NNPDF

CLOSURE TESTS FOR PARTON DISTRIBUTIONS

STEFANO FORTE

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PDF4LHC

CERN, DECEMBER 13, 2013

TOWARDS NNPDF3.0

OPTMIZATION

- FULL MIGRATION OF THE CODE TO C++
- STREAMLINING, OPTIMIZATION AND DEBUGGING OF THE WHOLE CODE INCLUDING GENETIC ALGORITHM, NUMERICAL METHODS, ETC
- FAST INTERFACES `FastKernel + APPLGRID/FASTNLO` USED SYSTEMATICALLY
- $\Rightarrow$ MORE DETAILED MINIMIZATION
  TYPICAL FIT: $\sim$ 4000 DATAPOINTS FOR 50000 ITERATIONS OF A GA WITH 80 MUTANTS:
  $\sim 10^{10}$ PREDICTIONS COMPUTED FOR EACH REPLICA
  (50H COMPUTING PER REPLICA ON CERN `lxplus`)

NEW DATA:

ALL LHC DATA WITH INFO ON SYSTEMATICS

- ATLAS: HIGH-MASS DRELL-YAN (2011); JETS 2.76 TEV
- CMS: W μ ASYM 5 fb^{-1}; CMS W+CHARM 5 fb^{-1}; DOUBLE-DIFFERENTIAL DRELL-YAN; INCLUSIVE JETS 5 FB^{-1}
- LHCB $Z \to e^+e^-$ RAPIDITY DISTN. (2011)
- HERA II COMBINED F_2^c
- H1 HERA-II INCLUSIVE F_2
- ZEUS HERA-II INCLUSIVE F_2
- ATLAS W p_T DISTN; ATLAS PROMPT PHOTON; LHCB $Z \to \mu^+\mu^-$ RAPIDITY DIST.; ATLAS+CMS TOP RAPIDITY DISTN.: UNDER CONSIDERATION (PRELIMINARY DATA, INTERFACES BEING DEVELOPED &C...)

MINIMIZATION STRATEGY BASED ON A CLOSURE TEST

CLOSURE TESTS

WHAT IS A CLOSURE TEST?

- ASSUME UNDERLYING PDFS KNOWN
- GENERATE DATA WITH GIVEN STATISTICAL AND CORRELATED SYSTEMATICS
- PERFORM A FIT & COMPARED TO "TRUTH"
- PREVIOUS STUDIES BY THORNE & WATT (2012) ALONG SIMILAR LINES

LEVELS

- DATA ARE GENERATED FOR THE SAME KINEMATICS OF ALL DATA IN NNPDF2.3 USING UNDERLYING MSTW08 PDFS (CT10 ALSO TRIED)
- LEVEL 0:
  - EACH DATAPOINT EQUAL TO THE MSTW "TRUE VALUE"; UNCERTAINTY ASSUMED TO COINCIDE WITH THE EXPERIMENTAL ONE
  - FIT → MUST FIND $\chi^2 = 0$ (GET BACK MSTW "TRUTH")
- LEVEL 2:
  - EACH DATAPOINT IS OBTAINED AS A RANDOM FLUCTUATION WITH GIVEN COVARIANCE MATRIX ABOUT MSTW "TRUTH"
  - GENERATE PSEUDODATA REPLICAS OF THESE "DATA"
  - THEN FIT PDF REPLICAS TO PSEUDODATA REPLICAS
  - FIT MUST FIND (PER DATAPOINT) $\chi^2 = 1$ (best-fit to data); $\langle E \rangle = 2$ (fit of each replica to data replica); $\langle \chi^{2\,(1)} \rangle = 1$ (fit of each replica to data)
  - MUST FIND THAT (PREDICTION)-(THEORY) IS COMPATIBLE WITH ZERO WITHIN ERRORS
  - MUST FIND THAT MSTW "TRUE PDFS" IS WITHIN ONE σ BAND IN 68% OF CASES

(LEVEL 1: SAME AS LEVEL 2, BUT WITHOUT PSEUDODATA REPLICAS)

STOPPING VS. WEIGHT PENALTY

- NNPDF OPTIMAL FIT CURRENTLY DETERMINED BY CROSS-VALIDATION: DATA RANDOMLY DIVIDED IN TWO SETS, χ^2 OF FITTED (TRAINING) DATASET KEEPS DECREASING BUT χ^2 OF NON-FITTED (VALIDATION) DATASET STARTS INCREASING
- MUST INTRODUCE THRESHOLDS FOR INCREASE & DECREASE BASED ON TYPICAL χ^2 FLUCTUATIONS
- ALTERNATIVE IDEA: INTRODUCE A MEASURE OF THE COMPLEXITY OF THE j-TH NN: $\Delta_j = \sum_{i=1}^{N_w} (w_i^j)^2$
- THEN ADD TO χ^2 A WEIGHT-PENALTY $f(w_i) = \sum_{j=1}^{N_{pdfs}} \alpha_j \Delta_j$ AND MINIMIZE χ^2
- CONSTANTS α_j DETERMINED BY EXPECTED COMPLEXITY OF THE j-TH NETWORK BASED ON PREVIOUS FIT: $\alpha_i = \left[\frac{\langle \Delta_i \rangle}{N_w}\right]^{-1}$
- ITERATE UNTIL CONVERGENCE
- FITS STOPS WHEN NETWORKS FIT THE DATA BUT ARE NOT TOO COMPLEX

