THEORY UNCERTAINTIES

IN

PDF DETERMINATION

STEFANO FORTE
UNIVERSITÀ DI MILANO & INFN

UNIVERSITÀ DEGLI STUDI DI MILANO
DIPARTIMENTO DI FISICA

Istituto Nazionale di Fisica Nucleare

PHYSICS AT TEV COLLIDERS

LES HOUCHES, JUNE 14, 2019

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SUMMARY

WHAT ARE PDF UNCERTAINTIES?

- PDFs AS PROXIES FOR OBSERVABLES
- NLO-NNLO SHIFT
- DIFFERENT SCALE CHOICES

THE THEORY COVARIANCE MATRIX

- MHOU AS NUISANCE PARAMETERS
- PRESCRIPTIONS
- THEORY CORRELATION
- VALIDATION: SHIFT VS COVARIANCE MATRIX

PDFs WITH THEORY UNCERTAINTIES

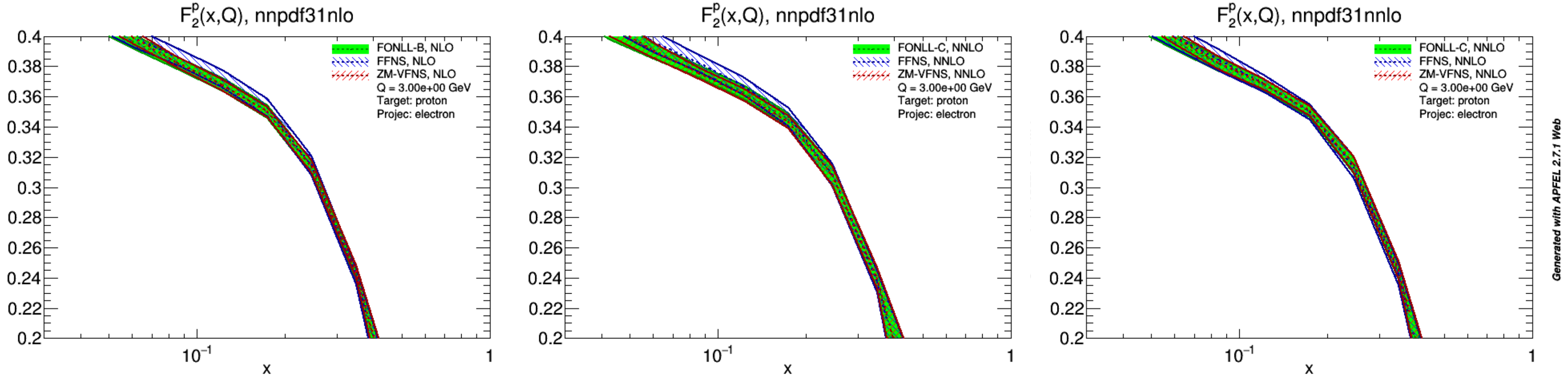
- FIT QUALITY AND TENSIONS
- DEPENDENCE ON THE PRESCRIPTION
- PHYSICAL OBSERVABLES

THE MISSING HIGHER ORDER UNCERTAINTY

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

F_2^p PROTON DIS STRUCTURE FUNCTION

NLO THEORY NLO PDFs | NNLO THEORY NLO PDFs | NNLO THEORY NNLO PDFs



MISSING HIGHER ORDER UNCERTAINTY ON FACTORIZED OBSERVABLES

$$\sigma = \hat{\sigma} \otimes f \otimes f$$

schematically

$$\sigma(M_w^2) = \hat{\sigma}(M_w^2)\left[\Gamma(M_w^2, Q^2)F_2(Q^2)\right]^2;\ \Gamma(M_w^2, Q^2) = \exp\int_{Q^2}^{M_W^2} \frac{d\alpha}{\beta(\alpha)}\gamma(\alpha)$$

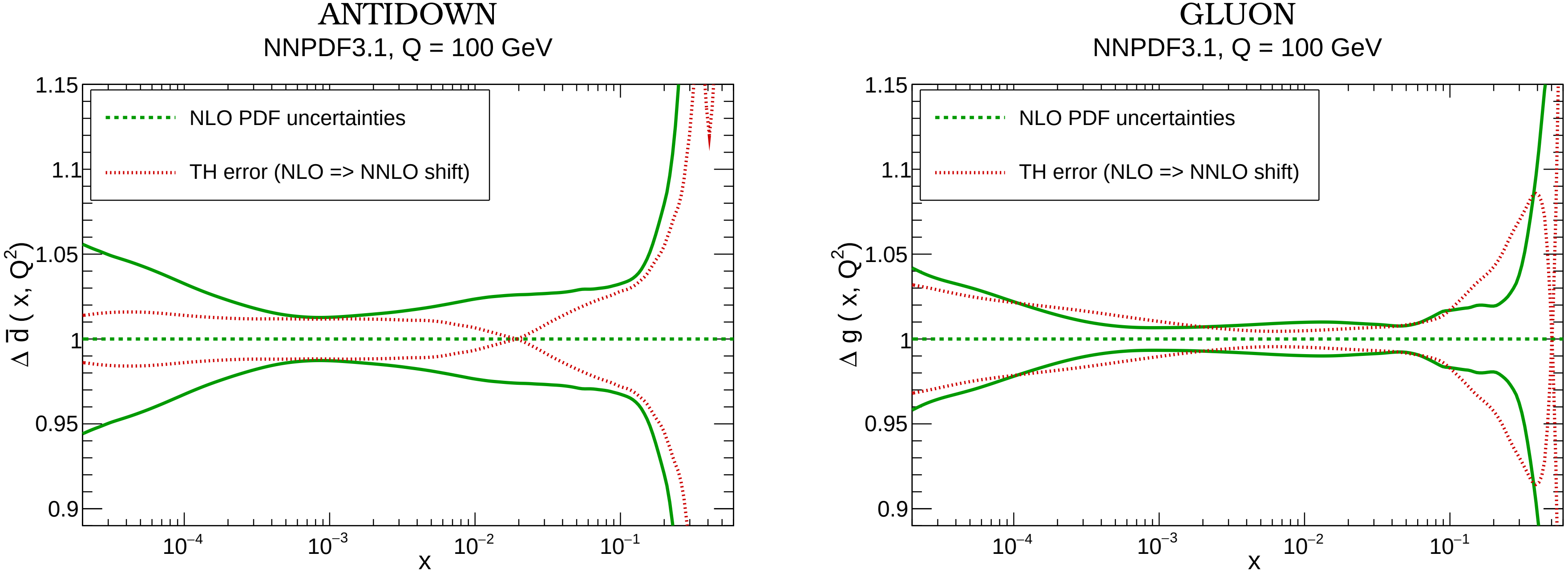
- HADRONIC XSECT= PARTONIC XSEC TIMES PDFs (CONVOLUTION)
- PDFs ARE A PROXY FOR ANOTHER PROCESS (DIS)
- MUST EVOLVE BETWEEN TWO PROCESSES

SOURCES OF MHOU UNCERTAINTY

- MHOU IN THE "DRELL-YAN" XSECT $\Rightarrow$ STANDARD SCALE VARN.
- MHOU IN THE STRUCTURE FUNCTIONS $\Rightarrow$ TH. UNCERTAINTY ON PDFs (1)
- MHOU IN THE EVOLUTION $\Rightarrow$ TH. UNCERTAINTY ON PDFs (2)

THE MISSING HIGHER ORDER UNCERTAINTY ON PDFs
HOW BIG IS IT?

