PDFS: FROM NN TO ML

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Machine Learning for Pheno

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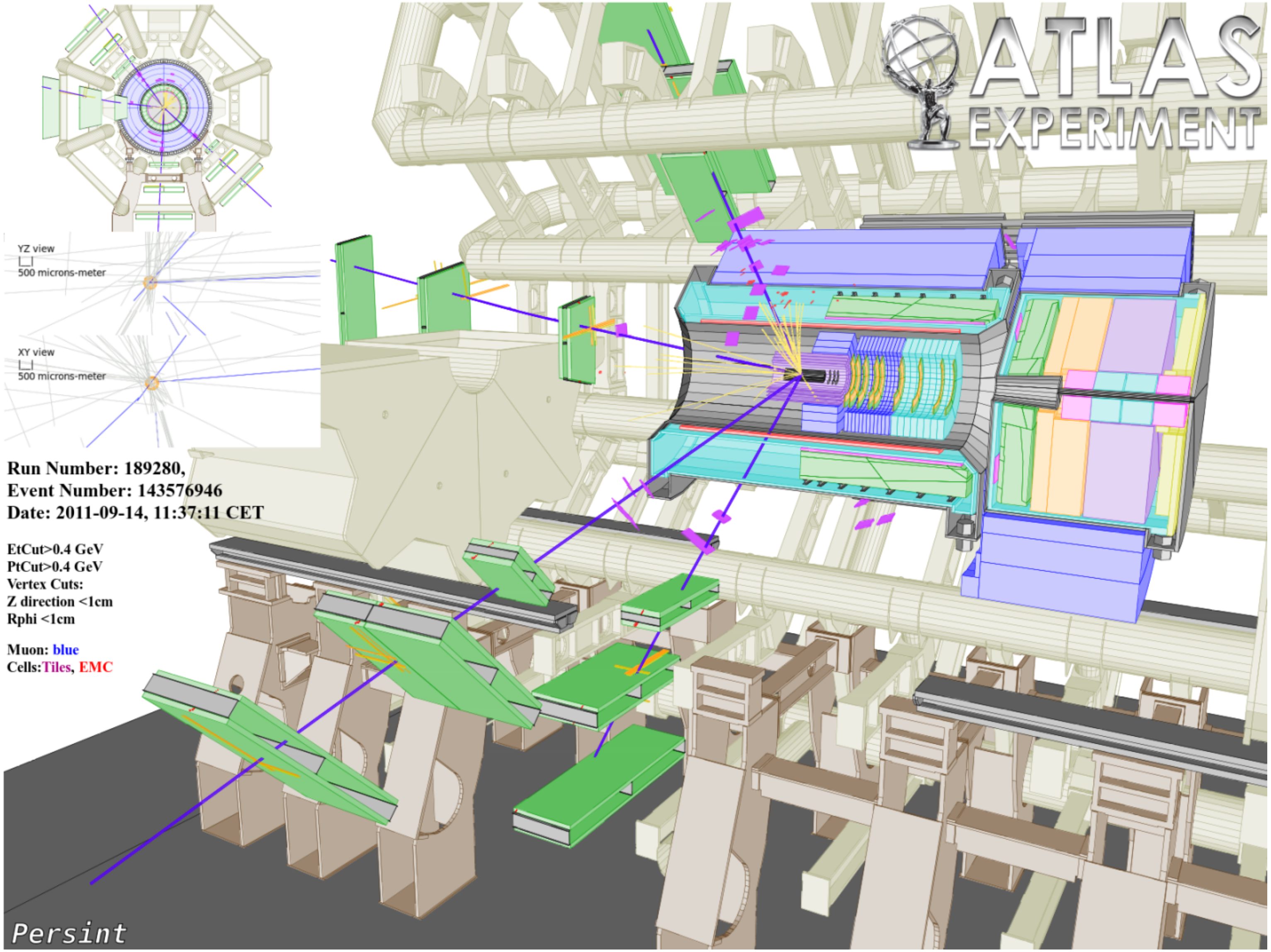
PHYSICS AT THE LHC



FACTORIZATION

THE PARTON LUMINOSITY

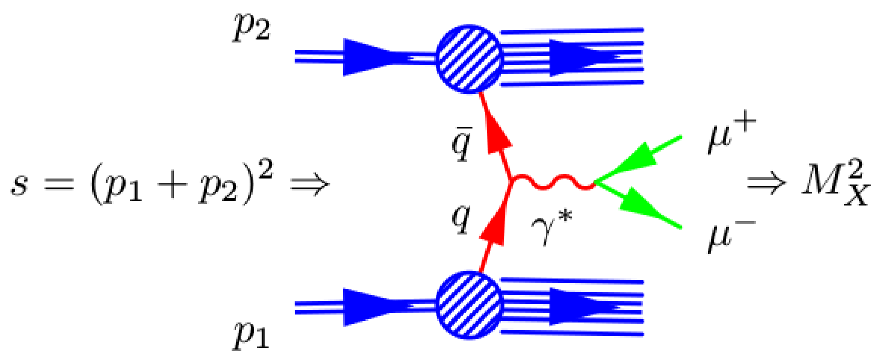
$$\sigma_X(s, M_X^2) = \sum_{a,b} \int_{x_{\min}}^1 dx_1\, dx_2\, f_{a/h_1}(x_1) f_{b/h_2}(x_2) \hat{\sigma}_{q_a q_b \to X}\left(x_1 x_2 s, M_X^2\right)$$

$$\sigma_X(s, M^2) = \sum_{a,b} \int_\tau^1 \frac{dx}{x} \mathcal{L}_{ab}\left(\frac{\tau}{x}\right) \hat{\sigma}\left(x, \alpha_s(M_H^2)\right) = \sum_{a,b} \mathcal{L}_{ab} \otimes \hat{\sigma}_{ab}$$

- PARTON LUMINOSITY $\mathcal{L}_{ab}(\tau) = \int_\tau^1 \frac{dx}{x} f_{a/h_1}(x) f_{b/h_2}(\tau/x) = f_a \otimes f_b$
- PARTONIC CROSS SECTION $\hat{\sigma}_{q_a q_b \to X}$