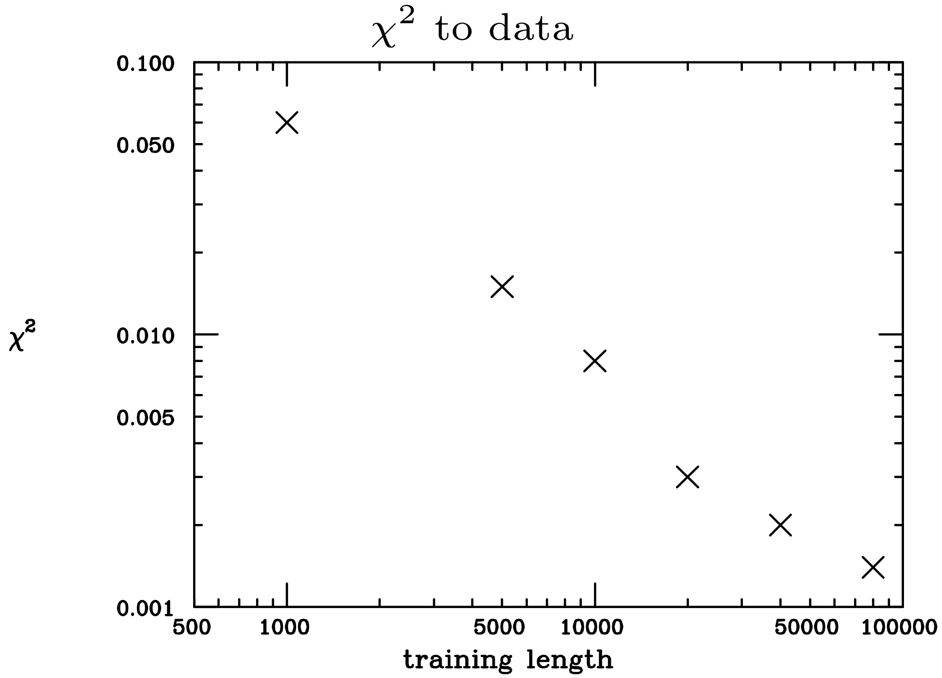
ADVANTAGES

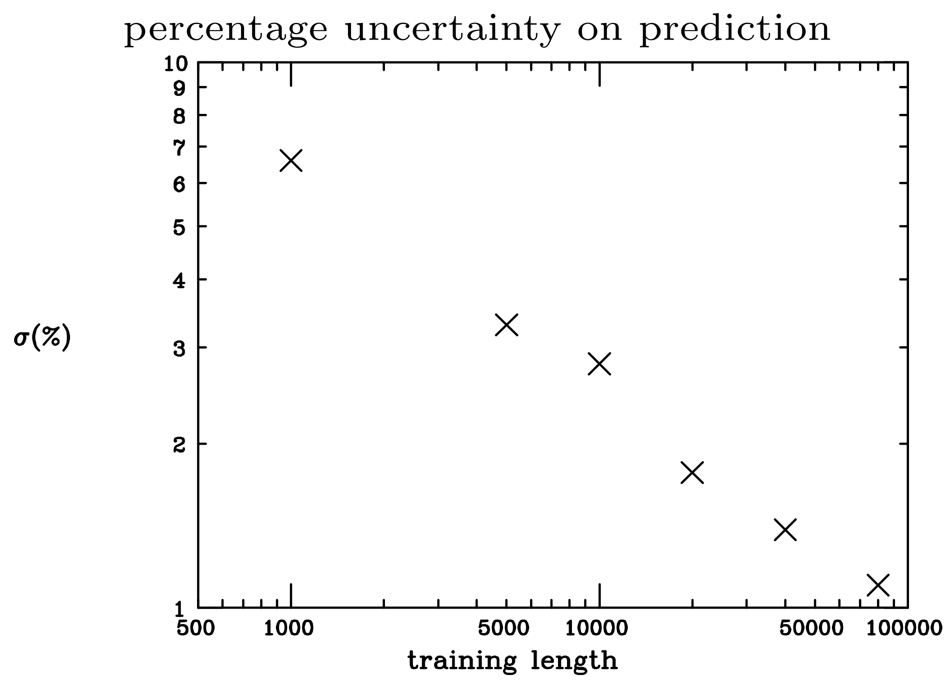
- OPTIMAL WEIGHTS DETERMINED SELF-CONSISTENTLY
- NO OVERLEARNING $\rightarrow$ NO STOPPING CRITERION NEEDED (JUST MAKE FIT LONG ENOUGH)
- NATURALLY SMOOTH PDF SHAPES