NLO-NNLO SHIFT VS. NLO PDF UNCERTAINTY (NNPDF3.1)



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

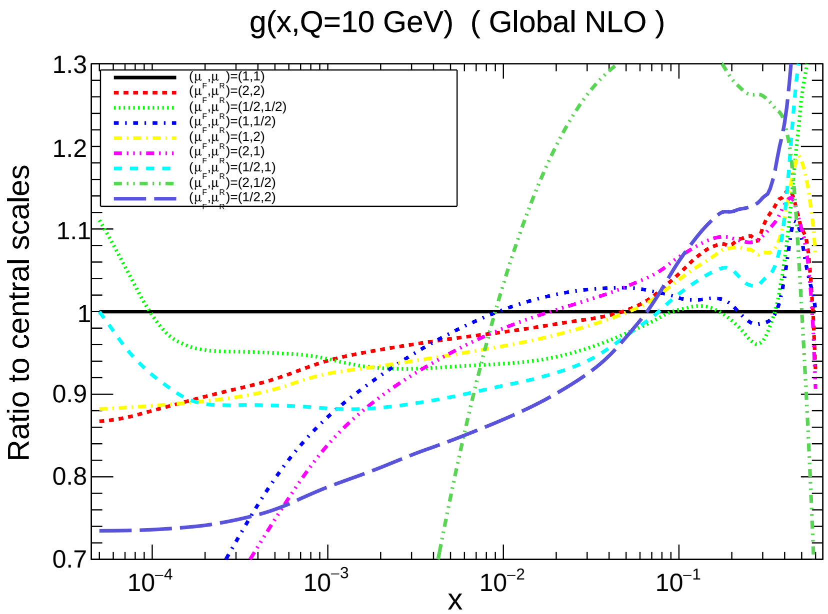
THE MISSING HIGHER ORDER UNCERTAINTY ON PDFs
CAN WE ESTIMATE IT?
SCALE VARIATION IN PDF FITTING

NAIVE IDEA FOR PDF MHOU ESTIMATE

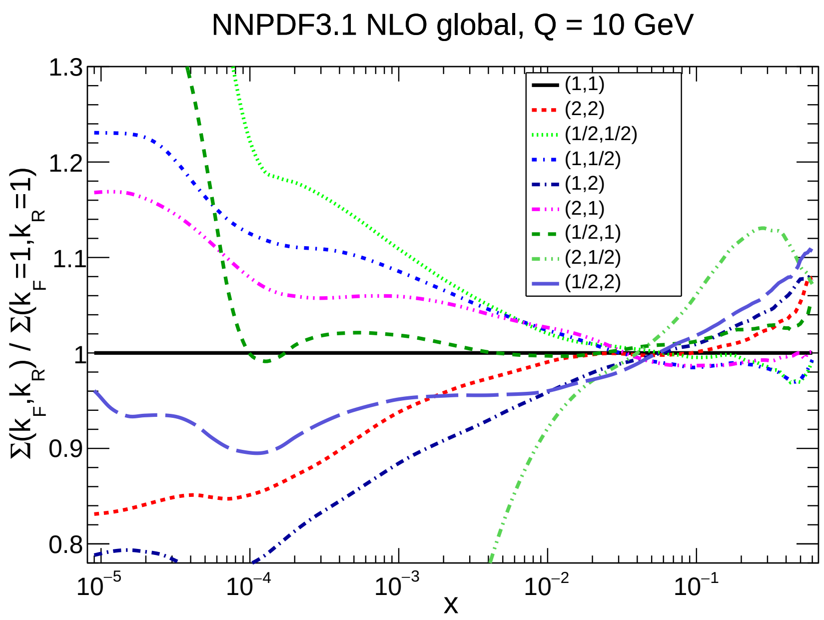
- PERFORM FIT WITH VARIOUS SCALE CHOICES
- TAKE ENVELOPE OF RESULTS
- 7-POINT ⇒ OK!; 9-POINT ⇒ UNSTABLE!
- RESULTS DEPEND STRONGLY ON THE CHOICE OF ENVELOPE

FITS WITH SCALE VARIATION

GLUON



QUARK SINGLET



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

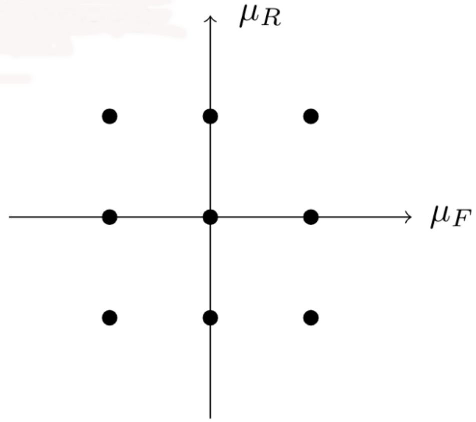
SCALE VARIATION

NINE-POINT SCALE VAR.

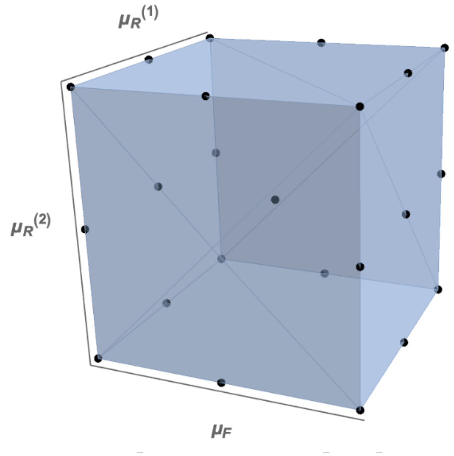
EXPERIMENTS AND PROCESSES

Process Type	Datasets
DIS NC	NMC, SLAC, BCDMS, HERA NC
DIS CC	NuTeV, CHORUS, HERA CC
DY	CDF, D0, ATLAS, CMS, LHCb (y, p_T, M_{ll})
JET	ATLAS, CMS inclusive jets
TOP	ATLAS, CMS total+differential cross-sections

SAME PROCESS



DIFFERENT PROCESSES



- CLASSIFY 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

PDF THEORY ERROR AS A FIT UNCERTAINTY

- PDFs ARE DETERMINED BY MAXIMIZING THE LIKELIHOOD

$$P = N \exp - \left(\frac{d - t}{2\sigma^2_{exp}} \right)$$

d, t ARE REALLY VECTORS AND $1/\sigma^2$ THE INVERSE COVARIANCE MATRIX

- CAN VIEW THIS AS THE PROBABILITY OF THE THEORY t BEING CORRECT GIVEN DATA d, WHICH BY BAYES IS
$$P(t|d) \propto P(d|t)P(t)$$

- IF THEORY WAS KNOWN EXACTLY, THEN $P(t) = \delta(t - t^{\mathrm{exact}})$

- IN ACTUAL FACT ONLY SOME PERTURBATIVE RESULT t_p IS EXACTLY KNOWN SO $t^{\mathrm{exact}} = t_p + \Delta_p$, WHERE Δ_p INCLUDES MHO

- ASSUMING Δ TO BE GAUSSIANLY DISTRIBUTED, WITH UNCERTAINTY σ_{th} AND INTEGRATING OUT
$$P = N \exp \left[\frac{d - t_p}{2\left(\sigma^2_{exp} + \sigma^2_{th}\right)} \right]$$

- THEORETICAL UNCERTAINTY ADDED IN QUADRATURE, PROPAGATES INTO PDF UNCERTAINTY UPON MINIMIZATION

- SCALE VARIATION FOR EACH DATA POINT $\Rightarrow$ EIGENVECTOR OF COVARIANCE MATRIX (NUISANCE PARM.)

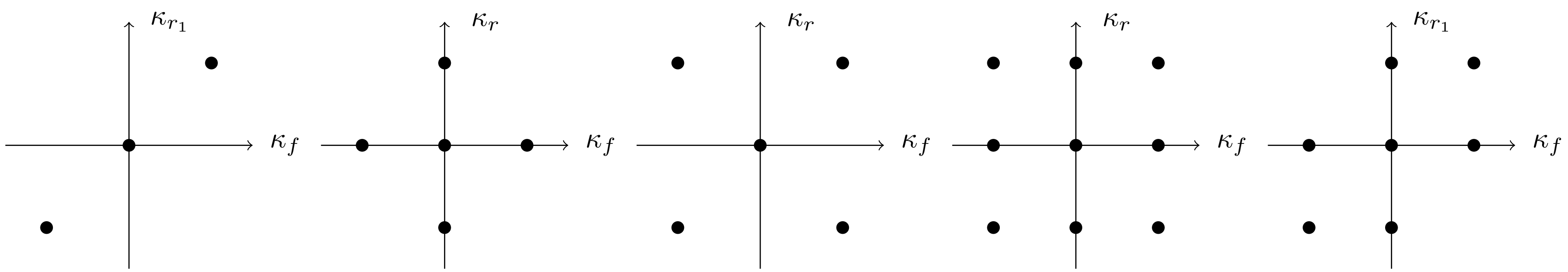
THE THEORY COVARIANCE MATRIX: PRESCRIPTIONS
FACTORIZATION VS RENORMALIZATION SCALE

Scale	MHOU	'Traditional' name	'Modern' name[PDG]
μ_r	in hard xsec	—	renormalization scale
μ_f	in PDF evolution	renormalization scale	factorization scale
$\widetilde{\mu}$	in physical xsec	factorization scale	scale of the process

- $\mu_r \Rightarrow$ MHOU IN HARD CROSS SECTION
- $\mu_f \Rightarrow$ MHOU IN ANOMALOUS DIMENSION