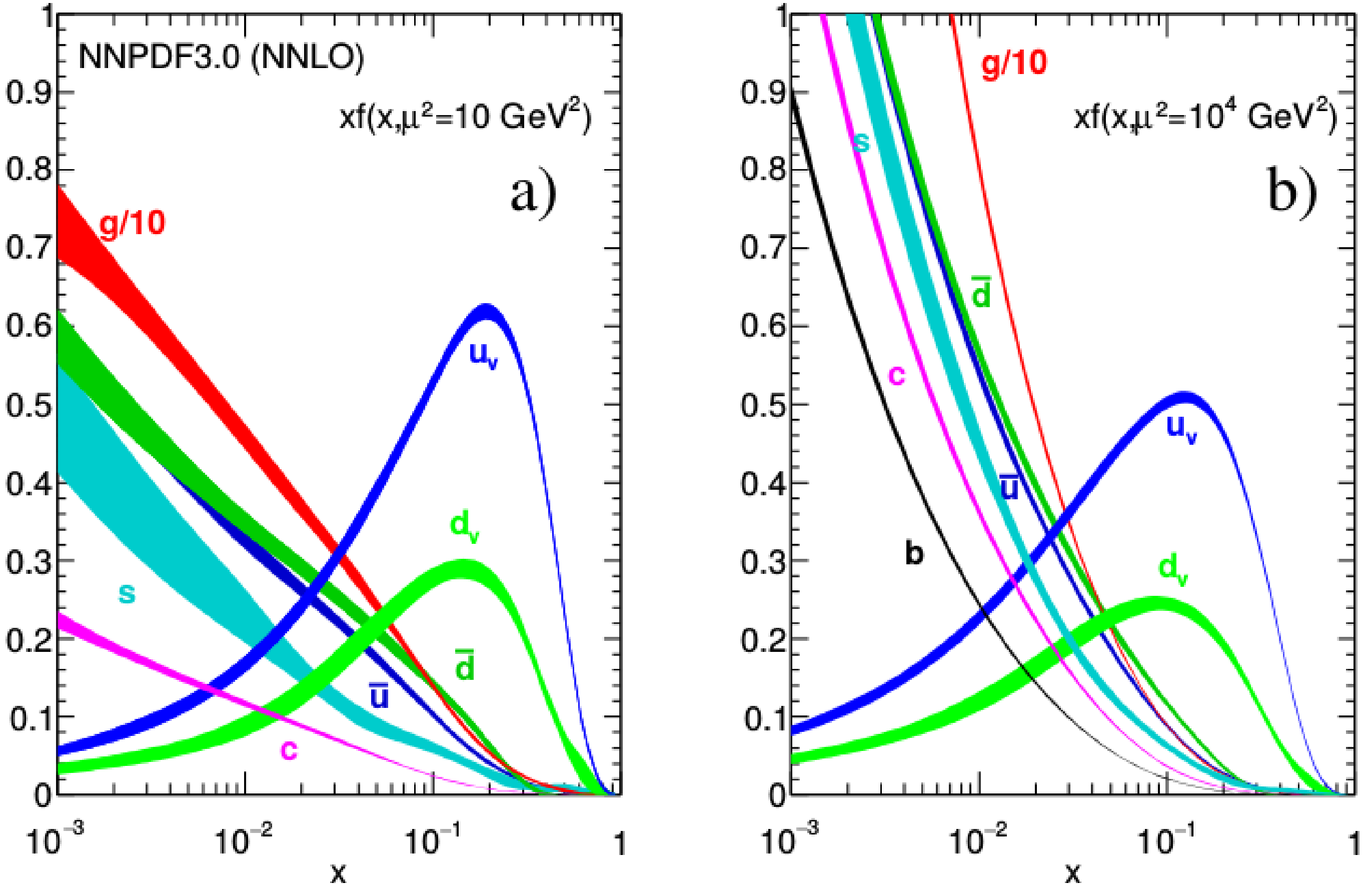
EXAMPLE: THE DRELL-YAN PROCESS

(LEADING ORDER)



- HADRONIC C.M. ENERGY: $s = (p_1 + p_2)^2$
- PARTONIC C.M. ENERGY: $\hat{s} = x_1 x_2 s$
- MOMENTUM FRACTIONS $x_{1,2} = \sqrt{\frac{\hat{s}}{s}} \exp \pm y$; AT LEADING ORDER $\hat{s} = M^2$

THE PDFs

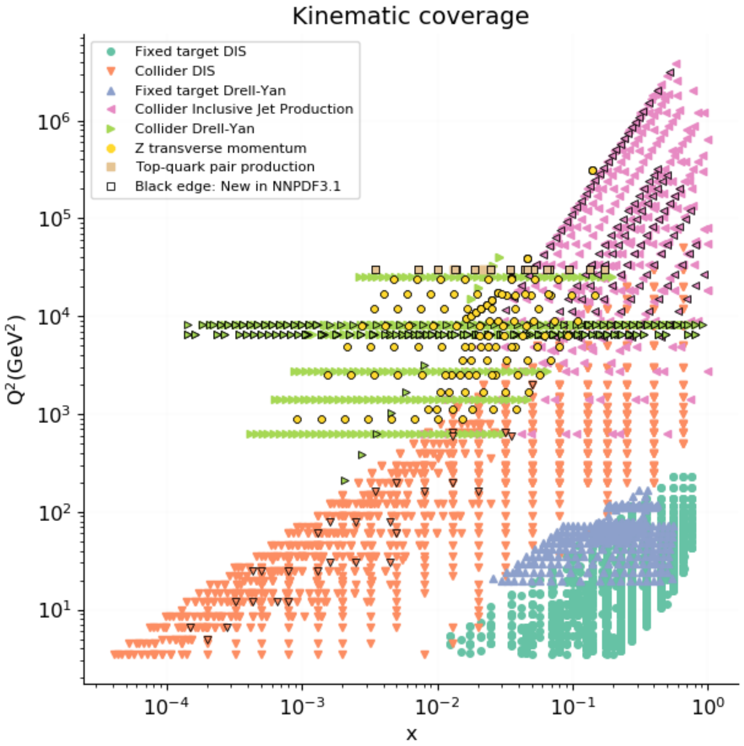


(PDG 2016)

- MOMENTUM PROBABILITY DENSITY $xf_i(x)$ AT TWO DIFFERENT SCALES (LEFT $\Rightarrow$ LOW SCALE; RIGHT $\Rightarrow$ HIGH SCALE)
- AS $x \geq 1$ KINEMATIC CONSTRAINT $f_i(x) = 0$
- VALENCE SUM RULES $\int dx(u(x) - \bar{u}(x)) = 2 \int dx(d(x) - \bar{d}(x)) = 2.$
- MOMENTUM SUM RULE $\sum \int dx x f_i(x) = 1$

PDF DETERMINATION

DATA $\rightarrow$ PARTON DISTRIBUTIONS



ISSUES:

TRIVIAL

- FROM PHYSICAL OBSERVABLES TO PDFs: SOLVE EVOLUTION EQUATIONS, CONVOLUTE WITH PARTON-LEVEL CROSS-SECTIONS
- DISENTANGLING PDFs: CHOOSE A BASIS OF PDFs ($2N_f$ QUARKS + 1 GLUON) & A SET OF SUITABLE PHYSICAL PROCESSES TO DETERMINE THEM ALL

