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THE ART OF SOLVING ILL-POSED PROBLEMS

STEFANO FORTE UNIVERSITÀ DI MILANO & INFN



UNIVERSITÀ DEGLI STUDI DI MILANO DIPARTIMENTO DI FISICA



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LHCP19

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SUMMARY PDFs NOW

- FROM PDF4LHC15 TO NEW GENERATION SETS
- THE IMPACT OF LHC DATA
- RESOLVING ISUES WITH DATA: STRANGENESS & CHARM

FITTING THE METHODOLOGY

- DATA VS. METHODOLOGY
- DATASET OPTIMIZATION
- METHODOLOGY OPTIMIZATION

THEORY UNCERTAINTIES

- PDF THEORY ERRORS
- SCALE VARIATION
- TESTING THEORY ERRORS

THE STATE OF THE ART

CONTEMPORARY PDF TIMELINE (ONLY PUBLISHED GLOBAL)

	2008		2009		2010		2011	2011 2012		2013		2014		2015 2017		017
SET	CTEQ6.6	NNPDF1.0	MSTW 01	ABKM09	NNPDF2.0	(NLO)	NNPDF2.1 (NNLO)	ABM11 (02)	NNPDF2.3	(NNLO)	ABM12 (10)	ONNPDF3.0	MMHT (12)	CT14 (06)	ABMP16	NNPDF3.10
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LHC JETS	×	×	×	×	×	×	×	×	~	×	×	 	~	 	×	✓
TOP TOTAL	X	×	×	×	X	×	X	×	×	×	~	~	×	×	~	 Image: A start of the start of
SINGLE TOP TOTAL	×	×	×	×	X	×	×	X	×	×	X	X	×	X	~	×
TOP DIFFERENTIAL	X	X	X	X	X	X	X	X	×	×	X	X	X	X	X	~
$W p_T$	x	X	X	X	X	X	X	x	x	x	x	~	X	X	X	X
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THEORY PROGRESS:

- MSTW, ABKM: all NNLO; NNPDF NNLO since 07/11 (2.1), CT since 02/13 (CT10); NNPDF THRESHOLD RESUMMATION (3.0RESUM, 07/15), SMALL *x* RESUMMATION (3.1SX, 10/17)
- MSTW, CT, NNPDF all GM-VFN; NNPDF since 01/11 (2.1); ABM FFN+ZM-VFN since 01/17 (ABMP16)
- NNPDF FITTED CHARM since 05/16 (NNPDF3IC)
- PHOTON PDF: (mrst2004qed), NNPDF2.3QED (08/13), NNPDF3.0QED (06/16), NNPDF3.1LUXQED (12/17)



- GLUON BETTER KNOWN AT SMALL x, VALENCE QUARKS AT LARGE x, SEA QUARKS IN BETWEEN
- TYPICAL UNCERTAINTIES IN DATA REGION $\sim 3-5\%$
- SWEET SPOT: VALENCE Q G; DOWN TO 1%
- UP BETTER KNOWN THAN DOWN; FLAVOR SINGLET BETTER THAN INDIVIDUAL FLAVORS
- NO QUALITATIVE DIFFERENCE BETWEEN NLO AND NNLO

DATASET WIDENING NNPDF3.0 vs NNPDF3.1

Kinematic coverage



NEW DATA: (BLACK EDGE)

- HERA COMBINED F_2^b
- D0 W LEPTON ASYMMETRY
- ATLAS *W*, *Z* 2011, HIGH & LOW MASS DY 2011; CMS *W*[±] RAPIDITY 8TEV LHCB *W*, *Z* 7TEV & 8TEV
- ATLAS 7TEV JETS 2011, CMS 2.76TEV JETS
- ATLAS & CMS TOP DIFFERENTIAL RAPIDITY
- ATLAS $Z p_T$ DIFFERENTIAL RAPIDITY & INVARIANT MASS 8TEV, CMS $Z p_T$ DIFFERENTIAL

RAPIDITY 8TEV

THE IMPACT OF LHC DATA PDF UNCERTAINTIES IN DETAIL: NNPDF3.0 (NNLO)