PRESCRIPTIONS

- **3 POINT**: $\widetilde{\mu} = \mu_r = \mu_f$ UNCORRELATED BETWEEN PROCESSES
- **5 POINT**, $\overline{5}$ **POINT**, **9 POINT**: μ_r μ_f VARIED INDEPENDENTLY, μ_r UNCORRELATED, μ_f CORRELATED
- **7 POINT**: $\widetilde{\mu}$ ADDED TO 5 POINT



9 point, off-diagonal: $S^{(9\mathrm{pt})}_{i_1 j_2} = \frac{1}{24}\{2(\Delta^{+0}_{i_1} + \Delta^{++}_{i_1} + \Delta^{+-}_{i_1})(\Delta^{+0}_{j_2} + \Delta^{++}_{j_2} + \Delta^{+-}_{j_2}) + 2(\Delta^{-0}_{i_1} + \Delta^{-+}_{i_1} + \Delta^{--}_{i_1})(\Delta^{-0}_{j_2} + \Delta^{-+}_{j_2} + \Delta^{--}_{j_2})\} + 3(\Delta^{0+}_{i_1} + \Delta^{0-}_{i_1})(\Delta^{0+}_{j_2} + \Delta^{0-}_{j_2})\}.$

THE THEORY COVARIANCE MATRIX: CORRELATIONS

- INDEPENDENT NUISANCE PARAMETERS $\Rightarrow$ TH. AND EXP. ERRORS COMBINE IN QUADRATURE
  $\chi^2 = \sum_{i,j=1}^{N_{\rm dat}} \left(D_i - T_i^{(0)}\right) [S+C]_{ij}^{-1} \left(D_i - T_i^{(0)}\right)$

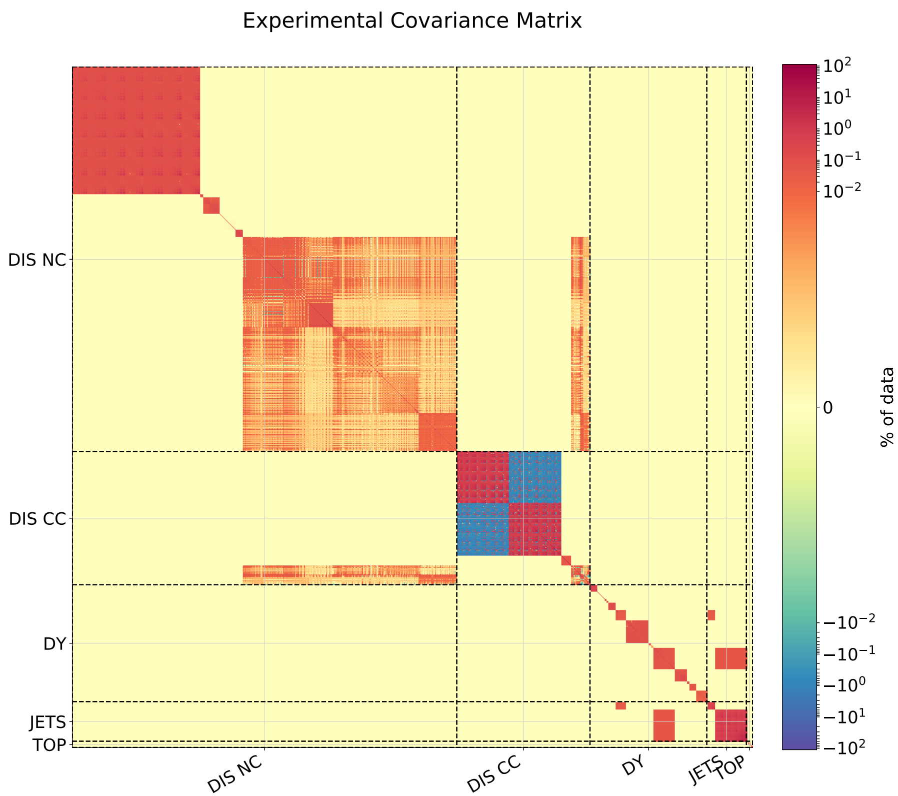
- REN. SCALE $\Rightarrow$ CORRELATIONS INDUCED BETWEEN EXPERIMENTALLY UNRELATED MEASUREMENTS OF SAME PROCESS

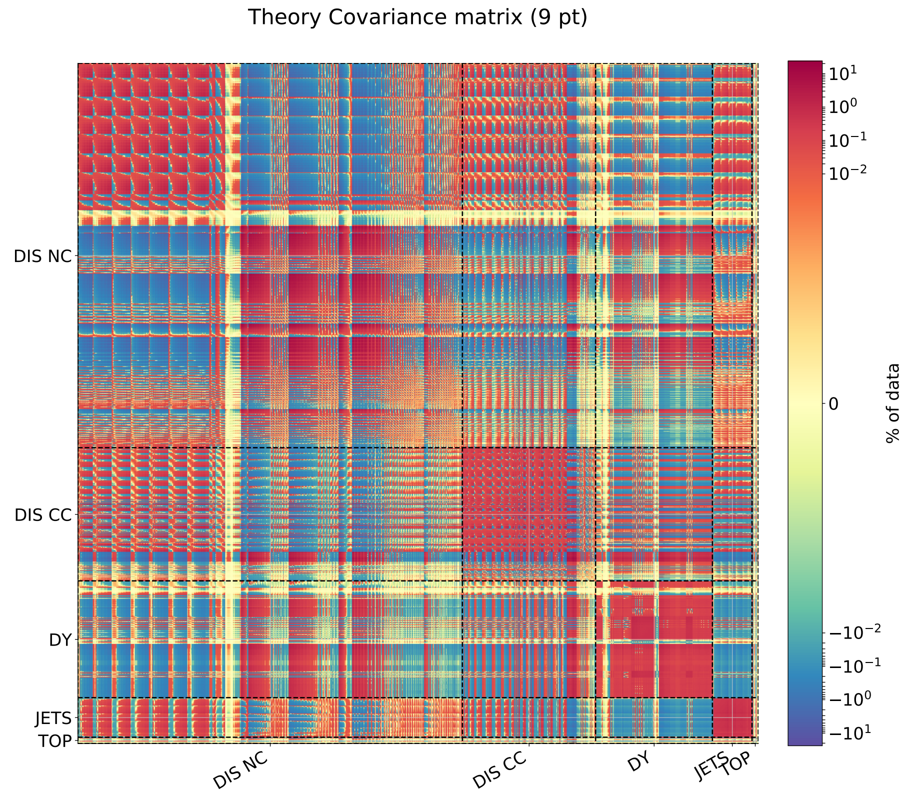
- FACT. SCALE $\Rightarrow$ CORRELATIONS INDUCED BETWEEN DIFFERENT PROCESSES

THE COVARIANCE MATRIX

EXPERIMENT

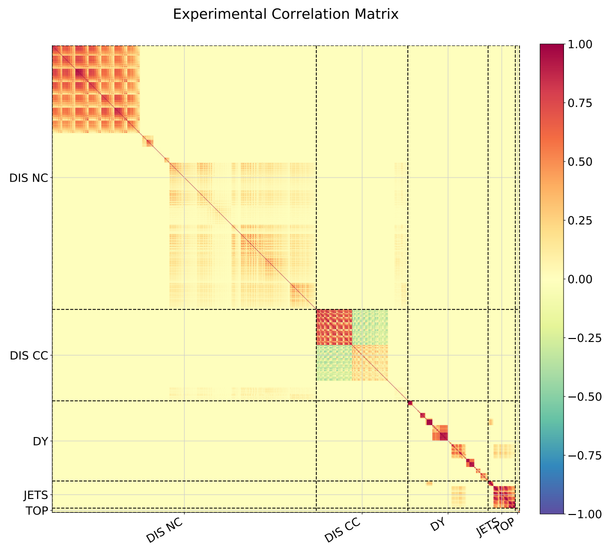
THEORY (9 PT)