LEVEL-0 CLOSURE

- FITS PRODUCED WITH INCREASING (FIXED) TRAINING LENGTH
- ALL FITS WITH SAME DATA AND SAME RANDOM SEED (RANDOM SEED INDEP SEPARATELY TESTED)
- GOODNESS OF FIT TO DATA AND PERCENTAGE UNCERTAINTY ON PREDICTION STUDIED VS. TRAINING LENGTH
- χ^2 MUST GO TO ZERO; σ MUST GO TO ZERO AT DATA LEVEL, NOT AT PDF LEVEL

FIT QUALITY





PERFECT FIT!

LEVEL-2 CLOSURE

FIXED-LENGTH FITS TO 100% OF DATA (NO CROSS-VALIDATION)

FIT QUALITY

- AT 10K GA ITERATIONS, $\chi^2 = 0.96$, $\langle E \rangle = 2.0$ (NOTE $\chi^2_{mstw} = 0.96$)
- CHECKED AGAIN AT 20K, 40K, 80K: SAME PERFECT VALUES (TO TWO DECIMAL PLACES)

AGREEMENT WITH THEORY (DATA LEVEL)

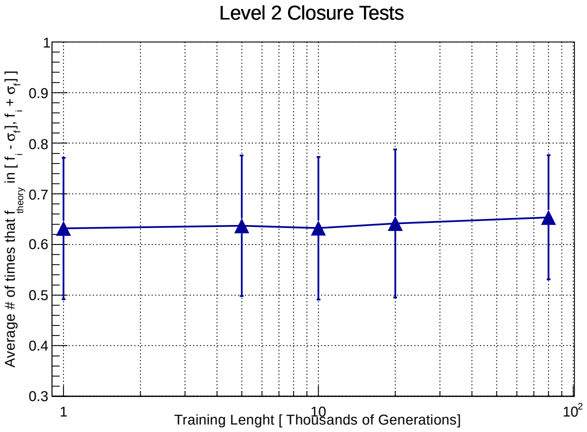
- COMPARE PREDICTION TO THEORY $$\frac{\left(F_i^{(0),\mathrm{nnpdf}} - F_i^{\mathrm{mstw}}\right)^2}{\left(\Delta F_i^{\mathrm{nnpdf}}\right)^2}$$
- AVERAGE OVER DATAPOINTS, DIFFERENT TL & METHODS: PERFECT

	NO WP	WP
10K	0.948 ± 0.854	0.638 ± 0.714
20K	0.966 ± 0.916	0.613 ± 0.732
40K	1.01 ± 1.00	0.622 ± 0.788

AGREEMENT WITH THEORY (PDF LEVEL)

- COMPARE PDF TO THEORY $\left[q_l^{(k)}(x_i) - \Delta q_l^{(k)}(x_i), q_l^{(k)}(x_i) + \Delta q_l^{(k)}(x_i)\right]$ AT $x = 0.01, 0.1, 0.2, 0.3, 0.4, 0.5, 0.7$ FOR ALL PDFs
- FRACTION WHICH FALLS WITHIN ONE σ
- NO WP SHOWN, WP SIMILAR: PERFECT

fraction within one σ



OVERLEARNING

- IT LOOKS LIKE AT 10K A PERFECT FIT IS REACHED
- NO OVERLEARNING → NO STOPPING CRITERION NEEDED (EVEN W/O WP)
- IS IT POSSIBLE?
- PDFS SHOULD STOP CHANGING WITH TL?:

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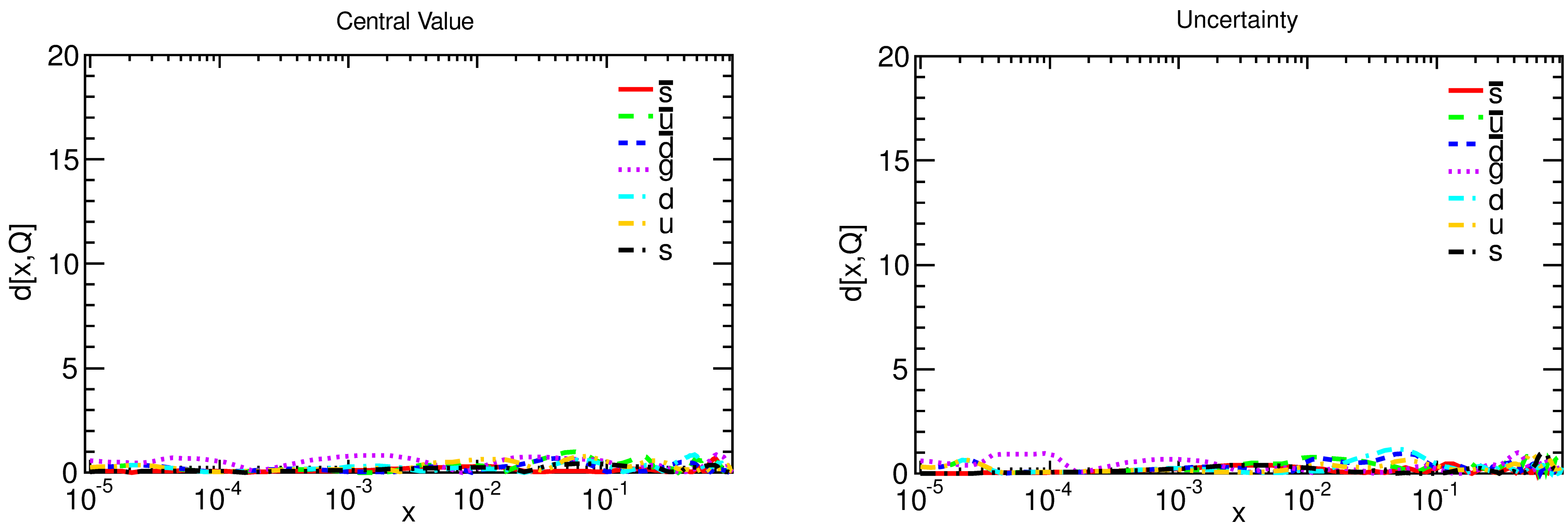
DISTANCES BETWEEN PDFs @ 10K AND 20K



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- PDFS SHOULD STOP CHANGING WITH TL?: THEY DO!
- UNCERTAINTIES MUST BE DRIVEN BY DATA FLUCTUATIONS
- TEST: REPEAT FIT WITH RESCALED UNCERTAINTIES
  $\Rightarrow$ FIT SHOULD BE UNCHANGED

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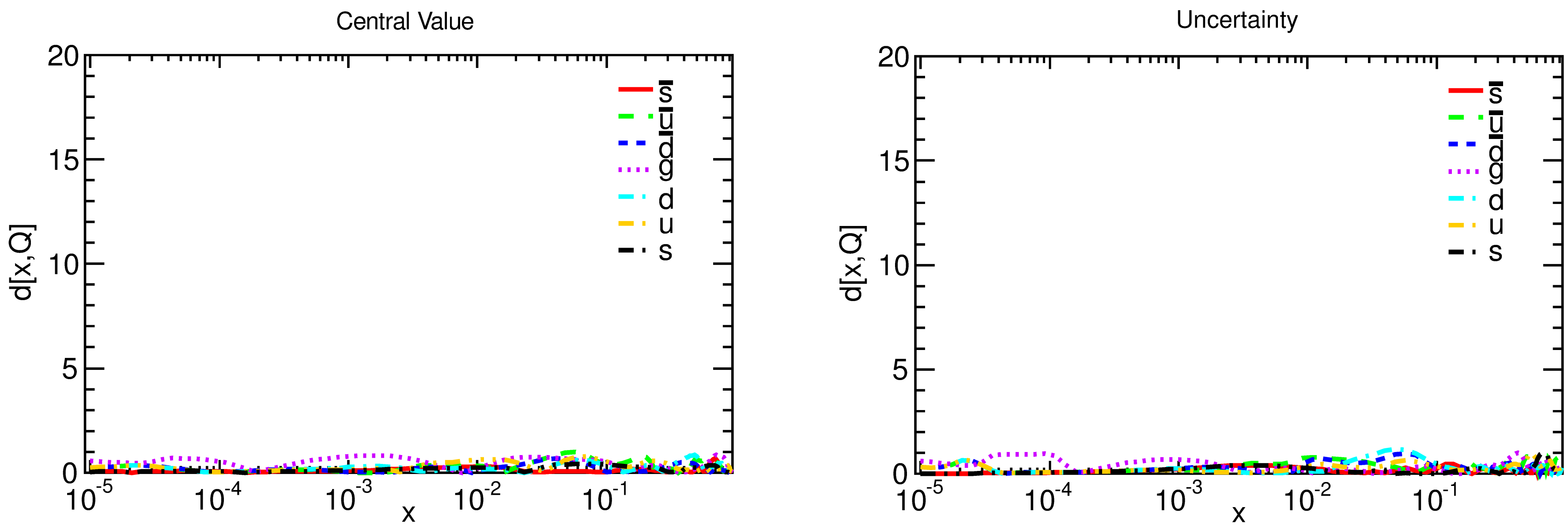

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- RESULT: UNRESCALED: $\chi^2 = 0.964$;
  RESCALED BY $\times 2$: $\chi^2 = 0.245$ $(0.964/4 = .241)$;
  RESCALED BY $\times 0.65$: $\chi^2 = 2.280$ $(0.964/.65^2 = 2.281)$: IT IS!

