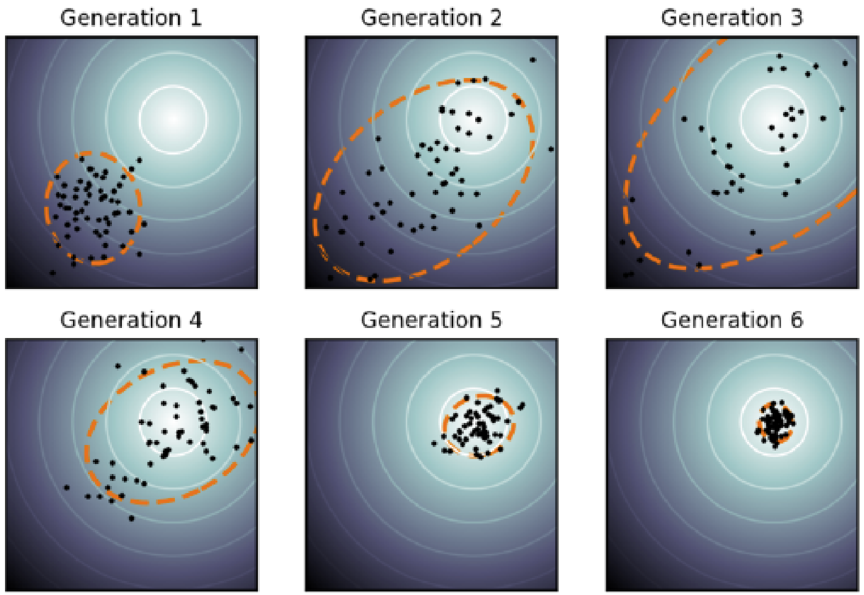
NNPDF: $2-5-3-1$ NN FOR EACH PDF: $37 \times 8 = 296$ PARAMETERS

SUPERVISED LEARNING

GENETIC ALGORITHMS

- BASIC IDEA: RANDOM MUTATION OF THE NN PARAMETER
- SELECTION OF THE FITTEST

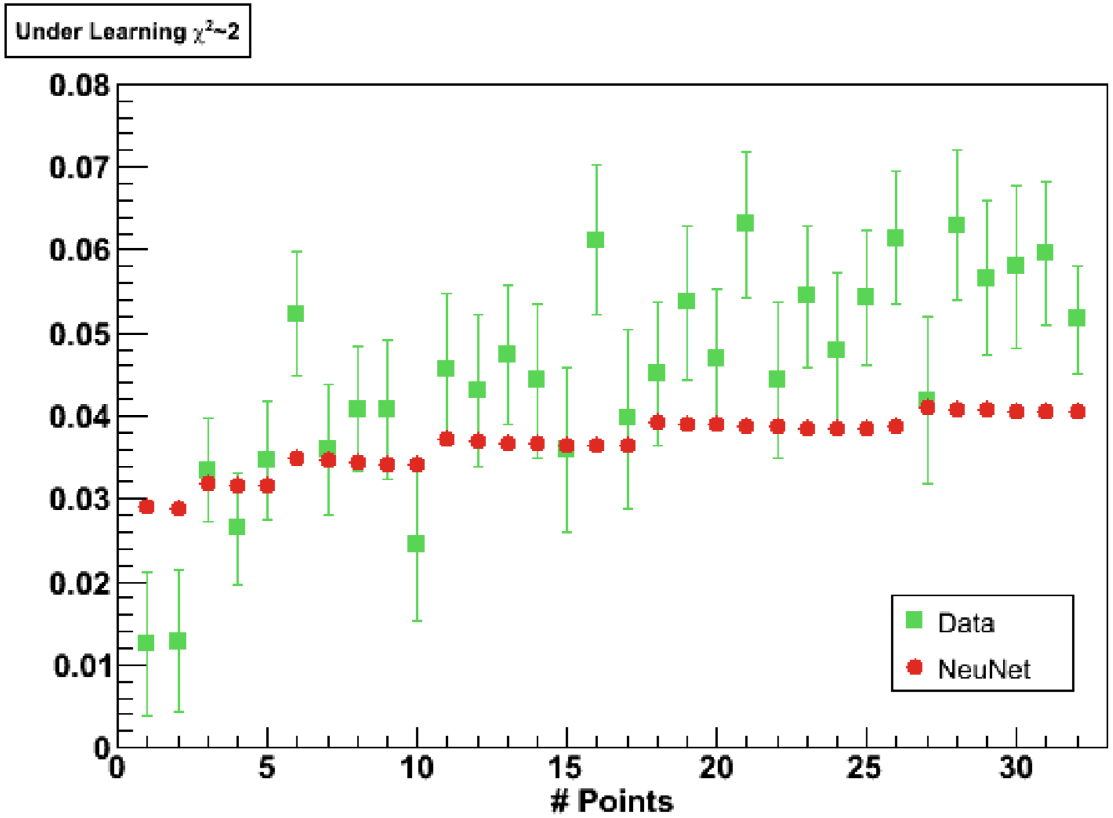




NEURAL LEARNING

- COMPLEXITY INCREASES AS THE FITTING PROCEEDS
- UNTIL LEARNING NOISE
- WHEN SHOULD ONE STOP?