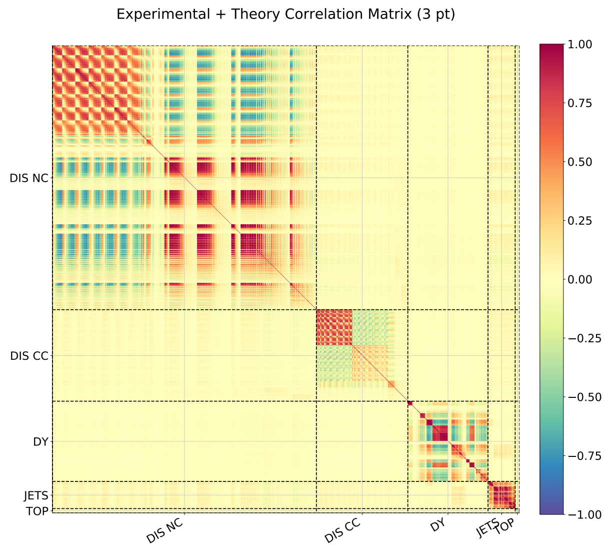


CORRELATION MATRICES

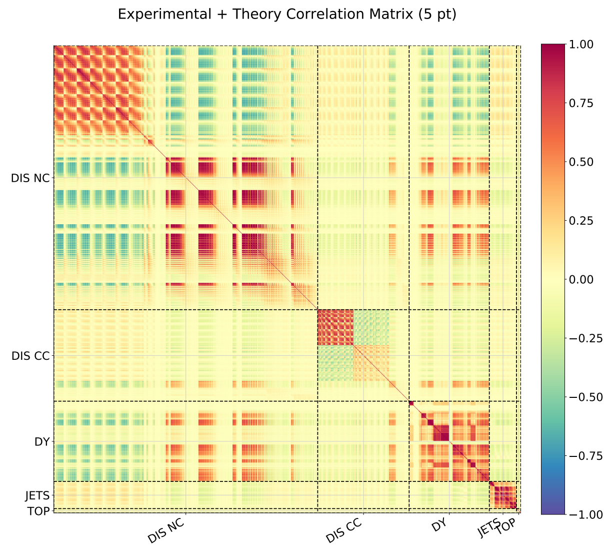
EXPERIMENT



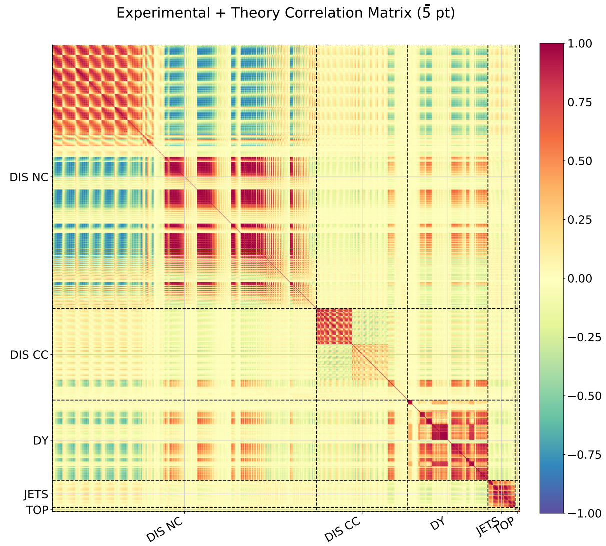
EXP+THEORY (3 PT)



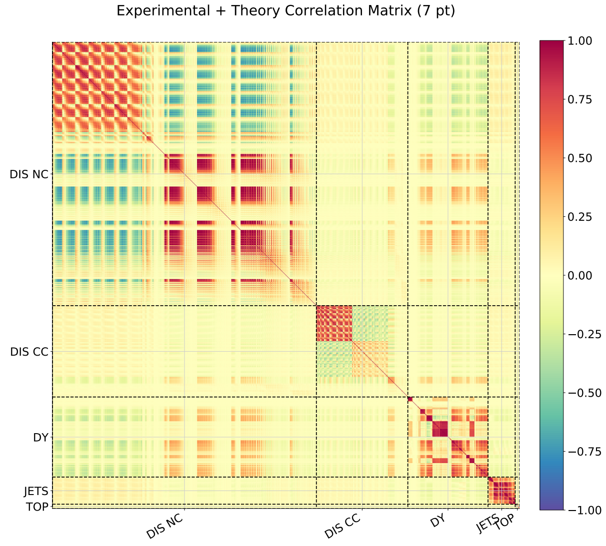
EXP+THEORY (5 PT)



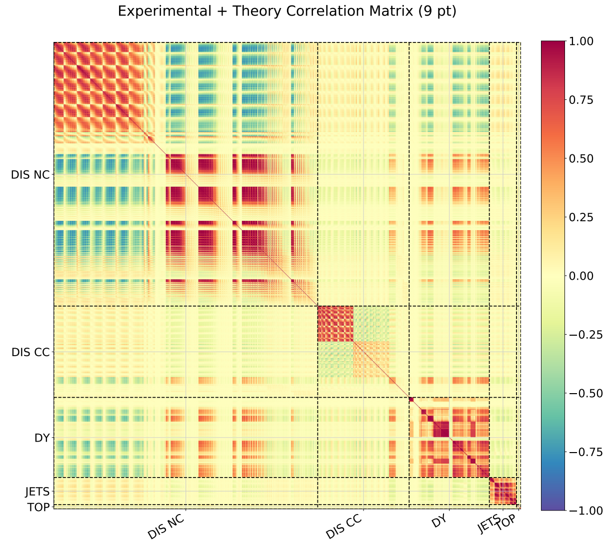
EXP+THEORY ($\bar{5}$ PT)



EXP+THEORY (7 PT)



EXP+THEORY (9 PT)

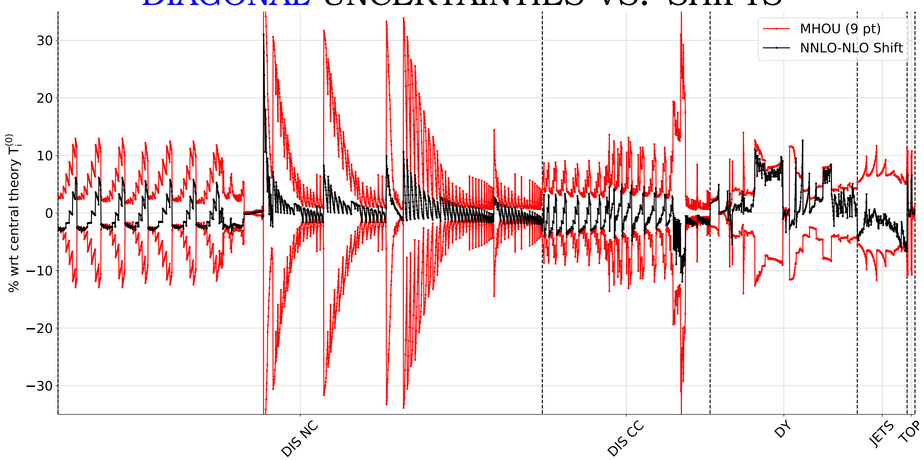


THE THEORY COVARIANCE MATRIX: VALIDATION

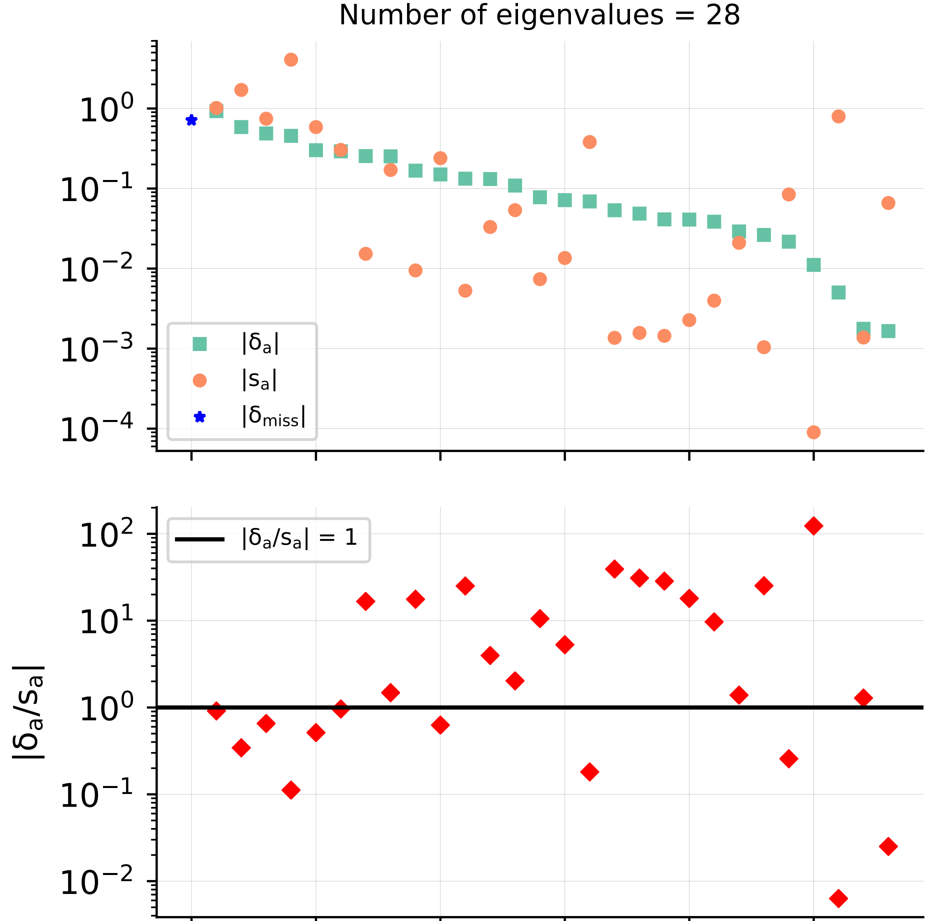
- COMPARE NLO THEORY COVMAT TO OBSERVED NLO-NNLO SHIFTS
- DETERMINE EIGENVECTORS e_i OF COVMAT $\Rightarrow$ 28 EVECS FOR 9PT, FIVE PROCESSES
- DETERMINE VECTOR OF SHIFTS δ
- DETERMINE PROJECTION OF δ IN SUBSPACE SPANNED BY e_i: IS IT CONTAINED IN IT?
- DETERMINE SIZE δ_i OF PROJECTIONS OF δ ALONG e_i: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