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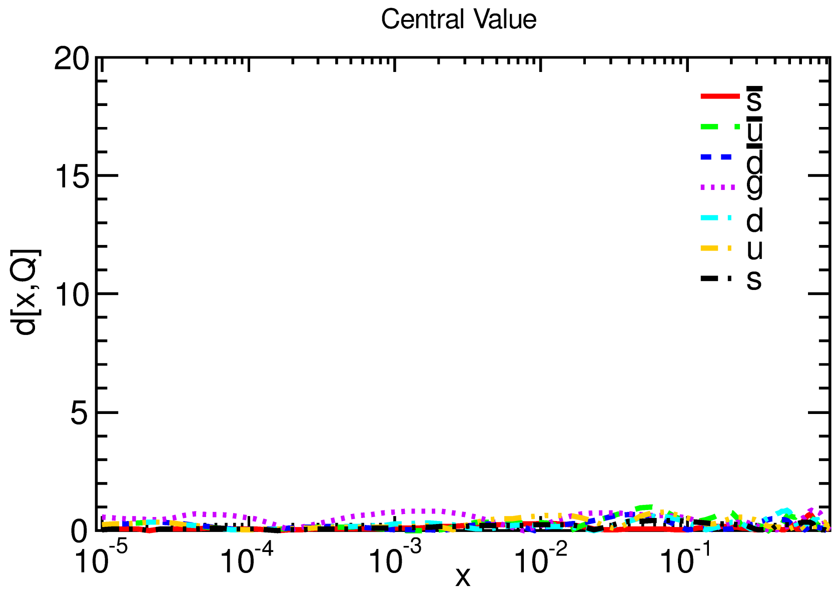

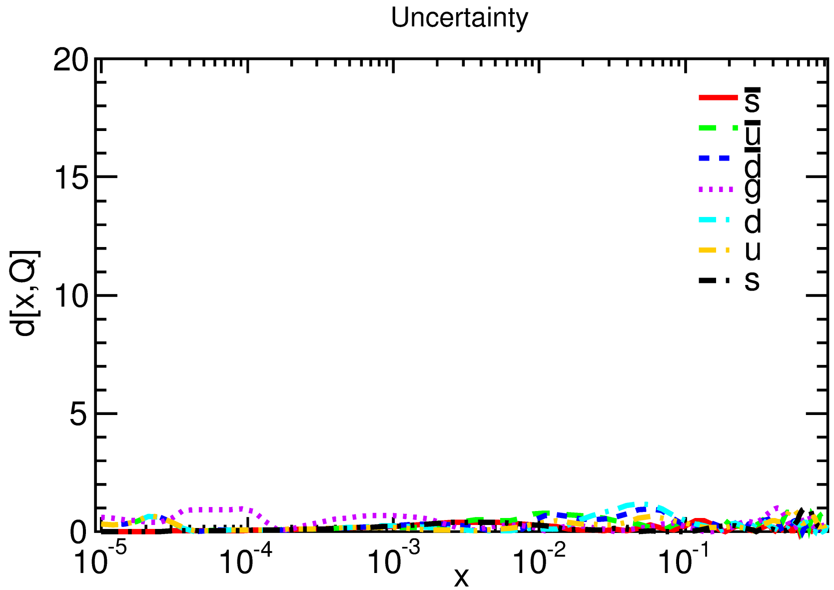

WHEN IS OVERLEARNING POSSIBLE?

- FOR ONE DATAPOINT, $\chi^2 = \frac{(t-d)^2}{\sigma^2}$, $\chi^2 = 0$ IF $t = d$
- BUT FOR TWO DATAPOINTS, $\chi^2 = \frac{(t-d_1)^2+(t-d_2)^2}{\sigma^2}$, minimum $\chi^2_{\min} = \frac{(d_1-d_2)^2}{4\sigma^2}$, IF d_i DRAWN FROM A RANDOM SAMPLE, $\chi^2_{\min} = \frac{1}{2}$
- FOR N DATAPOINTS, $\chi^2_{\min} = 1 - \frac{1}{N}$
  IF THERE ARE INFINITELY MANY MEASUREMENTS AT THE SAME POINT $\chi^2_{\min} = 1$
  $\Rightarrow$ NO OVERLEARNING