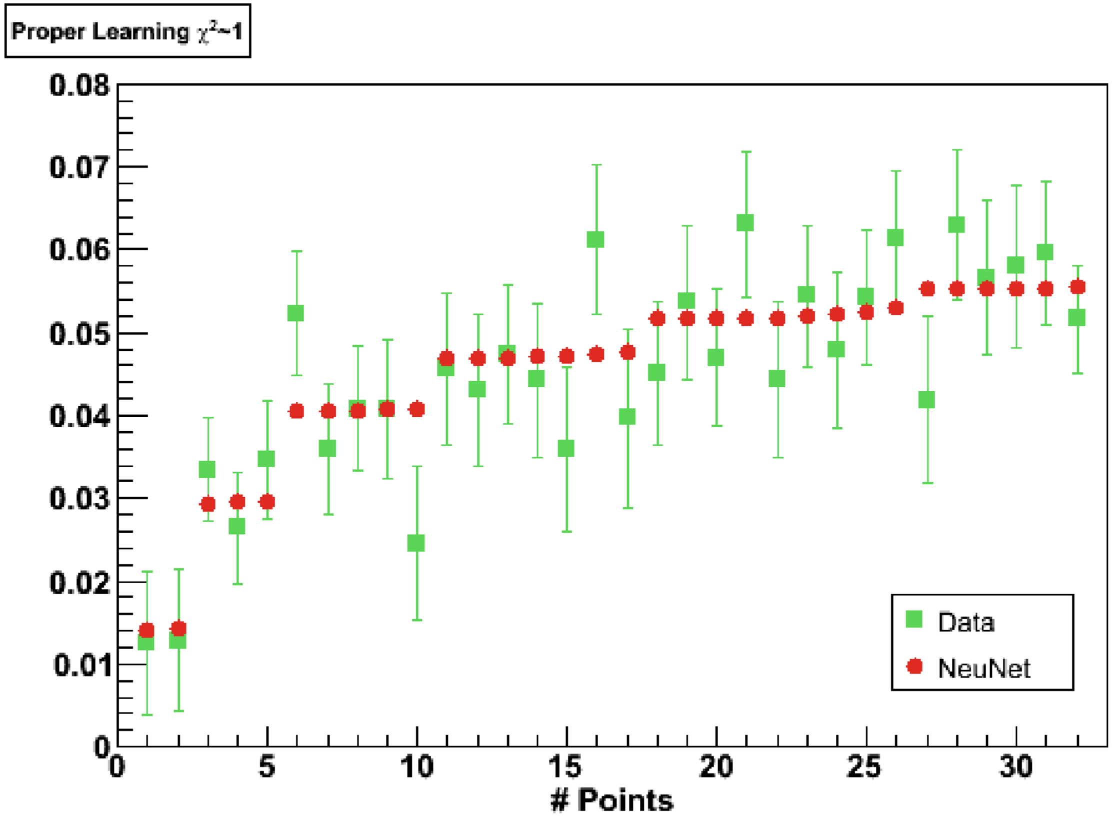
UNDERLEARNING



NEURAL LEARNING

- COMPLEXITY INCREASES AS THE FITTING PROCEEDS
- UNTIL LEARNING NOISE
- WHEN SHOULD ONE STOP?

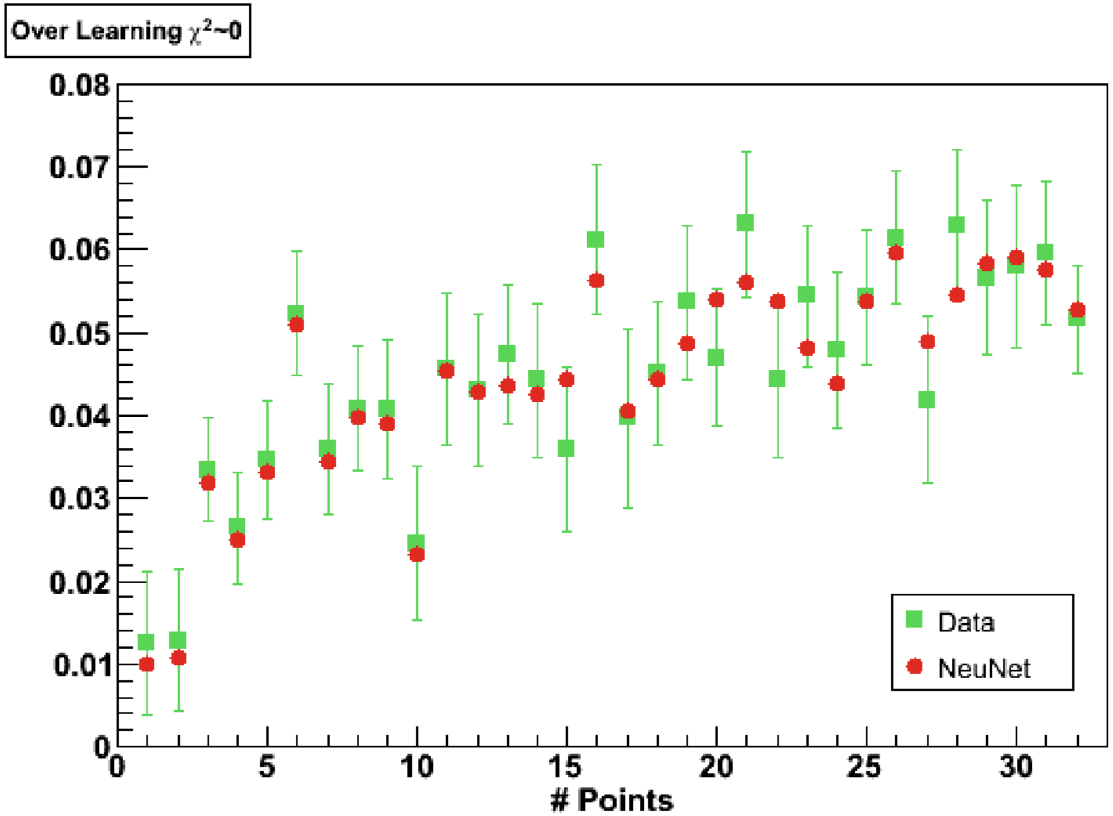
PROPER LEARNING



NEURAL LEARNING

- COMPLEXITY INCREASES AS THE FITTING PROCEEDS
- UNTIL LEARNING NOISE
- WHEN SHOULD ONE STOP?

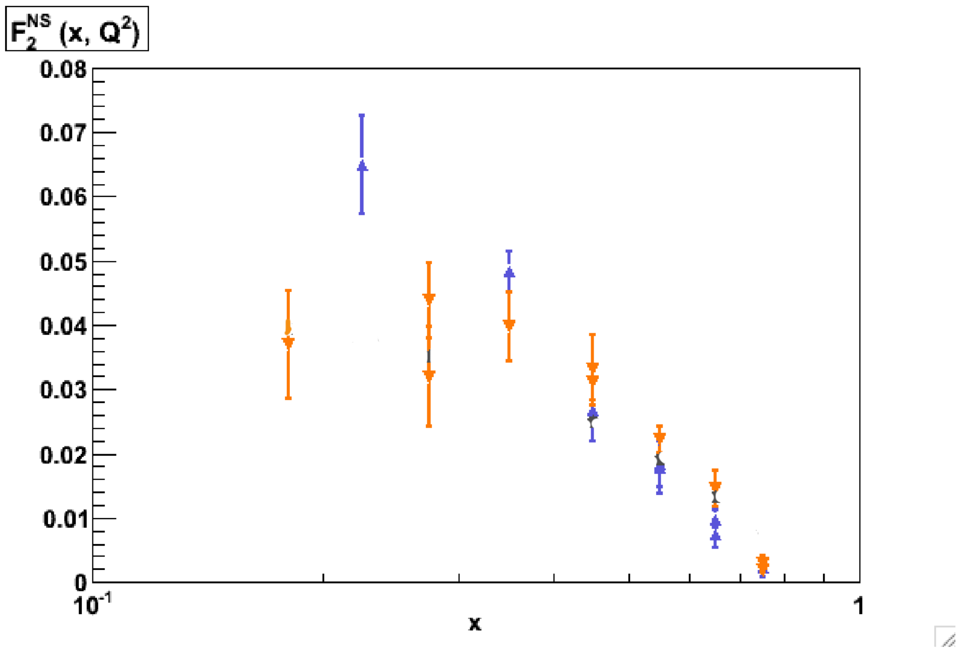
OVERLEARNING



OPTIMAL FIT: CROSS-VALIDATION

GENETIC MINIMIZATION:
AT EACH GENERATION, χ^2 EITHER UNCHANGED OR DECREASING

- DIVIDE THE DATA IN TWO SETS: TRAINING AND VALIDATION
- MINIMIZE THE χ^2 OF THE DATA IN THE TRAINING SET
- AT EACH ITERATION, COMPUTE THE χ^2 FOR THE DATA IN THE VALIDATION SET (NOT USED FOR FITTING)
- WHEN THE VALIDATION χ^2 STOPS DECREASING, STOP THE FIT