9PT PRESCRIPTION

DIAGONAL UNCERTAINTIES VS. SHIFTS



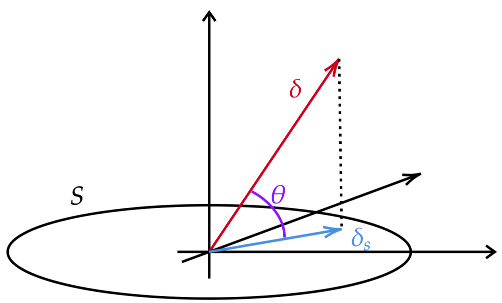
EIGENVALUES VS. SHIFT PROJECTIONS



ANGLE BETWEEN SHIFT AND PROJECTED SHIFT

- DIS NC: 32°
- DIS CC: 16°
- DY: 21°
- JETS: 15°
- TOP: 3°
- GLOBAL: 27°

SHIFT VECTOR VS PROJECTION



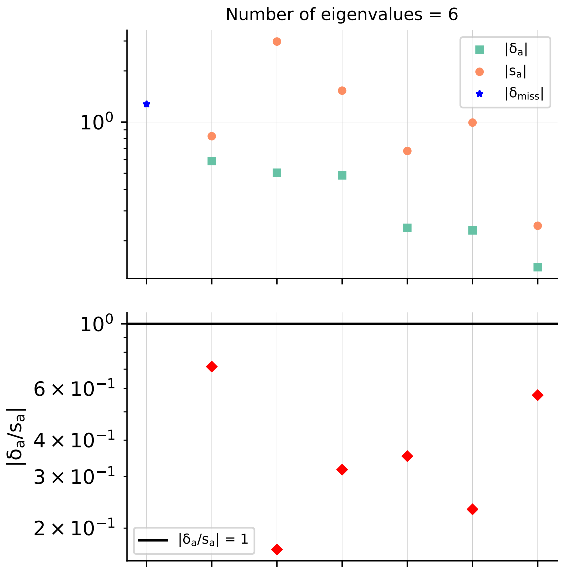
- ALL PRESCRIPTIONS BUT 3-PT PERFORM WELL
- ANGLE SCALES WITH NUMBER OF DATAPOINTS $\Rightarrow$ MORE POINTS, WORSE AGREEMENT
- ANGLE DOMINATED BY WORSE PROCESS

PRESCRIPTION	N_{sub}	θ
3-PT	6	52^{o}
5-PT	8	33^{o}
$\overline{5}$-PT	12	31^{o}
7-PT	14	29^{o}
9-PT	28	26^{o}

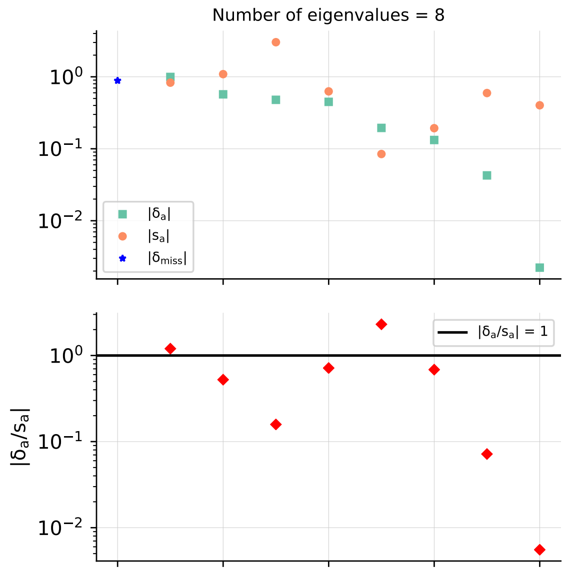
PRESCRIPTION	θ				
	DIS NC	DIS CC	DY	JET	TOP
3-PT	54^{o}	36^{o}	39^{o}	24^{o}	12^{o}
5-PT	39^{o}	21^{o}	25^{o}	17^{o}	11^{o}
$\overline{5}$-PT	38^{o}	17^{o}	23^{o}	22^{o}	10^{o}
7-PT	35^{o}	17^{o}	22^{o}	16^{o}	3^{o}
9-PT	32^{o}	16^{o}	22^{o}	14^{o}	3^{o}