NONTRIVIAL

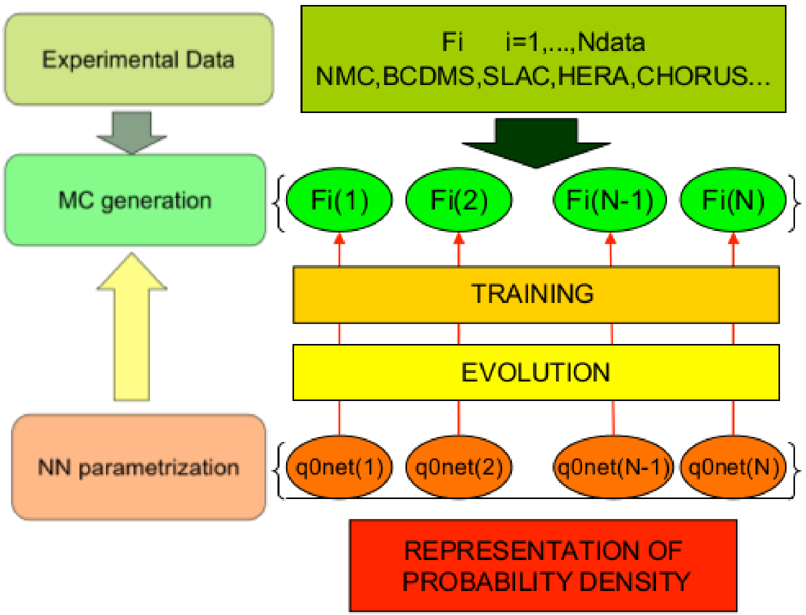
- (1) DETERMINE FUNCTIONS FROM A DISCRETE DATASET
- (2) DETERMINE A PROBABILITY FUNCTIONAL IN THE SPACE OF FUNCTIONS

THE NNPDF APPROACH

BASIC IDEA: MONTE CARLO SAMPLING OF THE PROBABILITY MEASURE IN THE (FUNCTION) SPACE OF PDFs

- GENERATE A SET OF MONTE CARLO REPLICAS $\sigma^{(k)}$ OF THE ORIGINAL DATASET $\sigma^{(\mathrm{data})}$
  $\Rightarrow$ REPRESENTATION OF $\mathcal{P}[\sigma]$ AT DISCRETE SET OF POINTS IN DATA SPACE
- FIT A PDF REPLICA TO A DATA REPLICA
  $\Rightarrow$ EACH PDF REPLICA $f_i^{(k)}$ IS A BEST-FIT PDF SET FOR GIVEN DATA REPLICA
- THE SET OF NEURAL NETS IS A REPRESENTATION OF THE PROBABILITY DENSITY:

$$\langle f_i \rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} f_i^{(k)}$$



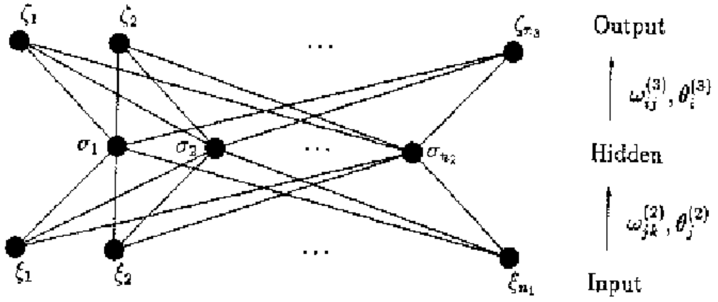
SOLUTIONS

- (1) FUNCTIONS FROM DISCRETE DATA $\Rightarrow$ NEURAL NETWORKS
- (2) PROBABILITY IN FUNCTION SPACE $\Rightarrow$ MONTE CARLO

NEURAL NETWORKS

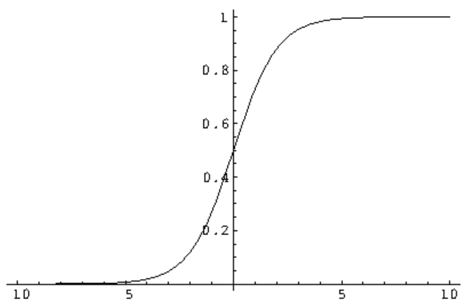
- EACH PDF REPLICA FITTED TO A DATA REPLICA
  $\Rightarrow$ NEED BEST-FIT, COVARIANCE MATRIX IN PARAMETER SPACE NOT NEEDED
- CAN USE VERY LARGE PARAMETRIZATION

NEURAL NETWORKS



MULTILAYER FEED-FORWARD NETWORKS

- Each neuron receives input from neurons in preceding layer and feeds output to neurons in subsequent layer
- Activation determined by weights and thresholds
  $$\xi_i = g\left(\sum_j \omega_{ij}\xi_j - \theta_i\right)$$
- Sigmoid activation function
  $g(x) = \frac{1}{1+e^{-\beta x}}$



EXAMPLE: A 1-2-1 NN

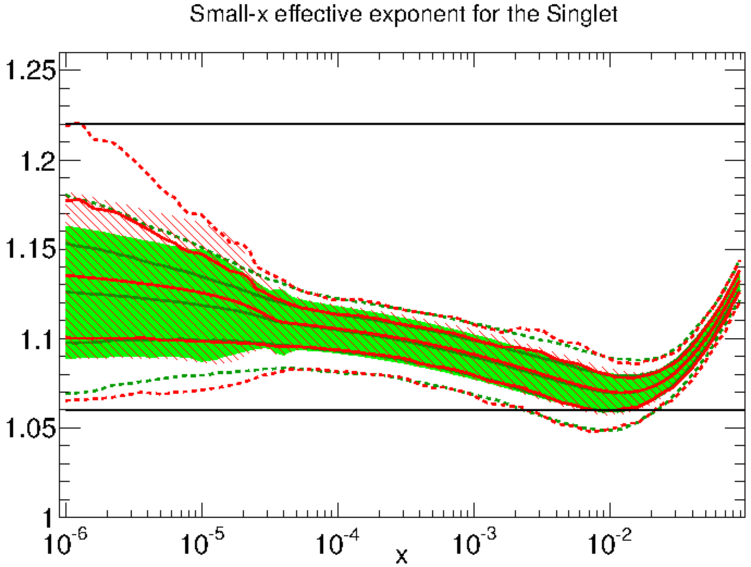
$$f(x) = \frac{1}{1+e^{\theta_1^{(3)} - \frac{\omega_{11}^{(2)}}{1+e^{\theta_1^{(2)} - x\omega_{11}^{(1)}}} - \frac{\omega_{12}^{(2)}}{1+e^{\theta_2^{(2)} - x\omega_{21}^{(1)}}}}}$$

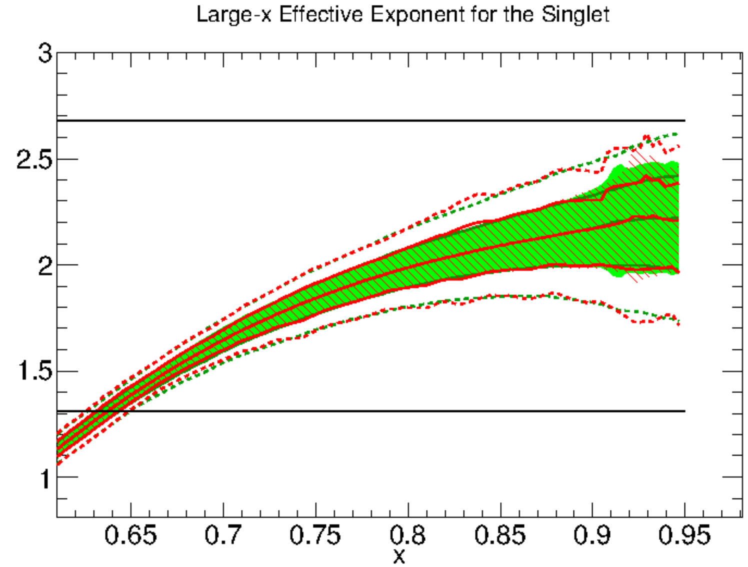
CURRENTLY: 2-5-3-1 NN FOR EACH OF 8 BASIS PDFS (37X8=296 FREE PARMS.)