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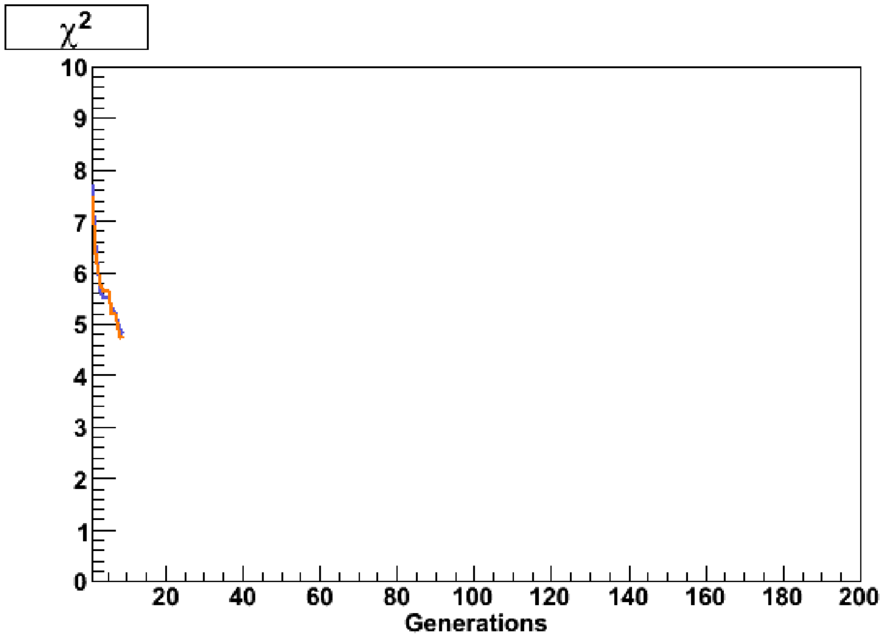
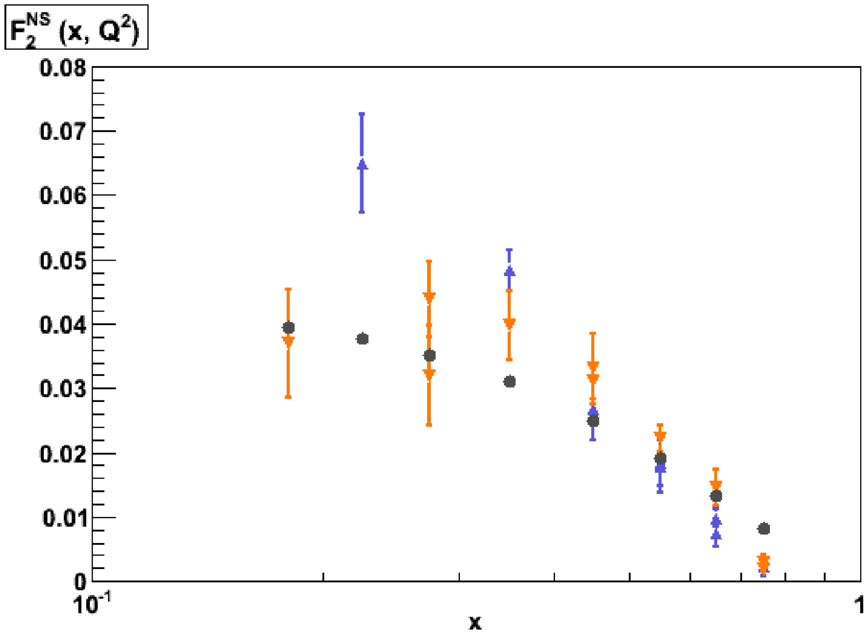
GO!





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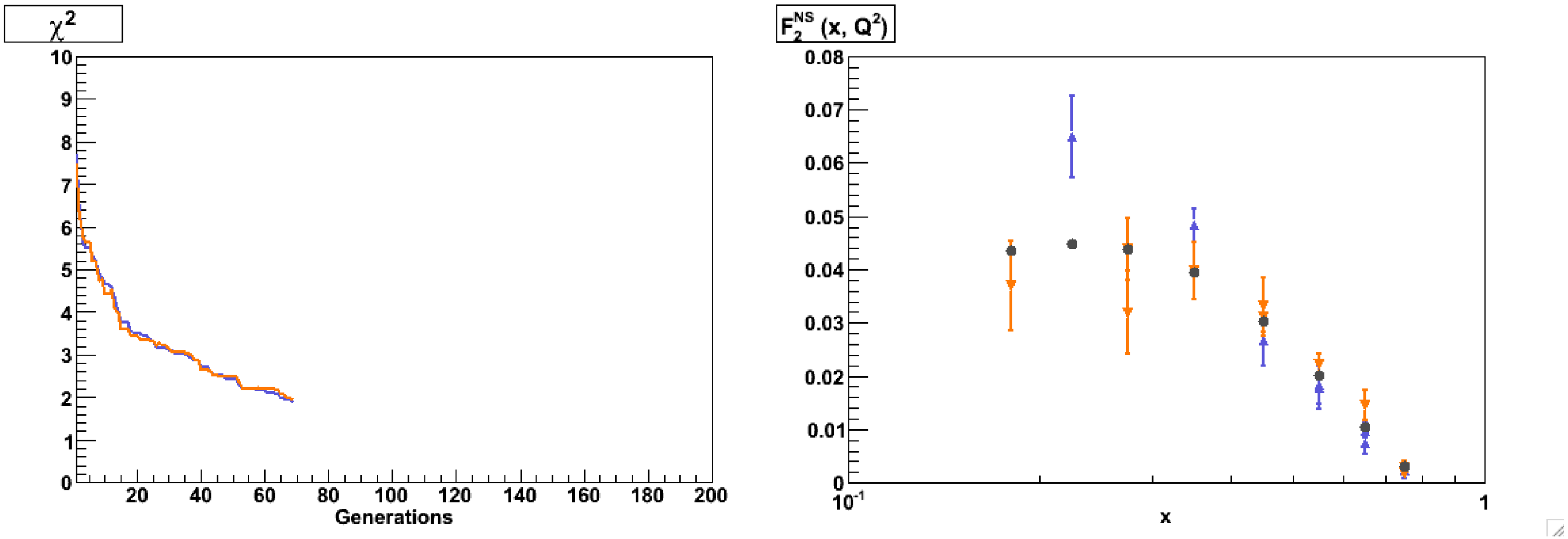
STOP!