• GLUON BETTER KNOWN AT SMALL x, VALENCE QUARKS AT LARGE x, SEA QUARKS IN BETWEEN

- TYPICAL UNCERTAINTIES IN DATA REGION $\sim 3-5\%$
- SWEET SPOT: VALENCE Q G; DOWN TO 1%
- UP BETTER KNOWN THAN DOWN; FLAVOR SINGLET BETTER THAN INDIVIDUAL FLAVORS



- GLUON BETTER KNOWN AT SMALL x, VALENCE QUARKS AT LARGE x, SEA QUARKS IN BETWEEN
- TYPICAL UNCERTAINTIES IN DATA REGION $\sim 1-3\%$
- SWEET SPOT: VALENCE Q G; 1% OR BELOW
- UP BETTER KNOWN THAN DOWN; FLAVOR SINGLET BETTER THAN INDIVIDUAL FLAVORS
- NEW LHC DATA \Rightarrow SIZABLE REDUCTION IN UNCERTAINTIES



- SIGNIFICANT UNCERTAINTY REDUCTION
- MANY PDFs CHANGE BY MORE THAN ONE SIGMA
- BOTH FLAVOR SEPARATION & GLUON SIGNIFICANTLY AFFECTED

DATA VS. THEORY/METHODOLOGY THE STRANGE PDF: DIS VS. W PRODUCTION

- STRANGE PDF CONTROLLED BY NEUTRINO DIS CHARM PRODUCTION + W PRODUCTION
- DIS DATA FAVOR "SUPPRESSED STRANGE" \Rightarrow SMALL $R_s \equiv \frac{s+\bar{s}}{\bar{u}+\bar{d}}$
- ATLAS FAVORS ENHANCED STRANGENESS
- ATLAS IMPACT EXAGGERATED IN XFITTER ANALYSIS
- EVERYTHING CONSISTENT WITHIN UNCERTAINTIES IN GLOBAL FIT



DATA VS. THEORY/METHODOLOGY THE STRANGE PDF: DIS VS. W PRODUCTION

- MASSIVE CORRECTIONS TO CHARGED CURRENT DIS HITERTO INCLUDED TO NLO MASSLESS TO NNLO
- Gao, $2018 \Rightarrow$ NNLO COMPUTED
- STRANGENESS ENHANCED BY NNLO CORRECTIONS





(Gao, 2108)

LESSONS:

- BEWARE OF XFITTER HERA+X FITS
- IN A GLOBAL FIT DIFFERENT DATA ALWAYS PULL IN DIFFERENT DIRECTIONS!
- TENSION CAN BE RESOLVED BY BETTER THEORY

DATA VS. THEORY/METHODOLOGY THE CHARM MASS AND TREATMENT CT18 \rightarrow CT18Z

- ATLAS W and Z 7TeV rapidity included
- CHARM MASS INCREASED
- x-dependent factorization scale



DATA VS. THEORY/METHODOLOGY THE CHARM MASS AND TREATMENT CHARM FROM DATA

• CHARM SHOULD NOT DEPEND STRONGLY ON CHARM MASS



• ITS SHAPE SHOULD NOT BE DETERMINED BY FIRST-ORDER MATCHING (NO HIGHER NONTRIVIAL ORDERS KNOWN)

• MIGHT EVEN HAVE A NONPERTURBATIVE COMPONENT

FITTED VS. PERTURBATIVE: SUPPRESSED AT MEDIUM-SMALL x, ENHANCED AT VERY SMALL, VERY LARGE x



- QUARK LUMI AFFECTED BECAUSE OF CHARM SUPPRESSION AT MEDIUM-x
- FLAVOR DECOMPOSITION ALTERED
- UNCERTAINTIES ON LIGHT QUARKS NOT SIGNIFICANTLY INCREASED
- AGREEMENT OF 13TeV W,Z PREDICTED CROSS-SECTIONS IMPROVES!



• W, Z CROSS-SECTIONS AT 13 TEV IN PERFECT AGREEMENT WITH DATA THANKS TO FITTED CHARM!