COVARIANCE EIGENVALUES vs. SHIFT PROJECTIONS

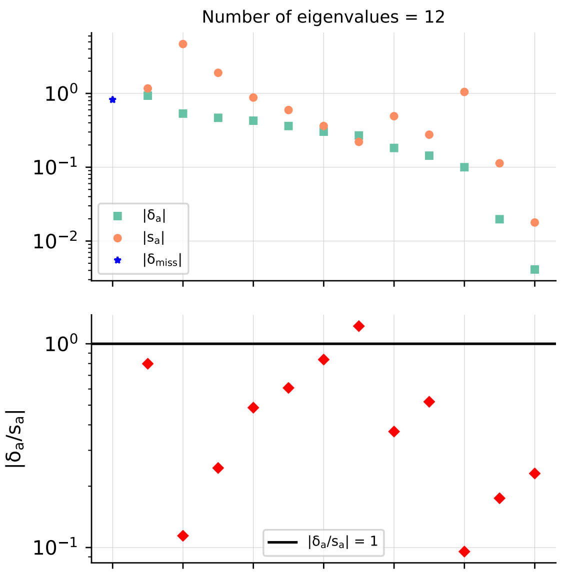
3 PT



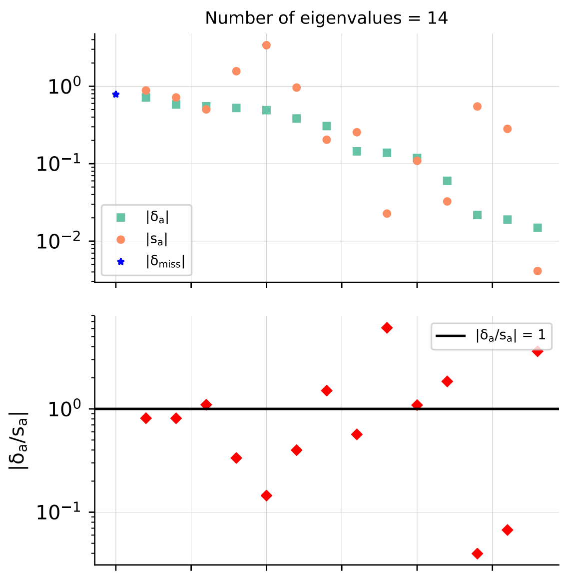
5 PT



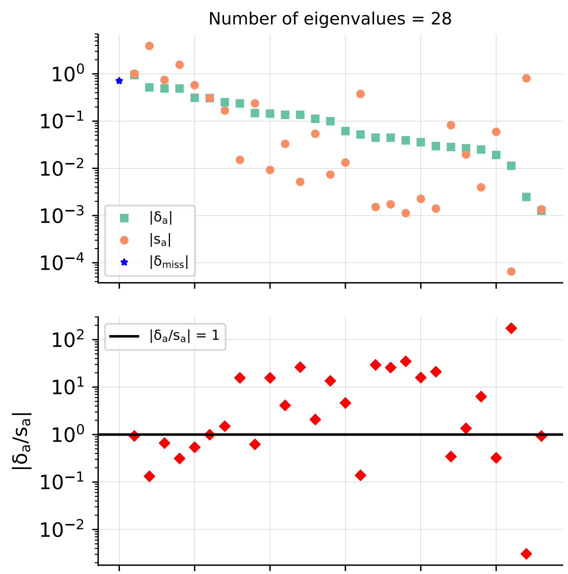
$\overline{5}$ PT



7 PT



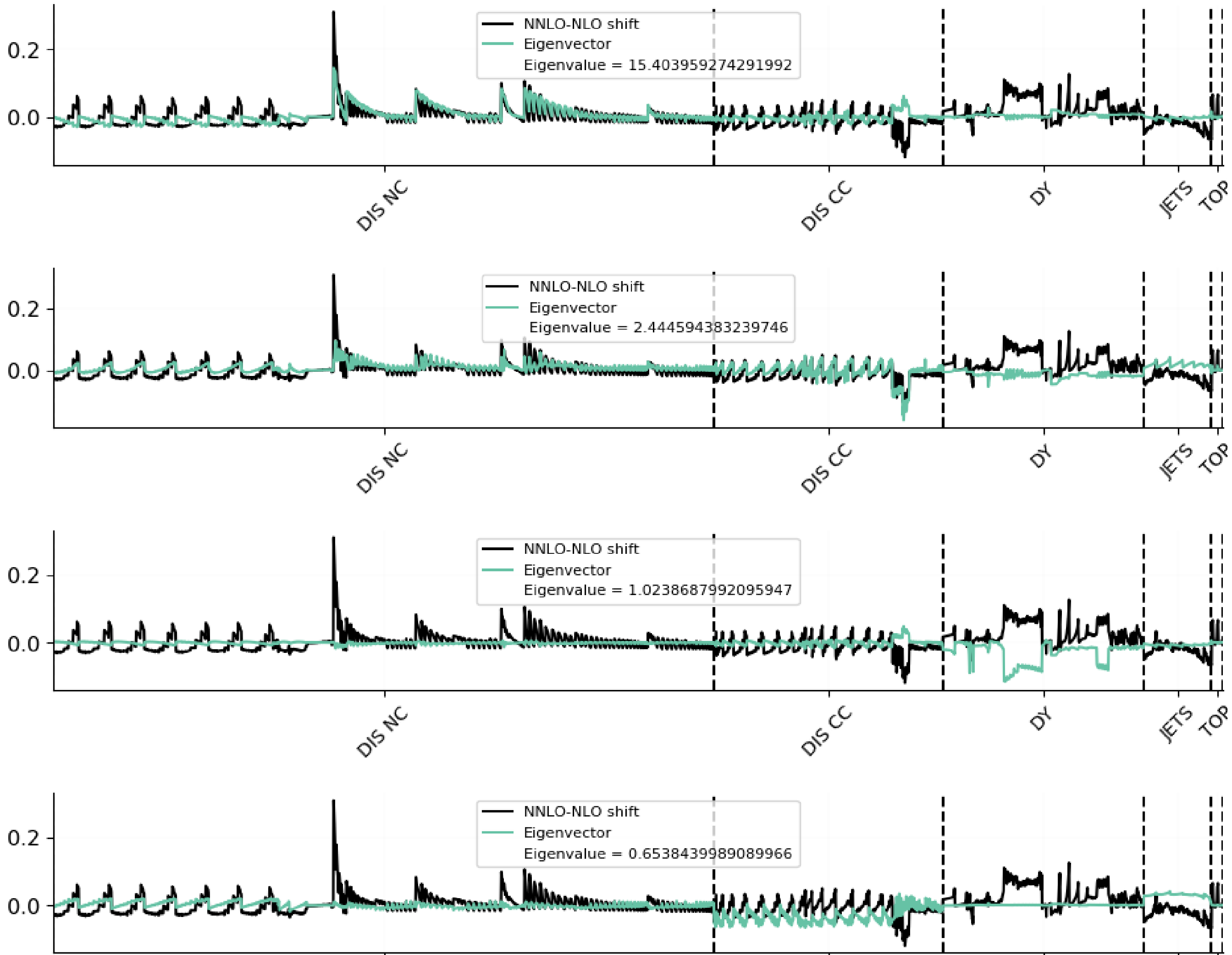
9 PT



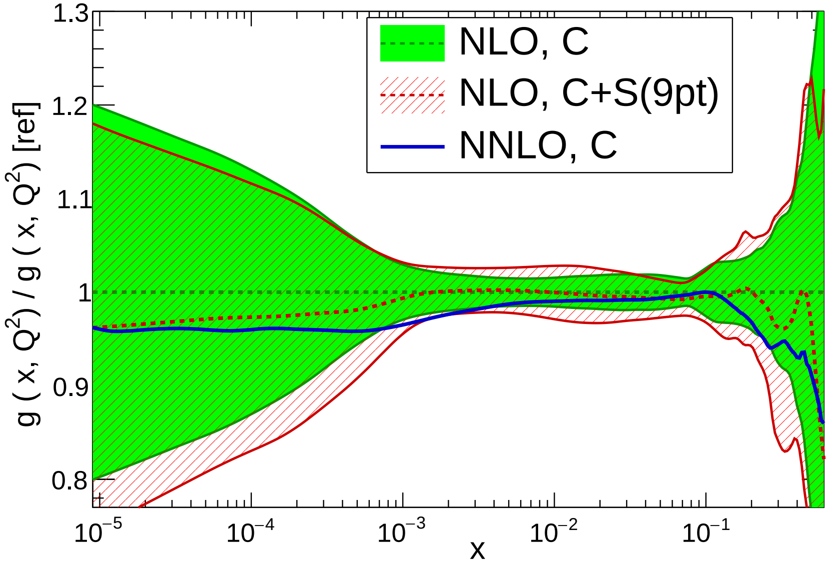
THE THEORY COVARIANCE MATRIX: VISUALIZING PROCESS IMPACT

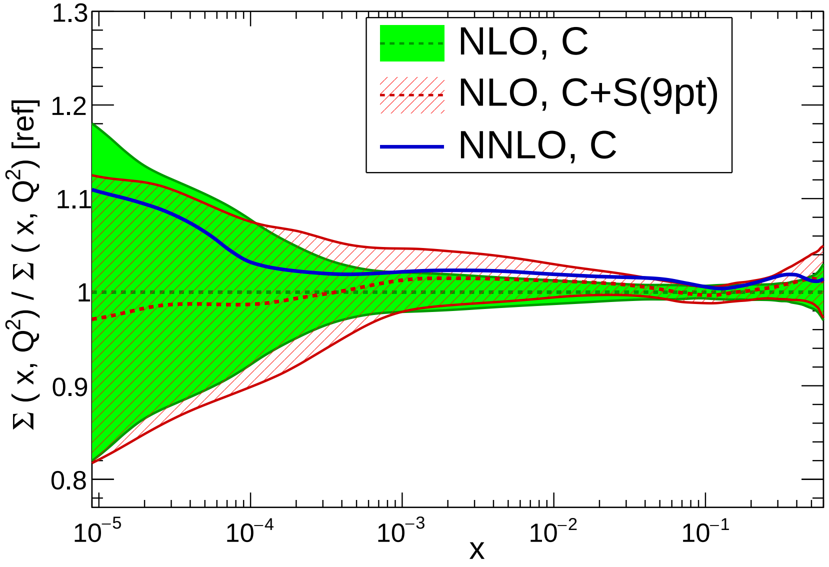
- PROJECT THE SHIFT VECTOR δ ON EACH EIGENVECTOR
- LOOK AT THE INDIVIDUAL ~ 3000 COMPONENTS
- GROUP POINTS BY PROCESS
- RELATION BETWEEN SCALE VARIATION EIGENVECTORS & PROCESSES