- TEST: REDUCE FRACTION OF FITTED DATA
- COMPUTE χ^2 OF FITTED & NON-FITTED DATA
- STUDY AS FUNCTION OF TRAINING LENGTH

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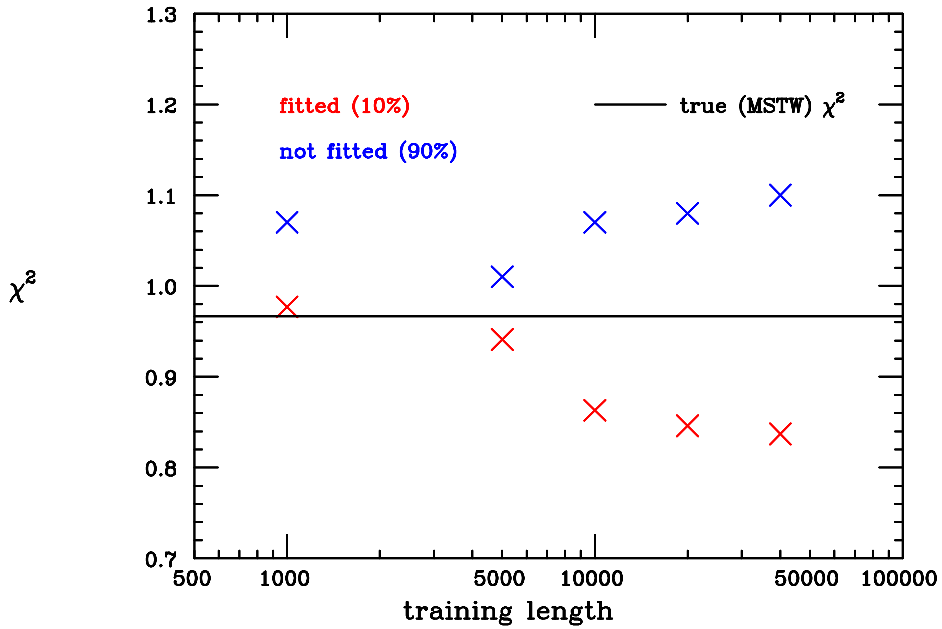
- TEST: REDUCE FRACTION OF FITTED DATA
- COMPUTE χ^2 OF FITTED & NON-FITTED DATA
- STUDY AS FUNCTION OF TRAINING LENGTH
- OVERLEARNING SETS IN AROUND 5000 GA ITERATIONS
- 'DATA REDUNDANCY' OF ORDER ~ 10

FIT TO 10% OF DATA



MICRO-OVERLEARNING

- EVEN IF NO OVERLEARNING VISIBLE
(PDFS DO NOT CHANGE IN STATISTICALLY SIGNIFICANT WAY)
CAN EXPLOIT KNOWLEDGE OF "TRUE" UNDERLYING THEORY
- $\Rightarrow$ COMPARE χ^2 OF FIT TO χ^2 OF "TRUTH": $\chi^2 = \chi^2_{\rm mstw}$
(REMEMBER PSEUDODATA FLUCTUATE ABOUT TRUTH, SO $\chi^2_{\rm mstw} \sim 1$)
- WHEN $\chi^2 < \chi^2_{\rm mstw}$ OVERLEARNING SETS IN

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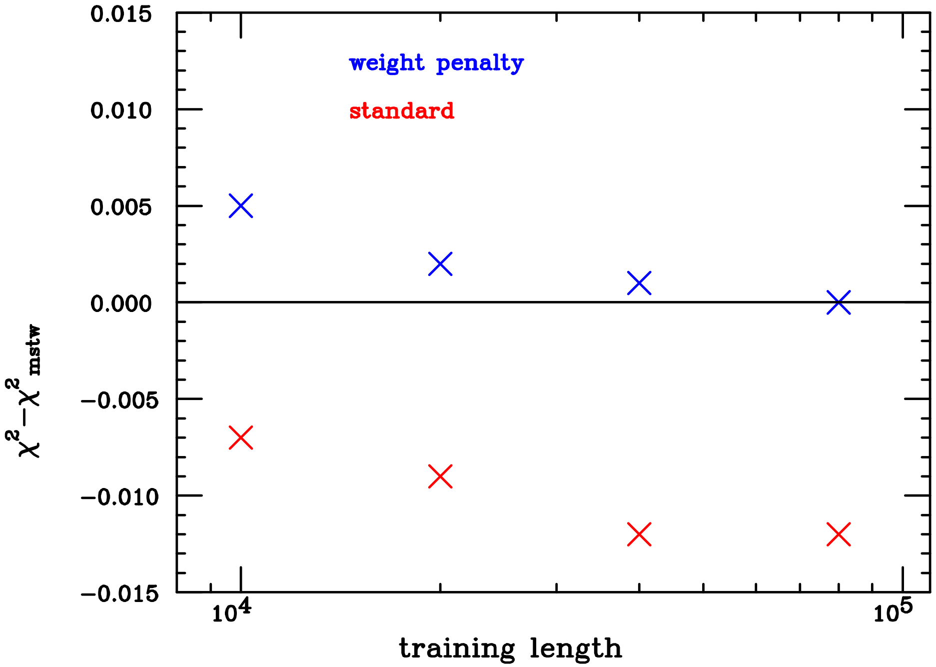
$\chi^2 - \chi^2_{\mathrm{mstw}}$ VS. TRAINING LENGTH



- DIFFERENCE COMPUTED BOTH FOR NON-WP & WP MIND SCALE ON y AXIUS!!
- NON-WP MICRO-OVERLEARNS SOMEWHERE AROUND 10K
- WP DOES NOT EVEN MICRO-OVERLEARN UP TO 80K
- MICRO-OVERLEARNING: MUCH SMALLER THAN STAT. FLUCTUATIONS ($\Delta\chi^2 \ll \sigma_{\chi^2}$)