LESSONS:

- TENSIONS CAN REVEAL METHODOLOGICAL ISSUES
- MORE LIKELY AS DATASET INCREASES, EXPERIMENTAL UNCERTAINTIES DECREASE
- RESOLVED BY MORE COMPLEX METHODOLOGY

OPTIMIZING THE METHODOLOGY

DATA vs. METHODOLOGY

- NEW DATA \Rightarrow MAJOR METHODOLOGICAL CHOICES \Rightarrow SIGNIFICANT IMPACT
- NNPDF3.1 vs NNPDF3.0: DATA AND METHODOLOGY HAVE SIMILAR IMPACT



$\begin{array}{c} \text{DATA} \Rightarrow \text{THEORY ISSUES} \\ \text{VISUALIZATION TOOLS} \\ \text{TRACING THE IMPACT OF DATA} \end{array}$

- DETERMINE THE SHIFT IN DATAPOINTS INDUCED BY CHANGES IN PDF
- CT14: 28 HESSIAN PARAMETER VARIATIONS
- VISUALIZE SHIFT VECTORS FOR 4000 datapoints
 - by PCA
 - BY TOUR



LESSONS FROM THE PAST: TWENTY YEARS BACK....

- NO PDF UNCERTAINTIES
- UNCERTAINTY \Leftrightarrow PDF SET VARIATION
- METHDOLOGY \leftrightarrow AGREEMENT WITH DATA

CDF JETS

GLUON UNCERTAINTY





(Carrazza, Cruz-Martinez, preliminary)

- EXPLORE METHODOLOGICAL ALTERNATIVES (ARCHITECTURE, MINIMIZATION, POSITIVITY,...)
- SCAN AUTOMATICALLY & ZOOM IN
- COULD BE DONE BY REINFORCEMENT LEARNING?



FITTING THE METHODOLOGY WHAT IS "PROPER LEARNING"?

- CROSS-VALIDATION \Rightarrow RANDOMLY DIVIDE DATA INTO TRAINING AND VALIDATION SETS
- MINIMIZE ON TRAINING; OPTIMIZE ON VALIDATION
- CORRELATIONS BETWEEN TRAINING AND VALIDATION
- HYPEROPTIMIZE ON VALIDATION \Rightarrow OVERLEARNING





FITTING THE METHODOLOGY WHAT IS "PROPER LEARNING"?

- NEED A COMPLETELY UNCORRELATED "TEST" SET
- OPTIMIZE ON WEIGHTED AVERAGE OF VALIDATION AND TEST \Rightarrow NO OVERLEARNING
- BETTER SOLUTIONS? WHAT IS "OPTIMAL"?





FITTING THE METHODOLOGY WHAT IS "PROPER LEARNING"?

- BETTER SOLUTIONS? WHAT IS "OPTIMAL"?
- ARE STATISTICAL PROPERTIES OF THE ENSEMBLE RELEVANT?
- SHOULD THEORY PREJUDICE PLAY A ROLE?

MENU V nature

NEWS • 08 JANUARY 2019

Machine learning leads mathematicians to unsolvable problem

Simple artificial-intelligence problem puts researchers up against a logical parc by famed mathematician Kurt Gödel.

Davide Castelvecchi





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THEORY UNCERTAINTIES

THE MISSING HIGHER ORDER UNCERTAINTY

- DOMINANT THEORY UNCERTAINTY ON QCD PREDICTIONS \Rightarrow MHOU (SCALE)
- NOT INCLUDED IN PDF UNCERTAINTY
- WHAT IS IT?





- TODAY: NLO PDF & MHOU UNCERTAINTIES COMPARABLE
- NEAR FUTURE: SHOULD WE WORRY ABOUT NNLO MHOU?

THE MISSING HIGHER ORDER UNCERTAINTY ON PDFS CAN WE ESTIMATE IT? SCALE VARIATION IN PDF FITTING

NAIVE IDEA FOR PDF MHOU ESTIMATE

- PERFORM FIT WITH VARIOUS SCALE CHOICES
- TAKE ENVELOPE OF RESULTS
- 7-POINT \Rightarrow OK!; 9-POINT \Rightarrow UNSTABLE!
- **RESULTS DEPEND STRONGLY** ON THE CHOICE OF ENVELOPE



THE THEORY COVARIANCE MATRIX

(NNPDF, 2019)