OPTIMAL FIT: CROSS-VALIDATION

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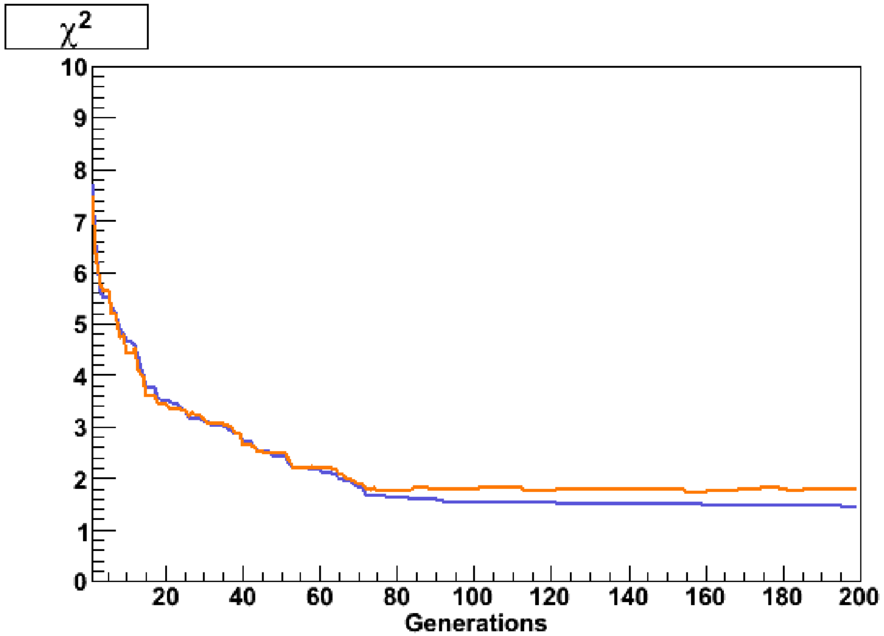
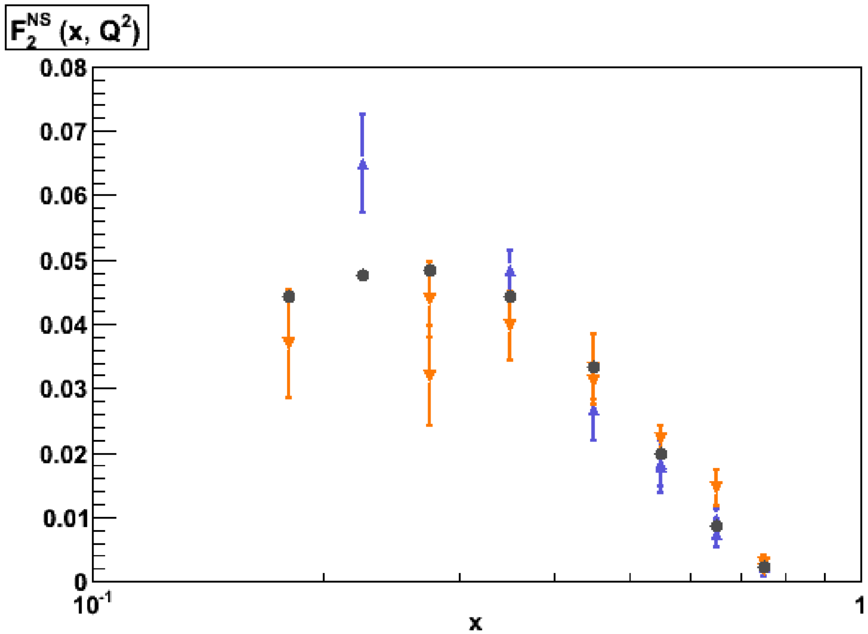
- WHEN THE VALIDATION χ^2 STOPS DECREASING, STOP THE FIT

TOO LATE!