PREPROCESSING

- PDFs ARE PARAMETRIZED WITH NEURAL NETWORKS TIMES PREPROCESSING FUNCTION: $f_i(x) = x^{\alpha_i}(1-x)^{\beta_i} NN(x)$
- GOAL IS TO SPEED UP TRAINING WITHOUT BIASING RESULT
- α_i, β_i RANDOM REPLICA BY REPLICA WITH UNIFORM DISTRIBUTION IN RANGE
- RANGE DETERMINED SELF-CONSISTENTLY AS TWICE THE RANGE OF EFFECTIVE EXPONENTS $\alpha_{\rm eff,i} = \frac{\ln f_i(x)}{\ln 1/x}$ $\beta_{\rm eff,i} = \frac{\ln f_i(x)}{\ln(1-x)}$
  EVALUATED AT $x = 0.95,\ 0.65$ (β); $x = 10^{-6},\ 10^{-3}$ (α)

EFFECTIVE EXPONENTS FOR QUARK SINGLET VS. PREPROCESSING RANGE
100 & 1000 REPLICAS





GENETIC MINIMIZATION

RANDOM MUTATION OF THE NN PARAMETERS STARTING FROM RANDOM VALUES

- LARGE NUMBER OF MUTANT (~ 100) PDF SETS GENERATED FROM PARENT
- FIGURE OF MERIT COMPUTED
- BEST-FIT KEPT & PASSED TO NEXT GENERATION

$$w \to w + \frac{\eta r_\delta}{N_{\rm ite}^{r_{\rm ite}}}$$

CHOICES

- MUTATION RATE η
- POINTLIKE VS. NODAL MUTATION
- NUMBER (POINTLIKE) OR PROBABILITY (NODAL) OF MUTATIONS
- TARGETED WT: WEIGTHS $p_i = E_i/E_i^{\rm targ}$
- GA EPOCHS: $N_{\rm gen}^{\rm mut}$

	$N_{\rm gen}^{\rm wt}$	$N_{\rm gen}^{\rm mut}$	$N_{\rm gen}^{\rm max}$	$E^{\rm sw}$	$N_{\rm mut}^{a}$	$N_{\rm mut}^{b}$
NNPDF 2.3	10000	2500	50000	2.3	80	30
NNPDF 3.0	–	-	30000	-	80	-

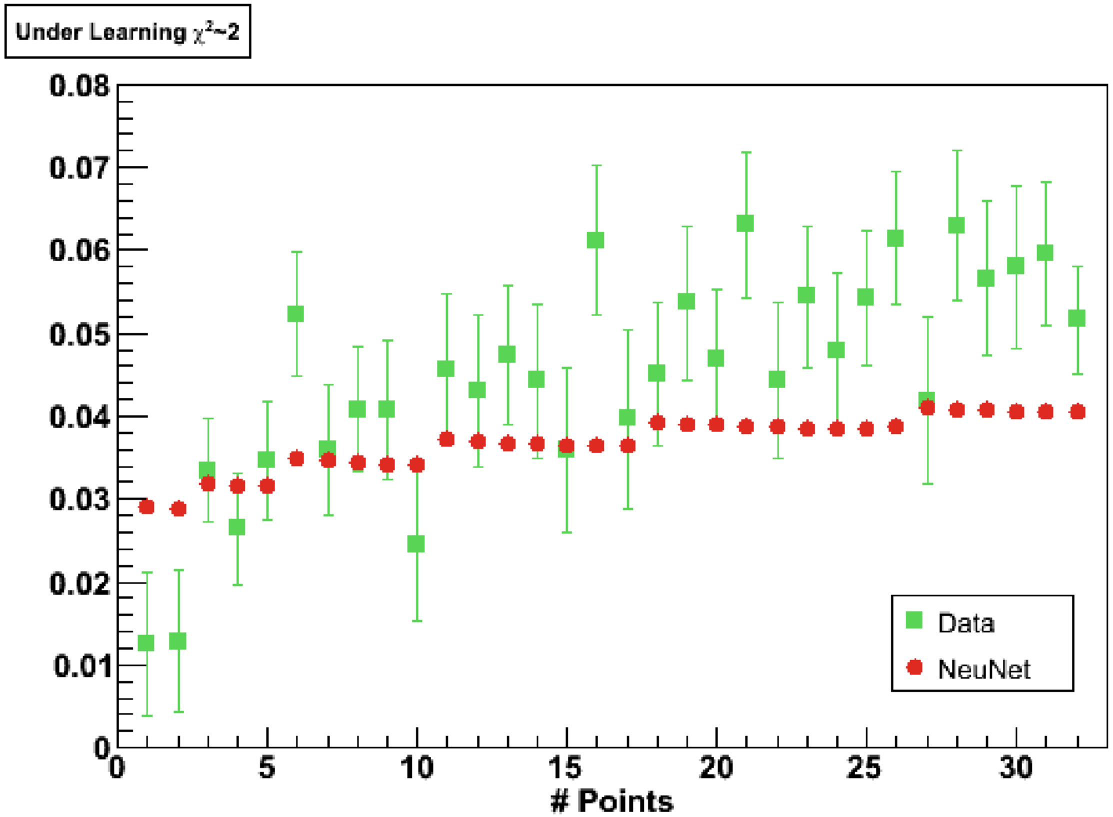
NNPDF2.3		
Single Parameter Mutation		
PDF	$N_{\rm mut}$	η
$\Sigma(x)$	2	10, 1
$g(x)$	3	10, 3, 0.4
$T_3(x)$	2	1, 0.1
$V(x)$	3	8, 1, 0.1
$\Delta_S(x)$	3	5, 1, 0.1
$s^+(x)$	2	5, 0.5
$s^-(x)$	2	1, 0.1

NNPDF3.0		
Nodal Mutation		
PDF	$P_{\rm mut}$	η
$\Sigma(x)$	5% per node	15
$g(x)$	5% per node	15
$V(x)$	5% per node	15
$V_3(x)$	5% per node	15
$V_8(x)$	5% per node	15
$T_3(x)$	5% per node	15
$T_8(x)$	5% per node	15

NN TRAINING: EXAMPLE

- HIGHLY REDUNDANT PARAMETRIZATION
- COMPLEXITY INCREASES AS THE FITTING PROCEEDS
- $\Rightarrow$ THE BEST FIT IS NOT THE ABSOLUTE MINIMUM:
  MUST LOOK FOR OPTIMAL LEARNING POINT