MORE TESTS

- ANALYSIS OF χ^2 PROFILES (INCLUDING FOR INDIVIDUAL EXPERIMENTS)
  $\Rightarrow$ NO STATISTICALLY SIGNIFICANT OVERLEARNING SEEN
- DETAILED COMPARISON BETWEEN WP & NON-WP
- DEPENDENCE ON TRAINING LENGTH
- DEPENDENCE ON RANDOM SEED
- DEPENDENCE ON THE UNDERLYING SET I: CTEQ VS MSTW
- DEPENDENCE ON THE UNDERLYING SET II: SINUSOIDAL OSCILLATION ADDED ON TOP OF MSTW
- FITS WITH HUGE NEURAL NETWORK ARCHITECTURE:
  2-20-15-1, I.E. 391 PARMS PER NETWORK, 2737 IN TOTAL
  $\Rightarrow$ RESULTS ARE NOT DRIVEN BY NEURAL NETWORK SIZE

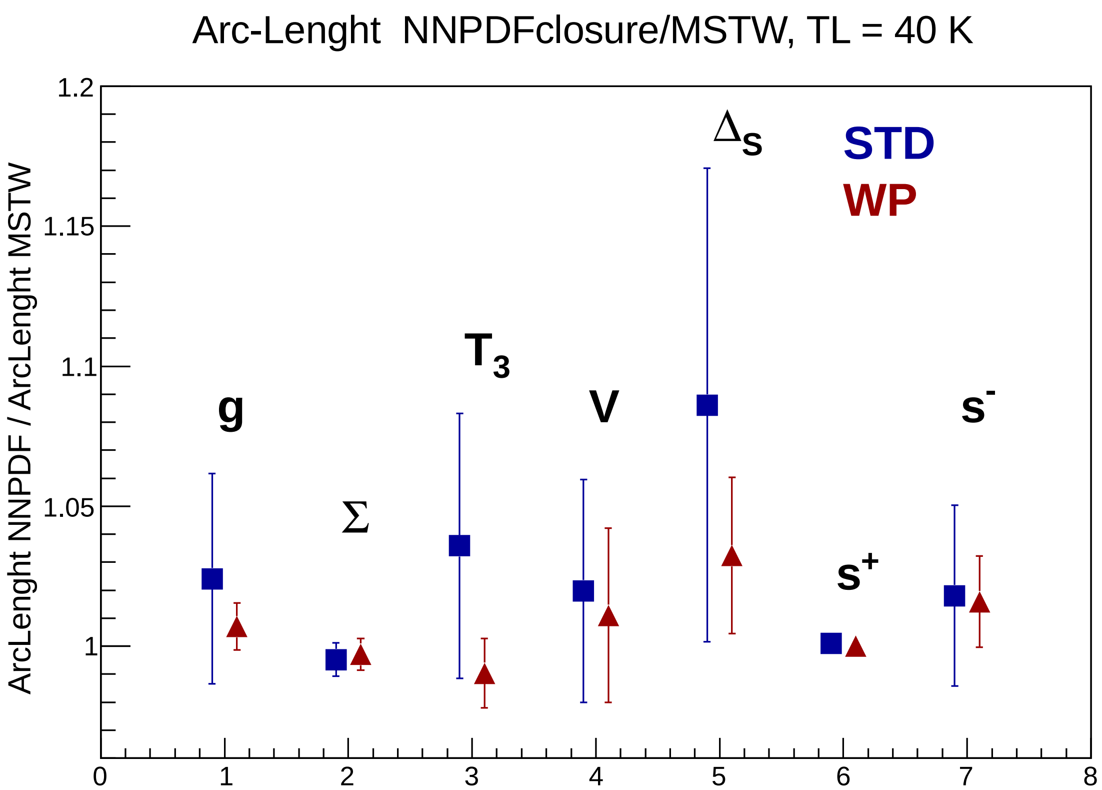
CONCLUSION

- FIXED-LENGTH FIT FULLY ADEQUATE,
- NO OVERLEARNING
- EFFECT OF WP VERY MODERATE

FLUCTUATIONS AND ARC-LENGTH

- DO WE REALLY NEED WEIGHT-PENALTY?
- LOOK AT ARC-LENGTH!: $L = \int_0^1 \sqrt{1 + \left(\frac{df}{dx}\right)^2} dx$
- SUGGESTED BY Moch, Glazov Radescu (2011) AS PENALTY FOR CHEBYSHEV POLY FITS: BUT HOW TO DETERMINE PENALTY? WP SELF-CONSISTENT!
- $\langle L \rangle$ SIMILAR FOR STANDARD AND WP, BUT σ_L RATHER SMALLER FOR WP; (ALSO, MORE STABLE W.R. TO TRAINING LENGTH)
  $\Rightarrow$ WP FIT MORE STABLE, & WITH SMALLER UNCERTAINTIES

ARC-LENGTH NORMALIZED TO "TRUTH"