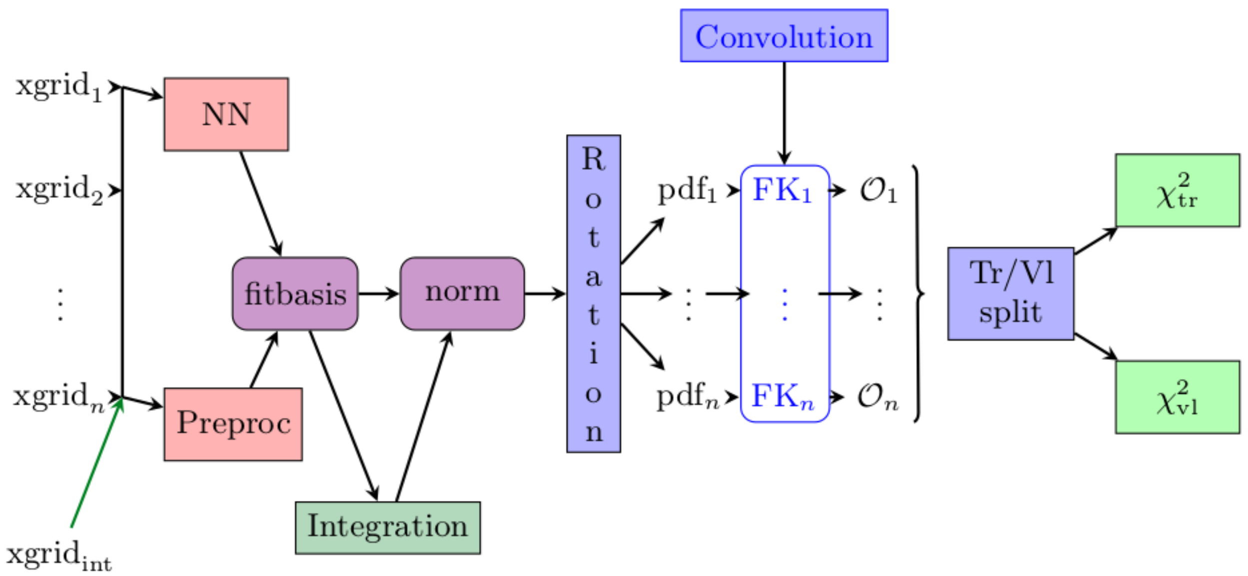




THE N3FIT PROJECT

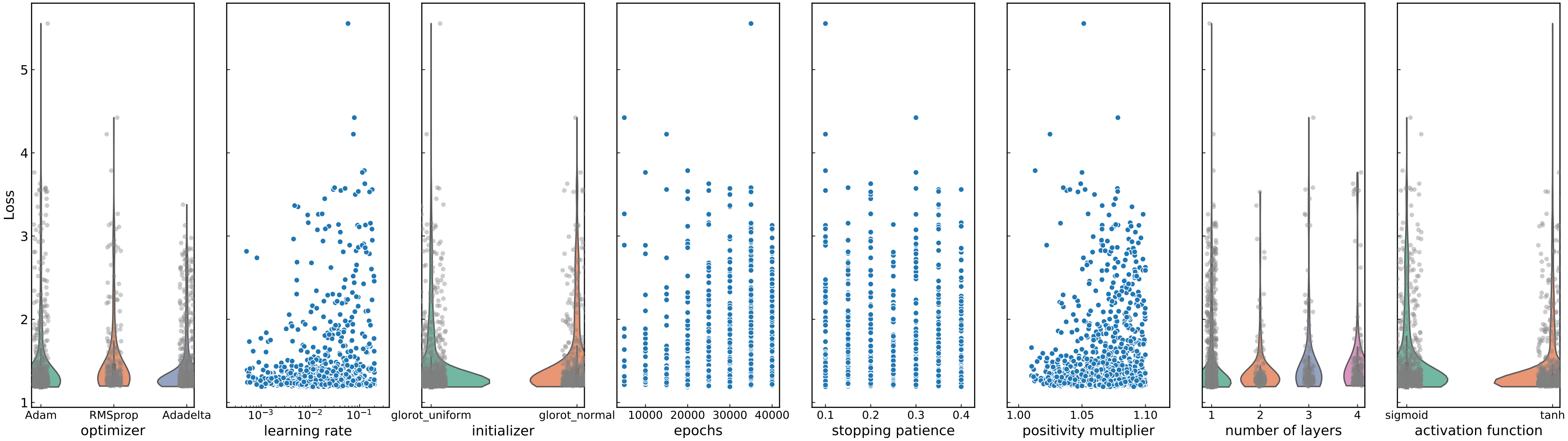
HOW DO WE KNOW THAT THE METHODOLOGY IS THE BEST?
"ACCUMULATED WISDOM" INEFFICIENT AND SLOW

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

FITTING THE METHODOLOGY
HYPEROPTIMIZATION SCANS



HYPEROPT PARAMETERS

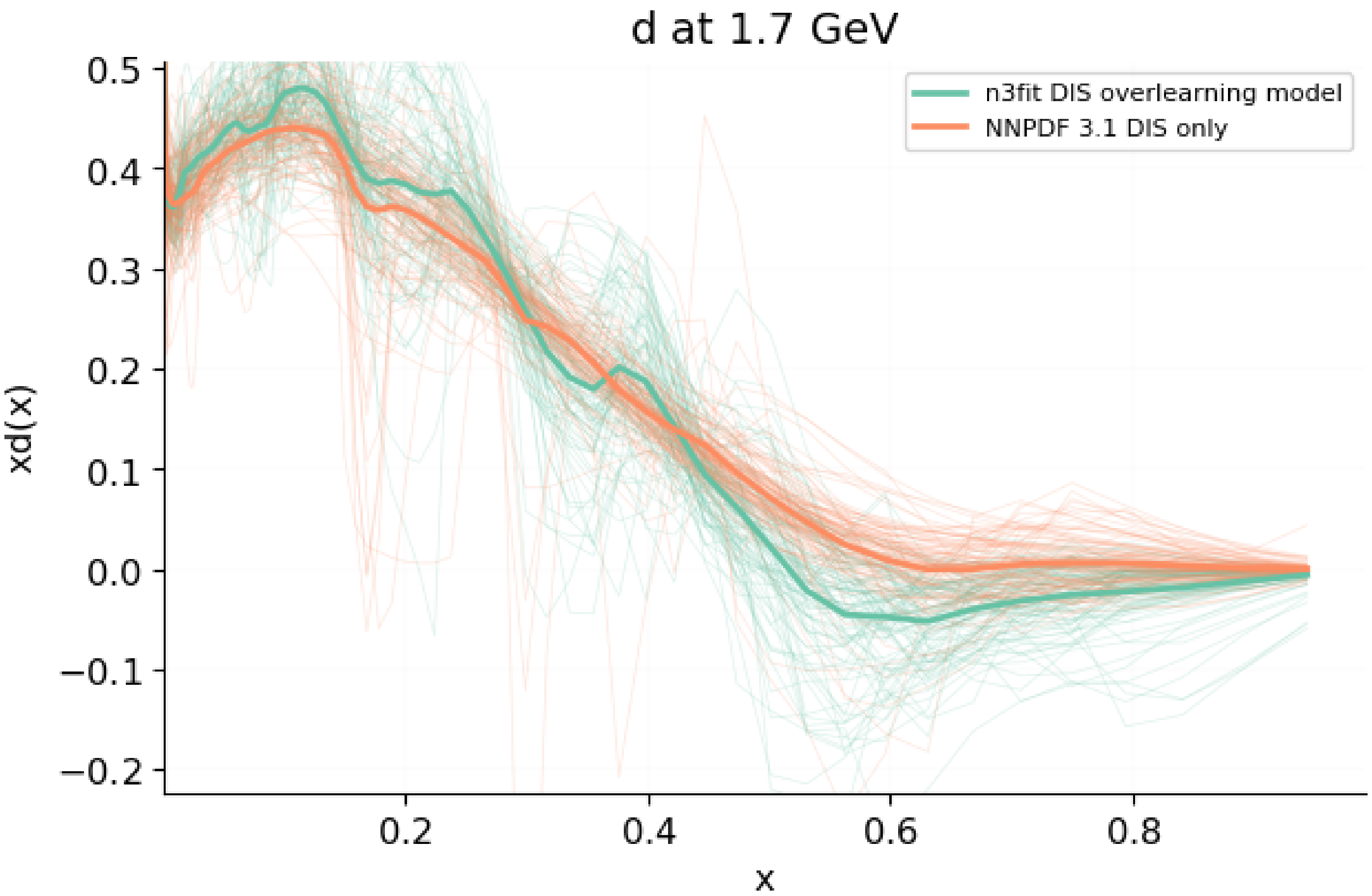
NEURAL NETWORK	FIT OPTIONS
NUMBER OF LAYERS (*)	OPTIMIZER (*)
SIZE OF EACH LAYER	INITIAL LEARNING RATE (*)
DROPOUT	MAXIMUM NUMBER OF EPOCHS (*)
ACTIVATION FUNCTIONS (*)	STOPPING PATIENCE (*)
INITIALIZATION FUNCTIONS (*)	POSITIVITY MULTIPLIER (*)

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

FITTING THE METHODOLOGY

THE OVERFITTING PROBLEM

DOWN QUARK: HYPEROPTIMIZED VS. STANDARD



- NNPDF3.1: 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?