UNDERLEARNING



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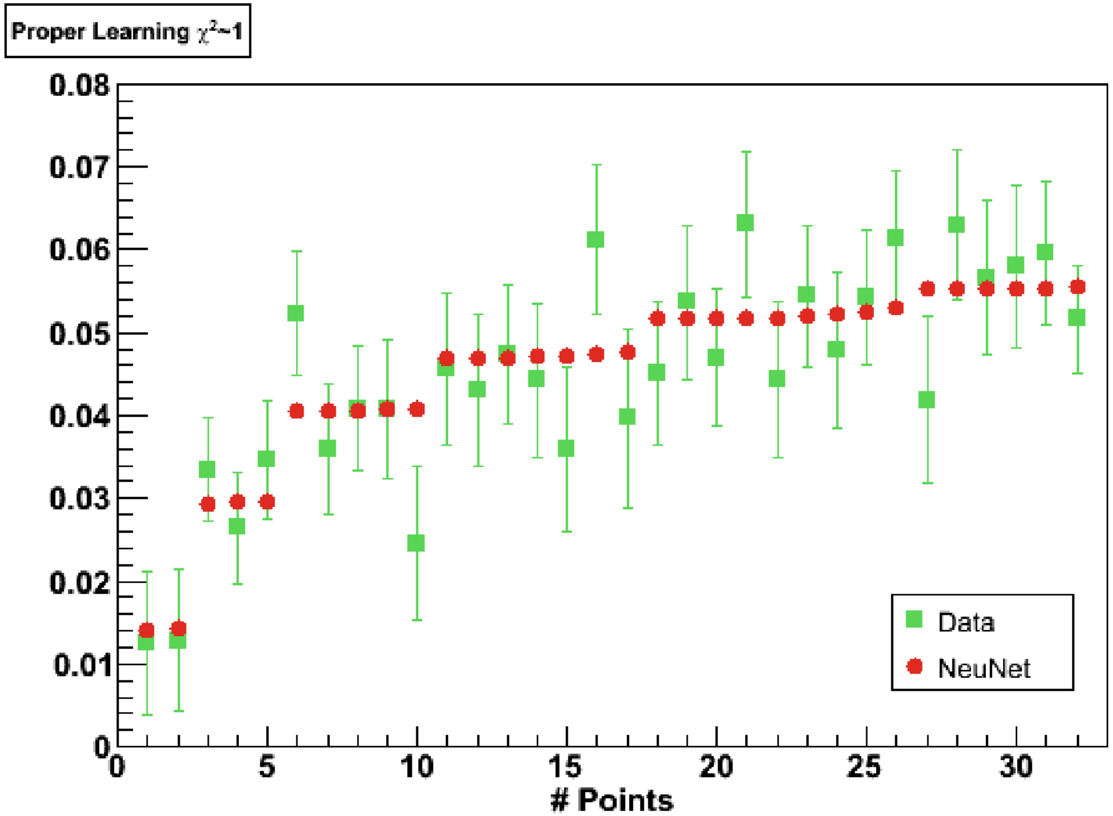
PROPER LEARNING



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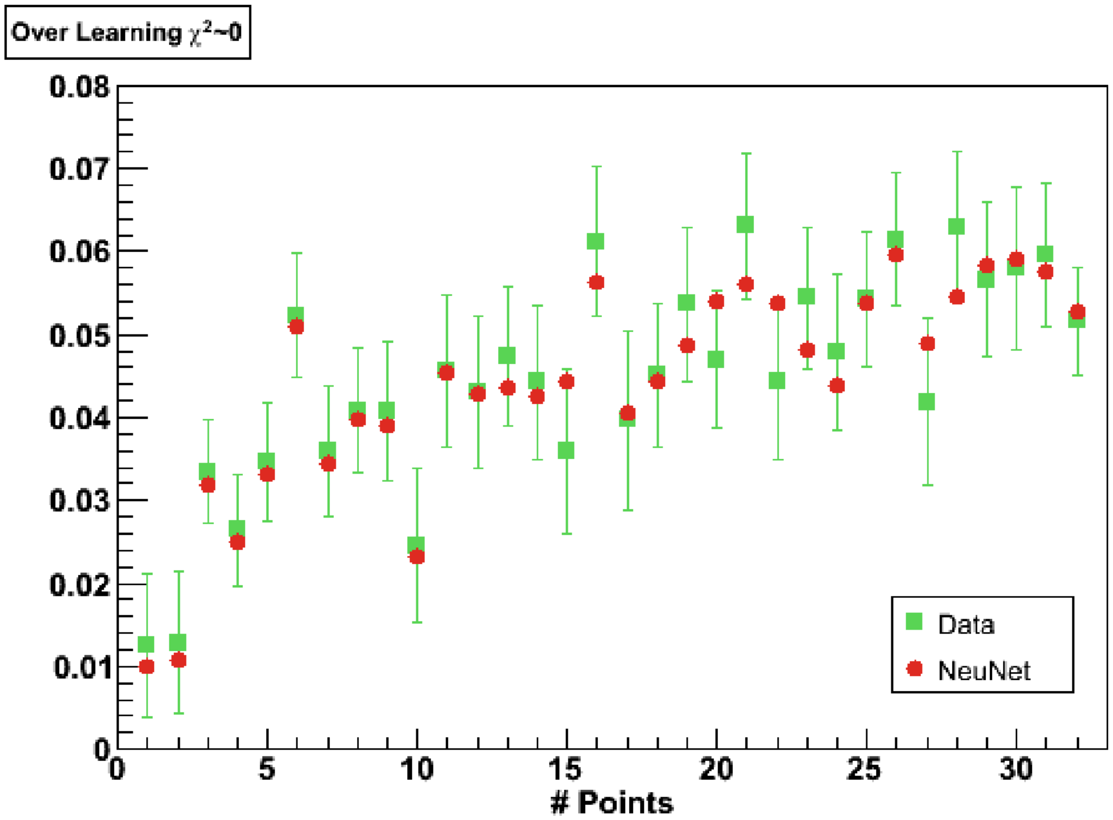
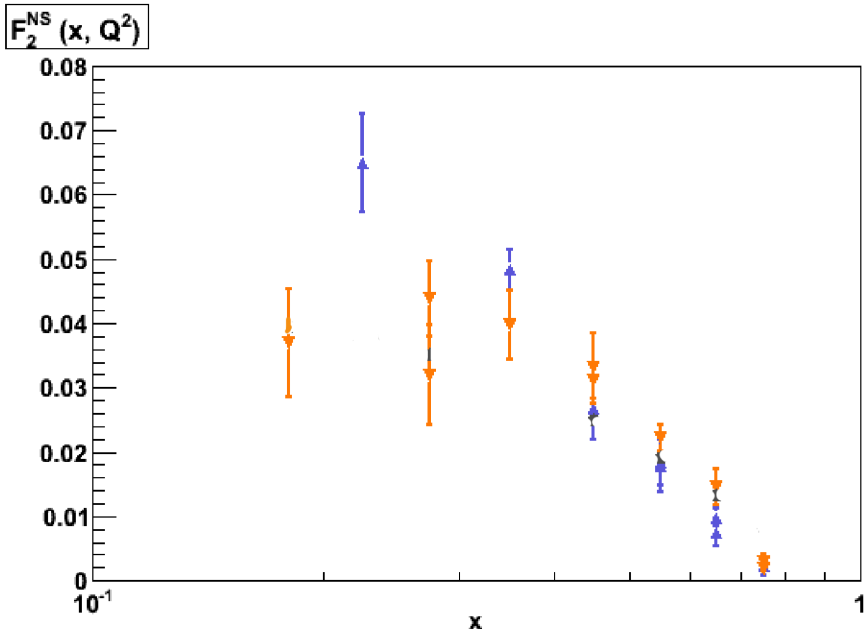
OVERLEARNING