- ASSOCIATE MHOU TO NUISANCE PARAMETER \Rightarrow THEORY COVARIANCE MATRIX S_{ij}
- $S_{ij} = \frac{1}{N} \sum_{k} \left(T_i^{(k)} T_i^{(0)} \right) \left(T_j^{(k)} T_j^{(0)} \right)$ $\left(T_i^{(k)} - T_i^{(0)} \right)$: k-th shift of *i*-th datapoint about central prediction $T_i^{(0)}$.
- SHIFT: GUESS FOR POSSIBLE MHO TERMS \Rightarrow Scale variation



- CLASSIFIY DATA INTO PROCESSES
- PICK A SET OF SCALE VARIATIONS
- DECIDE HOW TO CORRELATE SCALE VARIATION BETWEEN DIFFERENT PROCESSES
- **RENORMALIZATION** \Rightarrow **MATRIX ELEMENT**; FACTORIZATION \Rightarrow EVOLUTION

THE THEORY COVARIANCE MATRIX: CORRELATIONS

- INDEPENDENT NUISANCE PARAMETERS \Rightarrow TH. AND EXP. ERRORS COMBINE IN QUADRATURE $\chi^2 = \sum_{i,j=1}^{N_{\text{dat}}} \left(D_i T_i^{(0)} \right) [S+C]_{ij}^{-1} \left(D_i T_i^{(0)} \right)$
- REN. SCALE \Rightarrow CORRELATIONS INDUCED BETWEEN EXPERIMENTALLY UNRELATED MEASUREMENTS OF SAME PROCESS
- FACT. SCALE \Rightarrow CORRELATIONS INDUCED BETWEEN DIFFERENT PROCESSES



THE CORRELATION MATRIX



THE THEORY COVARIANCE MATRIX: VALIDATION

- COMPARE NLO THEORY COVMAT TO OBSERVED NLO-NNLO SHIFTS
- DETERMINE EIGENVECTORS e_i OF COVMAT $\Rightarrow 28$ EVECS FOR 9PT, FIVE PROCESSES
- DETERMINE VECTOR OF SHIFTS δ
- DETERMINE PROJECTION OF δ IN SUBSPACE SPANNED BY e_i : IS IT CONTAINED IN IT?
- DETERMINE SIZE δ_i OF PROJECTIONS OF δ ALONG e_i : ARE THEY OF COMPARABLE SIZE?





THE THEORY COVARIANCE MATRIX: VISUALIZING PROCESS IMPACT

- PROJECT THE SHIFT VECTOR δ on each eigenvector
- LOOK AT THE INDIVIDUAL $\sim 3000 \text{ components}$
- GROUP POINTS BY PROCESS
- RELATION BETWEEN SCALE VARIATION EIGENVECTORS & PROCESSES



projection of the shift vector along the four dominant eigenvectors NNLO-NLO shift 0.2 Eigenvector Eigenvalue = 15.403959274291992 0.0 DISNC JISCC NNLO-NLO shift 0.2 Eigenvector Eigenvalue = 2.444594383239746 0.0 DISNC DISCC 6° 28 2 NNLO-NLO shift Eigenvector 0.2 Eigenvalue = 1.0238687992095947 0.0 ASCC 715 NC 13 202 NNLO-NLO shift Eigenvector 0.2 Eigenvalue = 0.6538439989089966 0.0



- FIT QUALITY χ^2 IMPROVES
- Relative error ϕ on prediction does not change
- PDF UNCERTAINTY ALMOST UNCHANGED
- CENTRAL VALUE MOVES TOWARDS KNOWN NNLO

EQUALLY PRECISE BUT MORE ACCURATE RESULT!



PDFs with theory uncertainties

- Results mildly dep. on prescription \Rightarrow 3pt closer to result w/o theory uncertainty
- "UNSTABLE" SCALE VARIATIONS \Rightarrow NO IMPACT ON FIT
- 7PT ENVELOPE RATHER MORE CONSERVATIVE ENVELOPE DOES NOT INCLUDE EXP. UNCERTAINTY



OUTLOOK

SUMMARY

- BETTER DATA ⇔ BETTER THEORY AND BETTER METHODOLOGY
- CAN WE REDUCE ARBITRARINESS IN PDF METHPDOLOGY?
- CAN WE ASSESS ACCURATELY OUR THEORETICAL IGNORANCE?