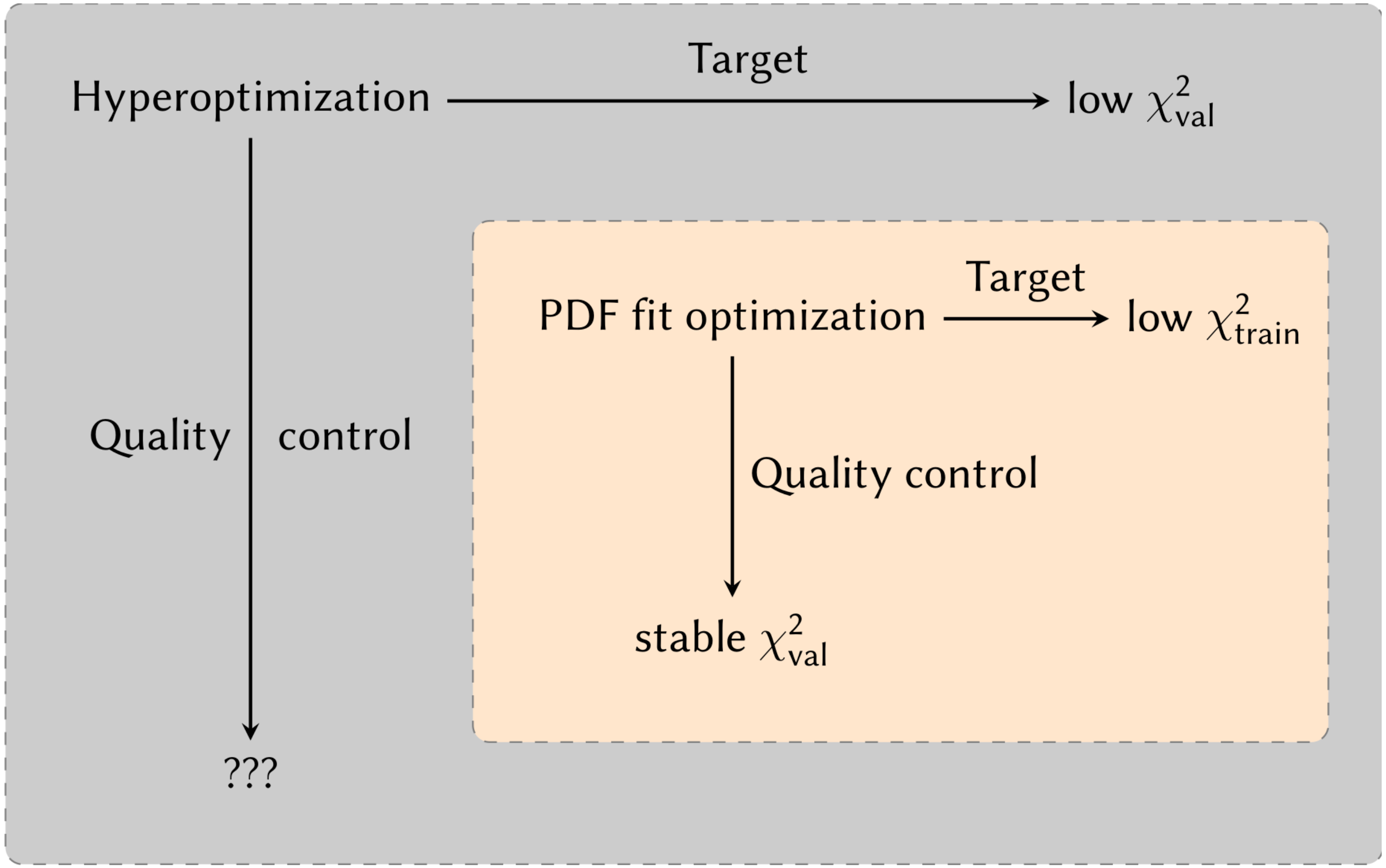
OPTIMIZATION

$$\begin{tikzcd}
\text{PDF fit optimization} \arrow[r, "\text{Target}"] \arrow[d, "\text{Quality control}"] & \text{low } \chi^2_{\text{train}} \\
\text{stable } \chi^2_{\text{val}} &
\end{tikzcd}$$

CROSS-VALIDATION SELECTS THE OPTIMAL MINIMUM

WHAT HAPPENED?