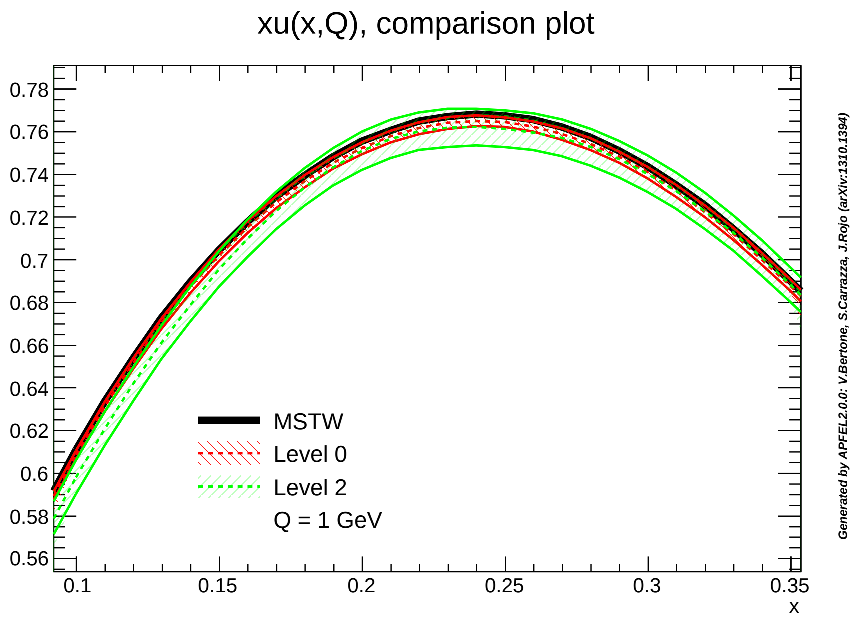


FUNCTIONAL VS. DATA UNCERTAINTY

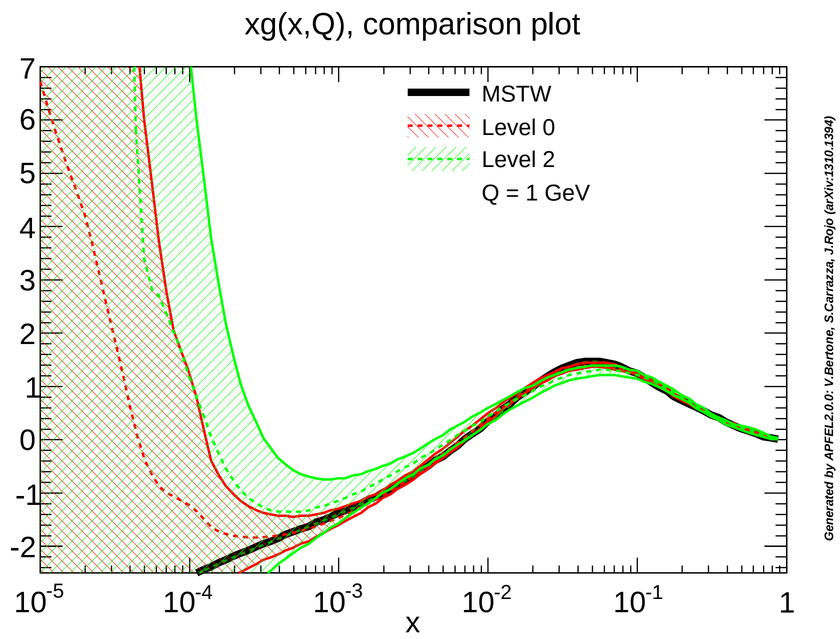
- LEVEL 2 UNCERTAINTY IS FAITHFUL REPRESENTATION OF UNDERLYING DATA UNCERTAINTY
- LEVEL 0 FIT UNCERTAINTY IS MINIMAL UNCERTAINTY WHEN DATA HAVE ZERO UNCERTAINTY → "FUNCTIONAL" UNCERTAINTY
- "TRUTH" (MSTW) IS CONTAINED WITHIN BOTH BANDS
- IN DATA REGION DATA UNC. $\ll$ FUNCTIONAL UNC.
  IN EXTRAPOLATION REGION DATA UNC. $\sim$ FUNCTIONAL UNC.

PDFS AT PARAMETRIZATION SCALE

up



gluon



OUTLOOK

- FURTHER STUDIES POSSIBLE/INTERESTING:
  - INTRODUCE "ARTIFICIAL INCONSISTENCIES" IN DATA (MISS OUT SOME SYSTEMATICS) & SEE HOW FIT BEHAVES
  - STUDY IN CONTROLLED SETTINGS IMPACT OF SPECIFIC DATASETS ON PDF KNOWLEDGE
  - DETERMINE $\Delta\chi^2$ CRITERIA $\Rightarrow$ BENCHMARKING
- CURRENT METHODOLOGY FULLY ADEQUATE FOR NNPDF3.0