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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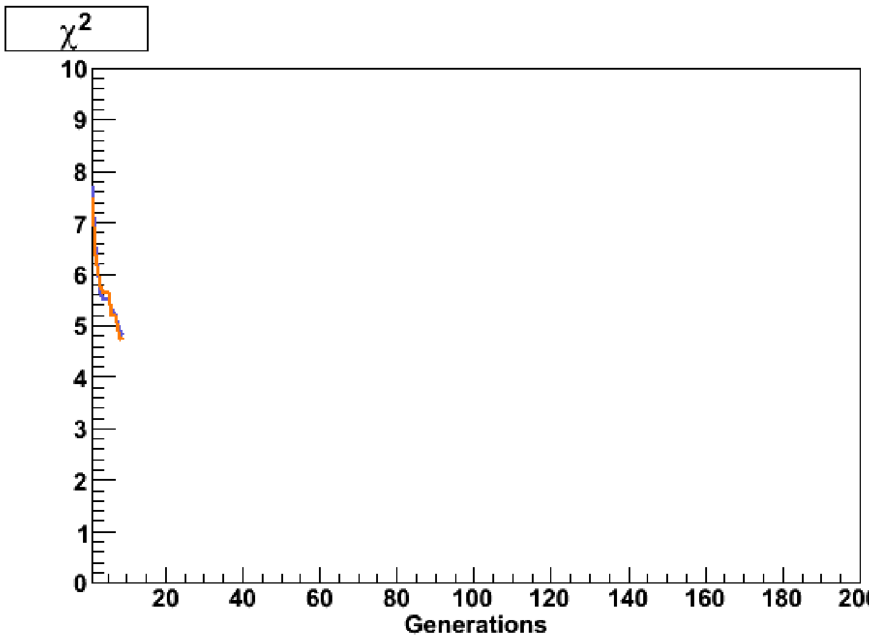
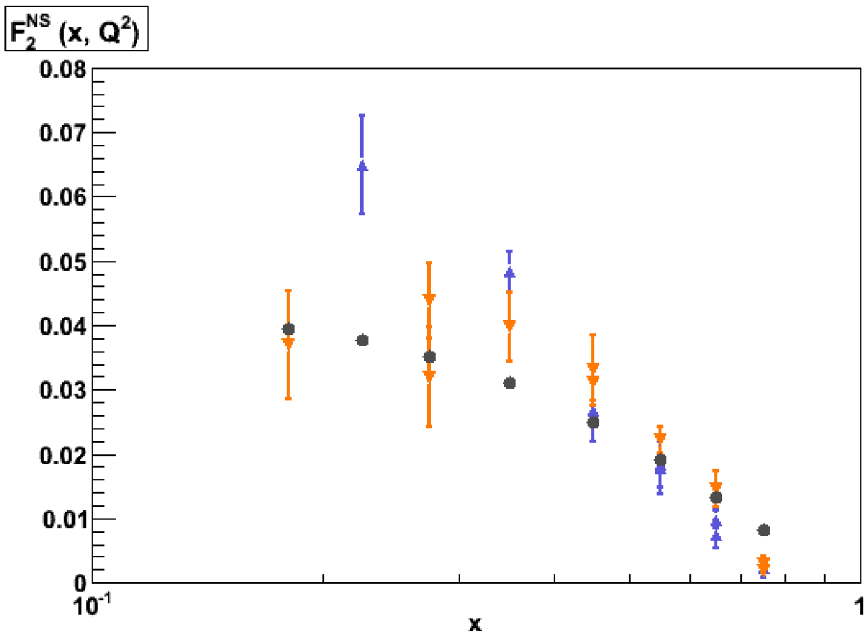
GO!





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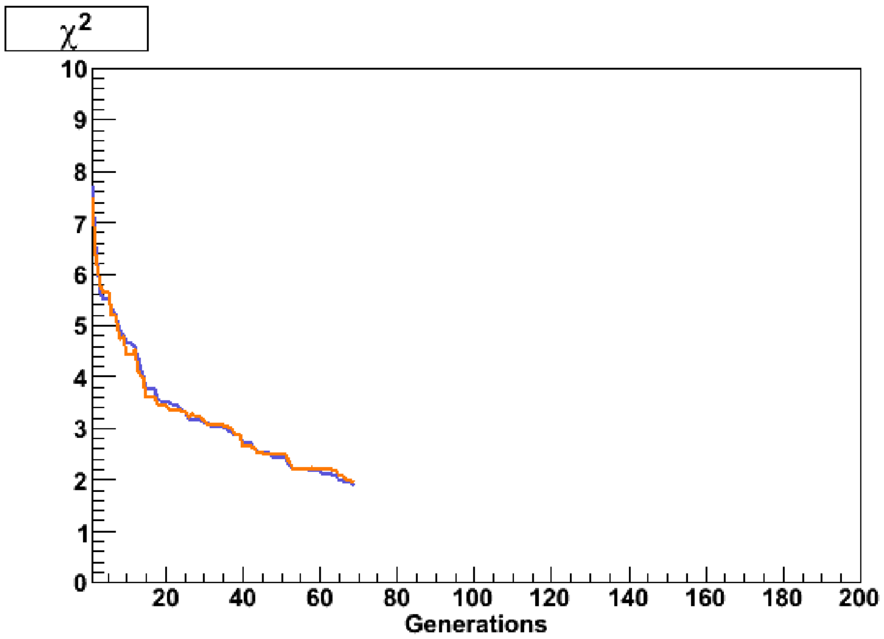
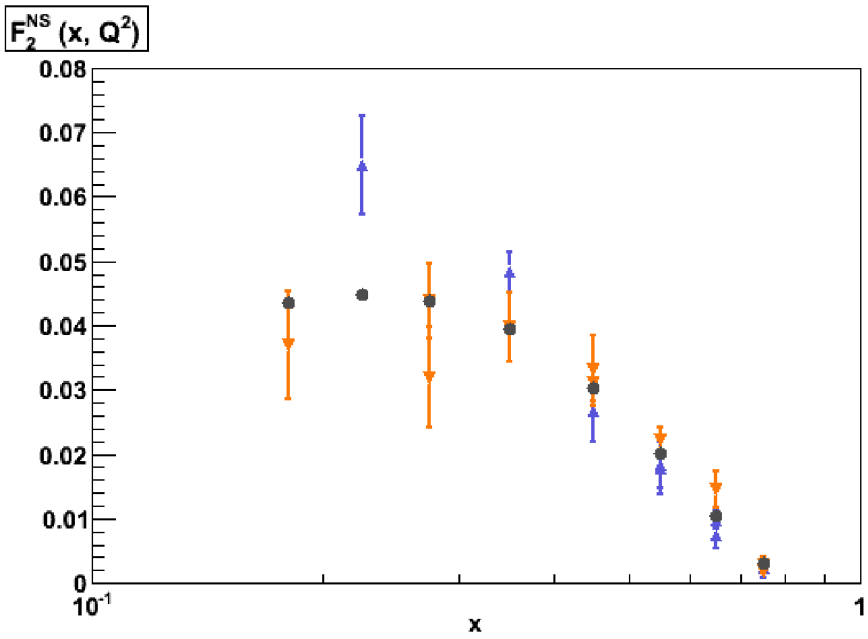
STOP!