HYPEROPTIMIZATION

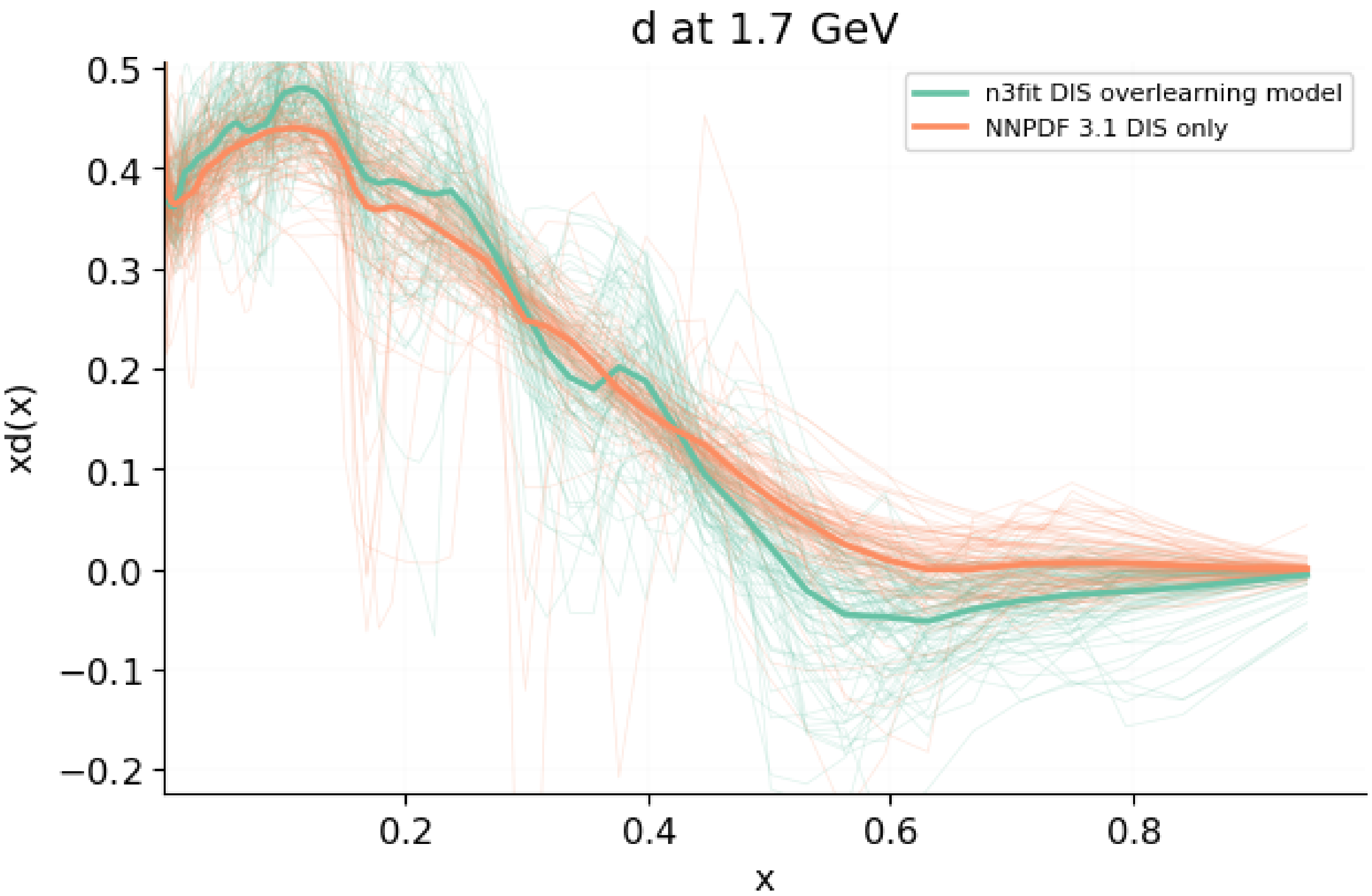


WE ARE MISSING A SELECTION CRITERION

FITTING THE METHODOLOGY

THE OVERFITTING PROBLEM

DOWN QUARK: HYPEROPTIMIZED VS. STANDARD

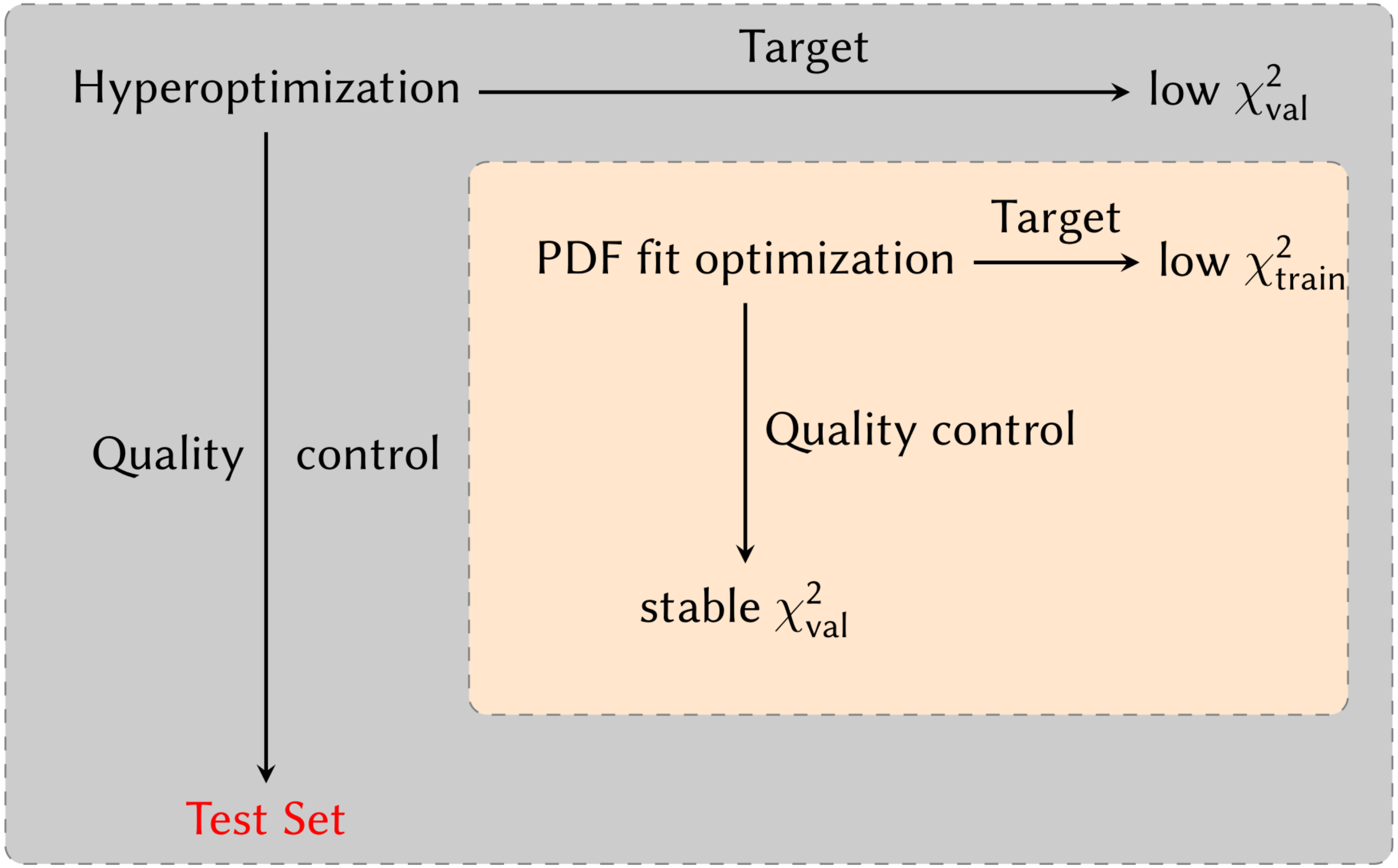


- NNPDF3.1: WIGGLES: FINITE SIZE $\Rightarrow$ WILL GO AWAY AS $N_{\rm rep}$ GROWS
- N3FIT: WIGGLY PDFS $\Leftrightarrow$ OVERFITTING $\Rightarrow$ WILL NOT GO AWAY ($\chi^2_{\rm train} \ll \chi^2_{\rm valid}$!!)
- CORRELATIONS BETWEEN TRAINING AND VALIDATION DATA