projection of the shift vector along the four dominant eigenvectors



PDFs with theory uncertainties 9pt



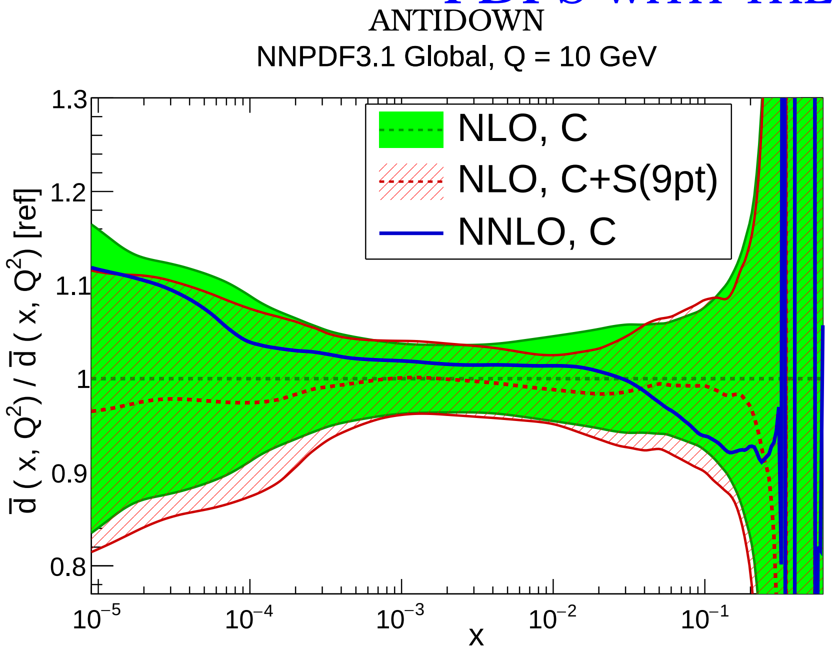


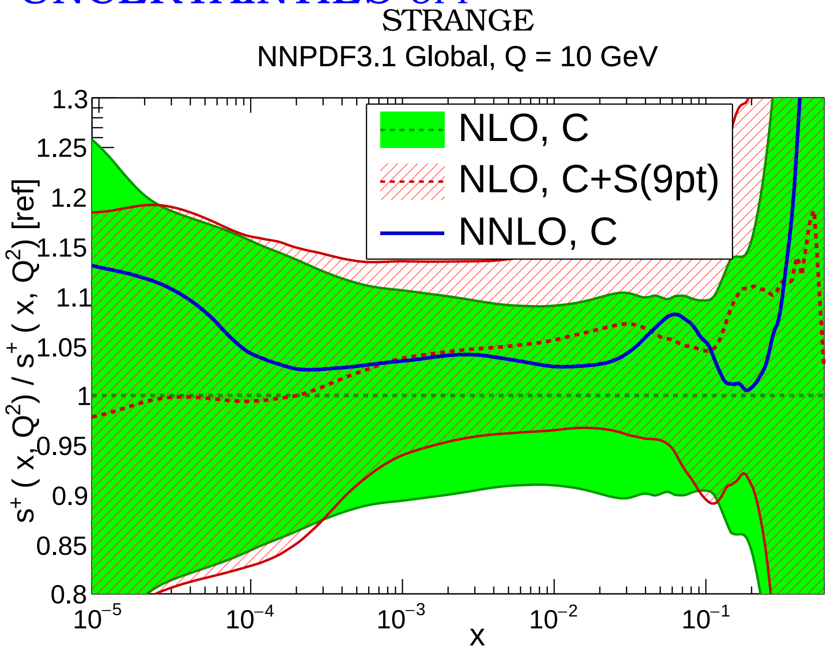
	C	$C + S^{(3\mathrm{pt})}$	$C + S^{(9\mathrm{pt})}$
χ^2	1.139	1.139	1.109
ϕ	0.314	0.310	0.315

- FIT QUALITY χ^2 IMPROVES
- RELATIVE ERROR ϕ ON PREDICTION DOES NOT CHANGE
- DATA REGION: PDF UNCERTAINTY ALMOST UNCHANGED
- EXTRAPOLATION REGION: PDF UNCERTAINTY SIGNIFICANTLY INCREASES
- CENTRAL VALUE MOVES TOWARDS KNOWN NNLO

EQUALLY PRECISE BUT MORE ACCURATE RESULT!

PDFs with theory uncertainties 9pt





	C	$C + S^{(3\text{pt})}$	$C + S^{(9\text{pt})}$
χ^2	1.139	1.139	1.109
ϕ	0.314	0.310	0.315

- Fit quality χ^2 improves
- Relative error ϕ on prediction does not change
- Data region: PDF uncertainty almost unchanged
- Extrapolation region: PDF uncertainty significantly increases
- Central value moves towards known NNLO

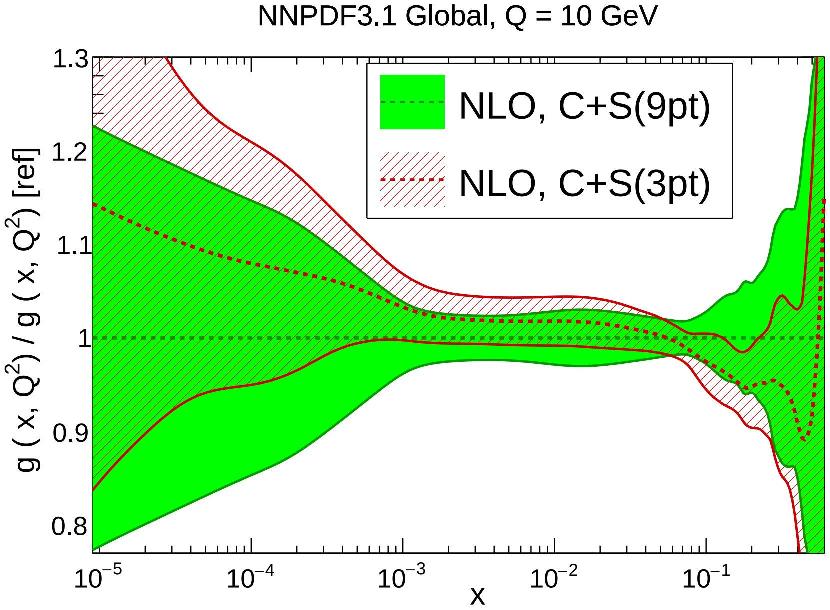
Equally precise but more accurate result!

PDFs WITH THEORY UNCERTAINTIES

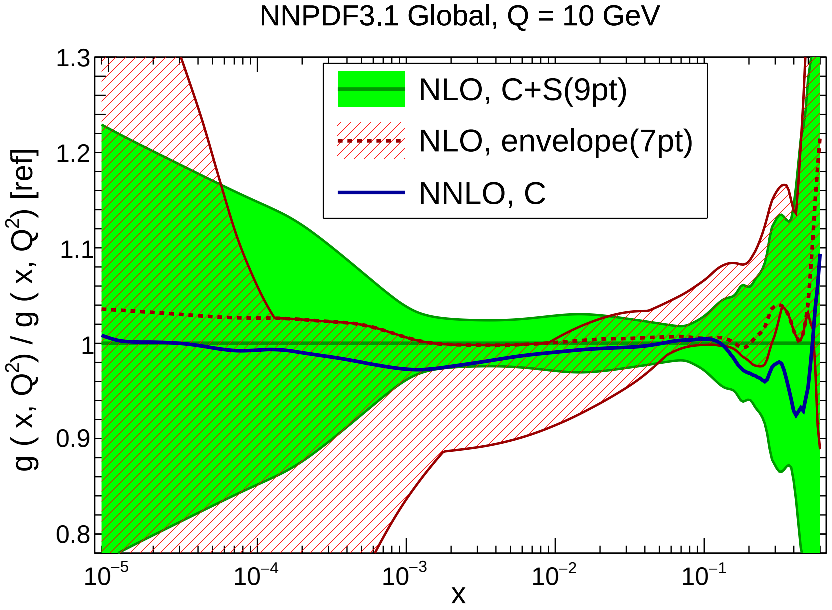
- RESULTS MILDLY DEP. ON PRESCRIPTION $\Rightarrow$ 3PT CLOSER TO RESULT W/O THEORY UNCERTAINTY
- "UNSTABLE" SCALE VARIATIONS $\Rightarrow$ NO IMPACT ON FIT
- 7PT ENVELOPE RATHER MORE CONSERVATIVE
  ENVELOPE DOES NOT INCLUDE EXP. UNCERTAINTY