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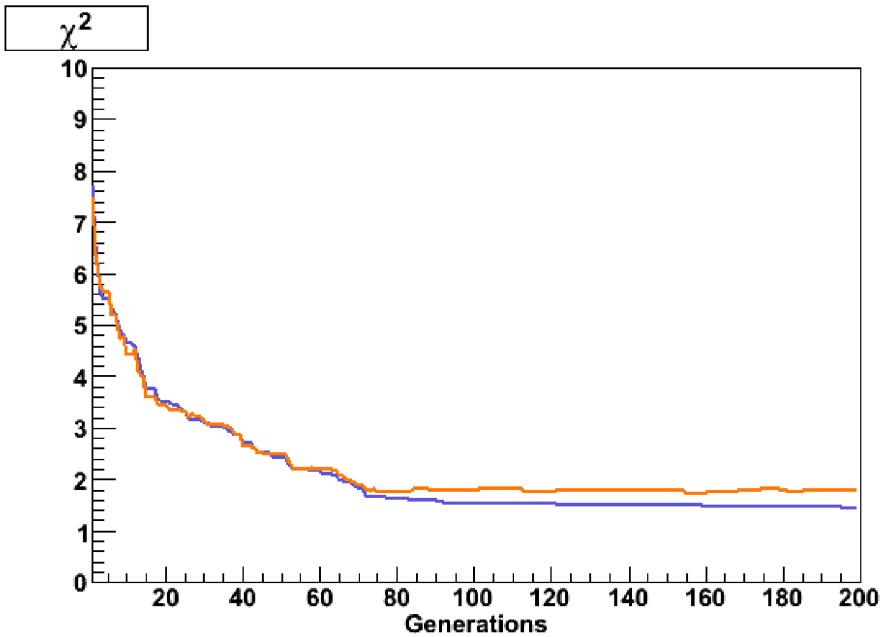
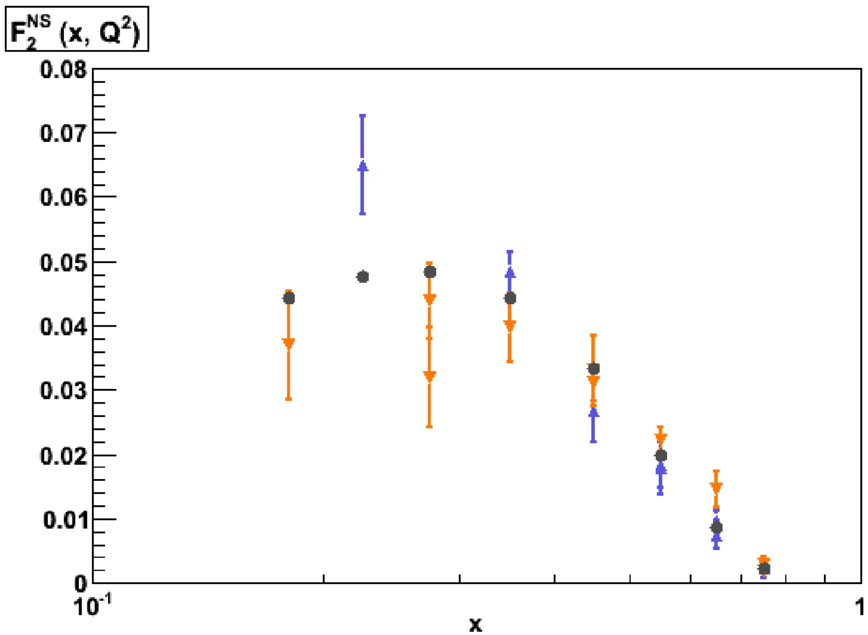
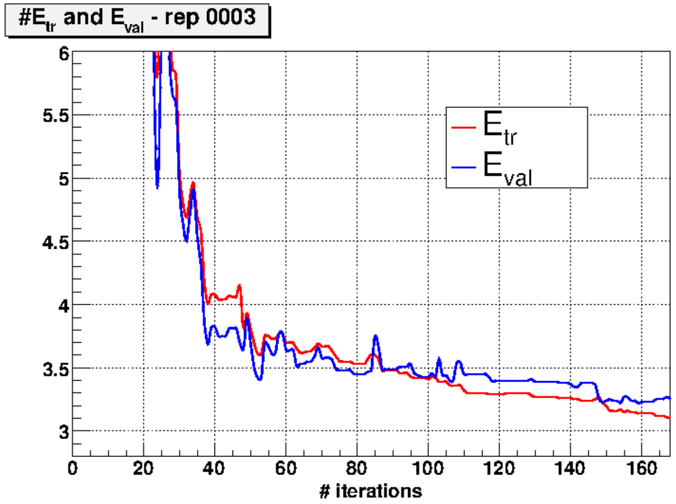
TOO LATE!

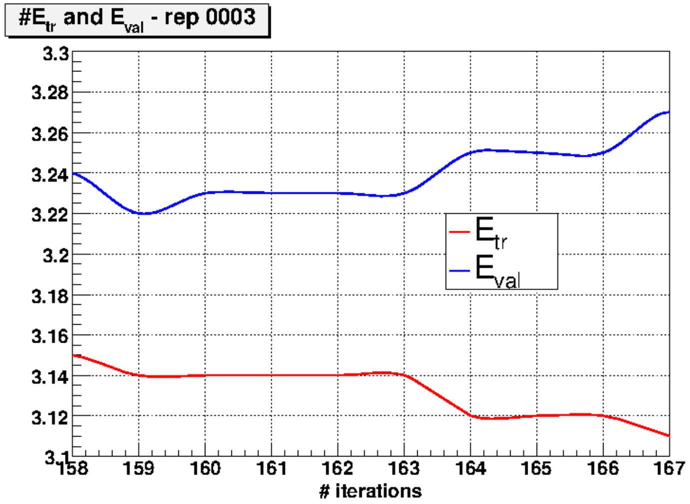




STOPPING CRITERIA

STOPPING FOR THE χ^2 OF ONE REPLICA





- UP TO NNPDF2.3 "INCREASING" AND "DECREASING" TRAINING AND VALIDATION χ^2 DEFINED IN TERMS OF THRESHOLD VALUES δ_{tr} AND δ_{val}:
  INCREASE: $\chi^2_{val}(N_{gen}+\Delta) > \chi^2(N_{gen}+\Delta) + \delta_{val}$
- FROM NNPDF3.0 USE LOOKBACK:
  FIT IS RUN UP TO SOME LARGE # OF GA GENERATIONS
  THEN ONE "LOOKS BACK" FOR ABSOLUTE MIN. OF VALIDATION χ^2
- CHECK THAT RESULTS ARE INDEPENDENT OF THE LARGE # OF GA GENS
- CHECK THAT RESULTS ARE INDEPENDENT OF FLUCTUATIONS IN VALUE OF ABSOLUTE MINIMUM
  DIFFERENT STOPPING POINTS, BUT INDISTINGUISHABLE PDFs