MACHINE LEARNING

THE SOLUTION

TUNED HYPEROPTIMIZATION



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

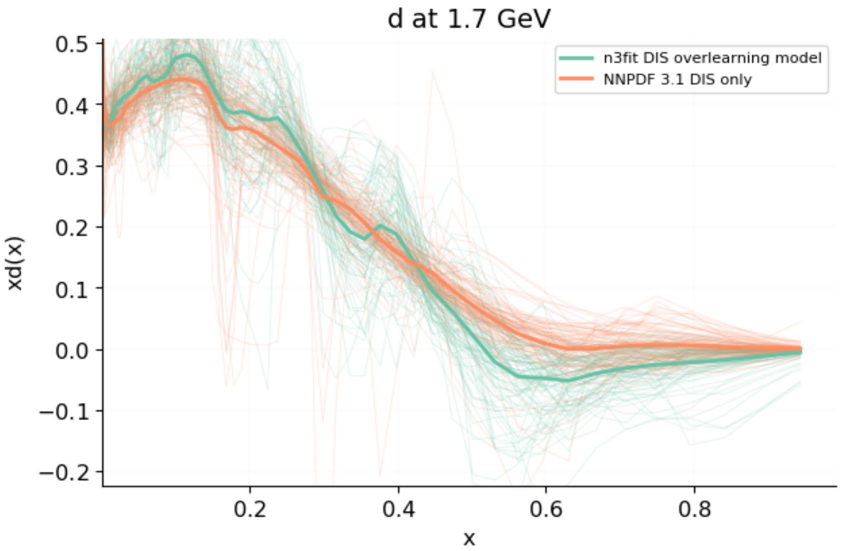
THE TEST SET METHOD

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

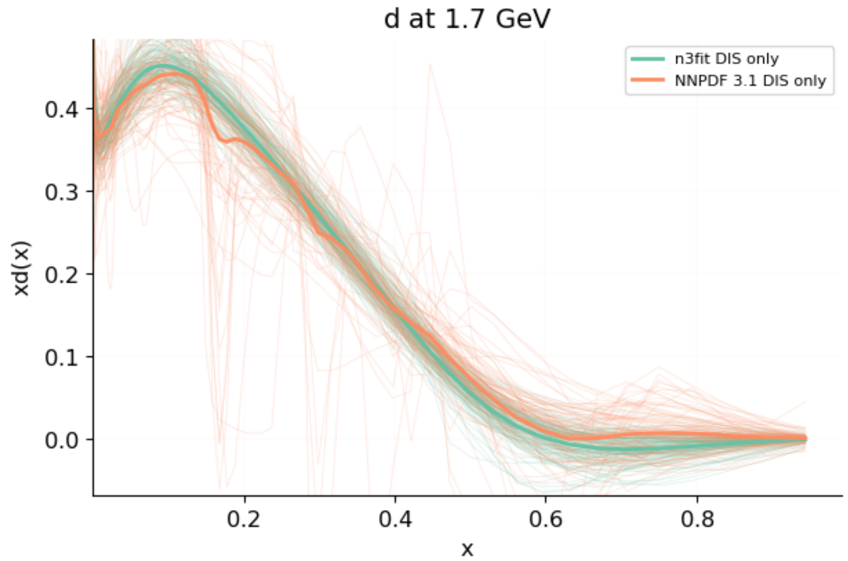
HYPEROPTIMIZED PDFs

DOWN QUARK

N3 OVERFIT vs NNPDF3.1



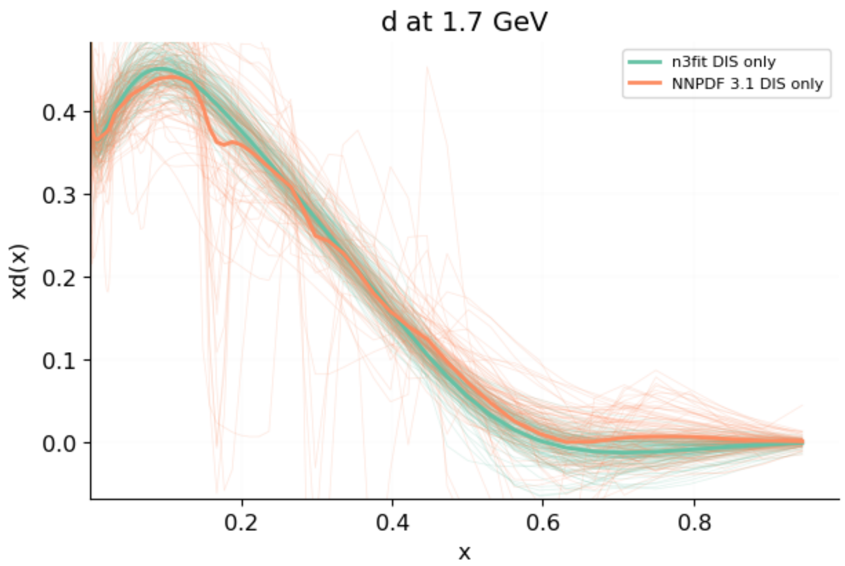
N3FIT vs NNPDF3.1



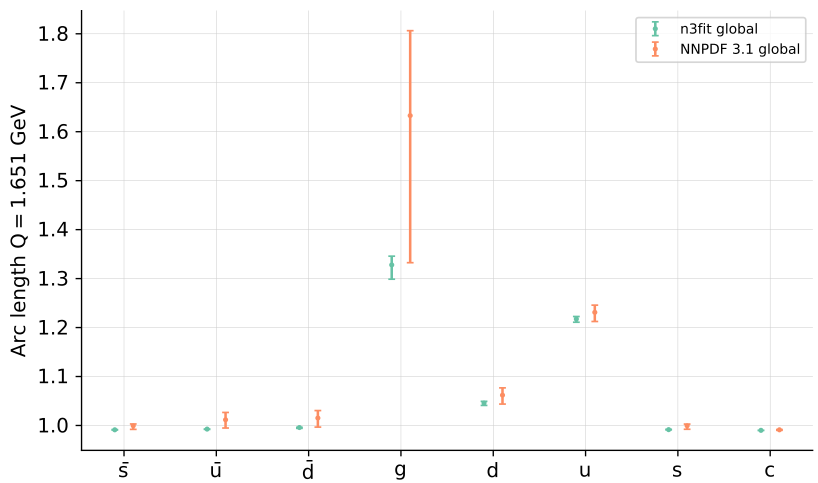
THE TEST SET METHOD

N3FIT vs NNPDF3.1

DOWN PDF



ARCLENGTHS



- NO OVERFITTING
- COMPARED TO NNPDF3.1
  - MUCH GREATER STABILITY $\Rightarrow$ FEWER REPLICAS FOR EQUAL ACCURACY
  - UNCERTAINTIES SOMEWHAT REDUCED