THE GLUON PDF

3PT VS 9PT PRESCRIPTION



9PT PRESCRIPTION VS ENVELOPE



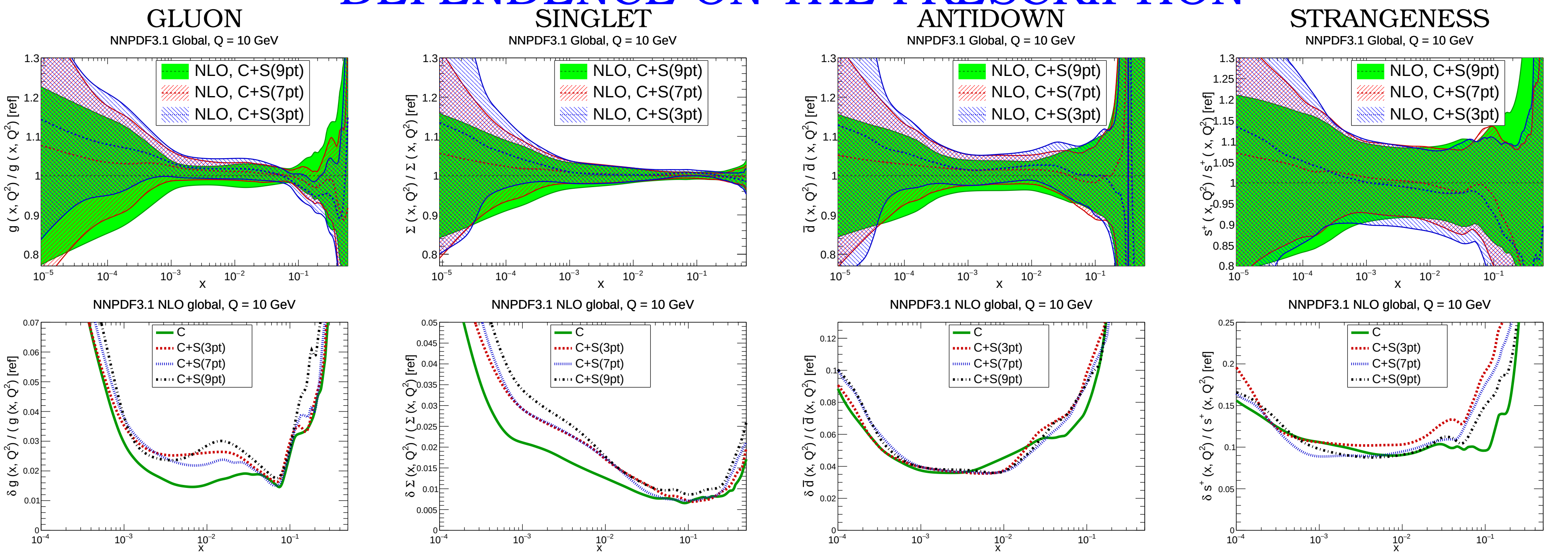
STATISTICAL INDICATORS

Process	$n_{\rm dat}$	$\chi^2/n_{\rm dat}$ in the NNPDF3.1 global fits NLO C	$C+S^{(9pt)}$	$C+S^{(7pt)}$	$C+S^{(3pt)}$	$C+S^{(9pt)}_{\rm fit}$	$C+S^{(9pt)}_{\rm sampl}$	NNLO C
DIS NC	1593	1.088	1.079	1.086	1.095	1.081	1.227	1.084
DIS CC	552	1.012	0.928	0.933	0.960	0.929	1.036	1.079
DY	484	1.486	1.447	1.485	1.483	1.461	1.434	1.231
JETS	164	0.907	0.839	0.858	0.901	0.848	0.911	0.950
TOP	26	1.260	1.012	1.016	1.077	1.001	1.264	1.068
Total	2819	1.139	1.109	1.129	1.139	1.113	1.217	1.105

Process	ϕ in the NNPDF3.1 global fits NLO C	$C+S^{(9pt)}$	$C+S^{(7pt)}$	$C+S^{(3pt)}$	$C+S^{(9pt)}_{\rm fit}$	$C+S^{(9pt)}_{\rm sampl}$	NNLO C
DIS NC	0.266	0.268	0.262	0.261	0.261	1.137	0.305
DIS CC	0.389	0.376	0.367	0.391	0.369	0.502	0.471
DY	0.361	0.343	0.340	0.358	0.349	0.603	0.380
JETS	0.295	0.312	0.279	0.291	0.298	0.461	0.392
TOP	0.375	0.352	0.318	0.331	0.319	0.612	0.363
Total	0.314	0.315	0.304	0.313	0.309	0.932	0.362

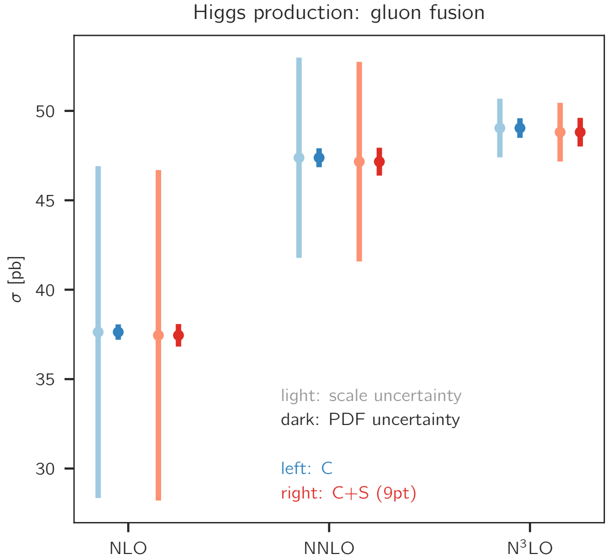
- MILD PRESCRIPTION DEPENDENCE
- COVMAT ONLY IN FITTING $\Rightarrow$ SAME CENTRAL VALUE, REDUCED UNCERTAINTY
  TH COVMAT RESOLVES TENSION

DEPENDENCE ON THE PRESCRIPTION

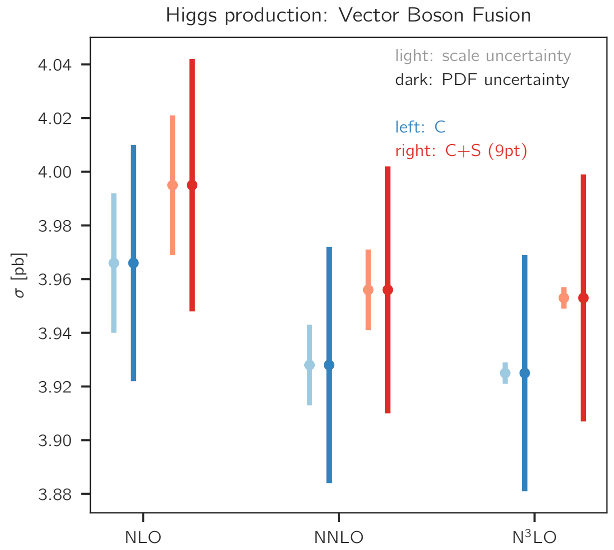


PHENOMENOLOGY (LHC 13)

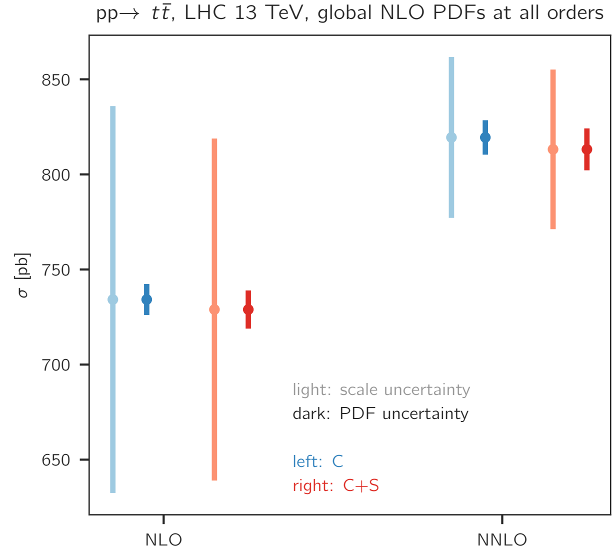
Higgs gg



Higgs VBF



TOP PAIRS



USAGE: JUST COMPUTE PDF ERROR AS USUAL & COMBINE WITH MHOU ON HARD MATRIX ELEMENT COMPUTED WITH YOUR PREFEREED RECIPRE

- MODERATE EFFECT ON UNCERTAINTIES
- VISIBLE SHIFT OF CENTRAL VALUES

OUTLOOK

- INCLUSION OF MHOU THROUGH COVARIANCE MATRIX
  REASONABLY STABLE
- MORE DETAILED SCALE VARIATION PATTERNS TO BE EXPLORED
- NEXT STEP: APPLICATION TO NNLO GLOBAL FITS

EXTRAS

CORRELATIONS

- Harland-Lang, Thorne 2018: FACTORIZATION SCALE VARIATION "DOUBLE COUNTED" BETWEEN PDF AND HARD PROCESS
- RECALL FACTORIZATION SCALE $\Rightarrow$ SCALE OF EVOLUTION
- INITIAL PDF SCALE AT SAME SCALE AS PROCESS $\Rightarrow$ NO EVOLUTION UNCERTAINTY
- WOULD NEED A PDF SET FOR EACH SCALE $\Rightarrow$ UNIVERSALITY BROKEN