CLOSURE TESTS:

THE BASIC IDEA

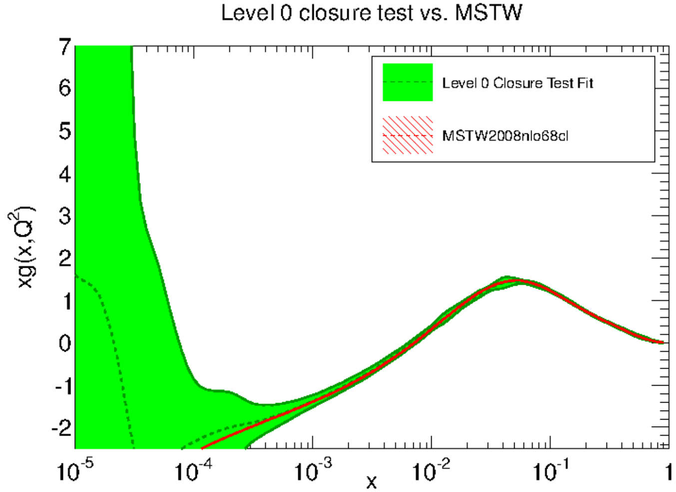
- ASSUME PDFs KNOWN: GENERATE FAKE EXPERIMENTAL DATA
- CAN DECIDE DATA UNCERTAINTY (ZERO, OR AS IN REAL DATA, OR . . .)
- FIT PDFs TO FAKE DATA
- CHECK WHETHER FIT REPRODUCES UNDERLYING "TRUTH":
  - CHECK WHETHER TRUE VALUE GAUSSIANLY DISTRIBUTED ABOUT FIT
  - CHECK WHETHER UNCERTAINTIES FAITHFUL
  - CHECK STABILITY

    (INDEP. OF METHODOLOGICAL DETAILS)

LEVEL-0 CLOSURE TESTS

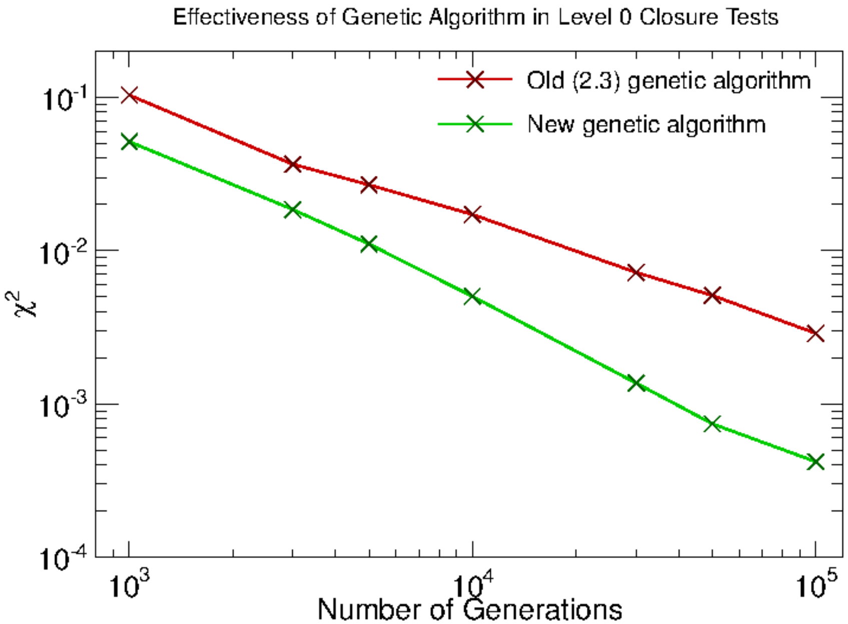
- ASSUME VANISHING EXPERIMENTAL UNCERTAINTY
- MUST BE ABLE TO GET $\chi^2 = 0$
- UNCERTAINTY AT DATA POINTS TENDS TO ZERO (NOT NECESSARILY ON PDF!)
  DEFINE $\phi \equiv \sqrt{\langle \chi^2_{rep} \rangle - \chi^2}$, EQUALS FIT UNCERTAINTY/DATA UNCERTAINTY; CHECK $\phi \to 0$
- BEST FIT ON TOP OF "TRUTH" IN DATA REGION

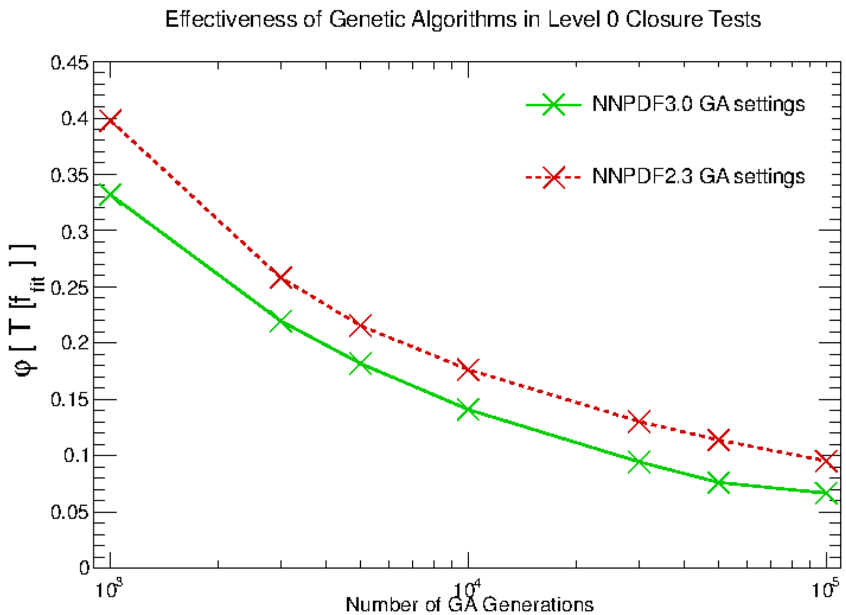
THE GLUON



FRACTIONAL UNCERTAINTY VS TRAINING LENGTH

χ^2 VS TRAINING LENGTH

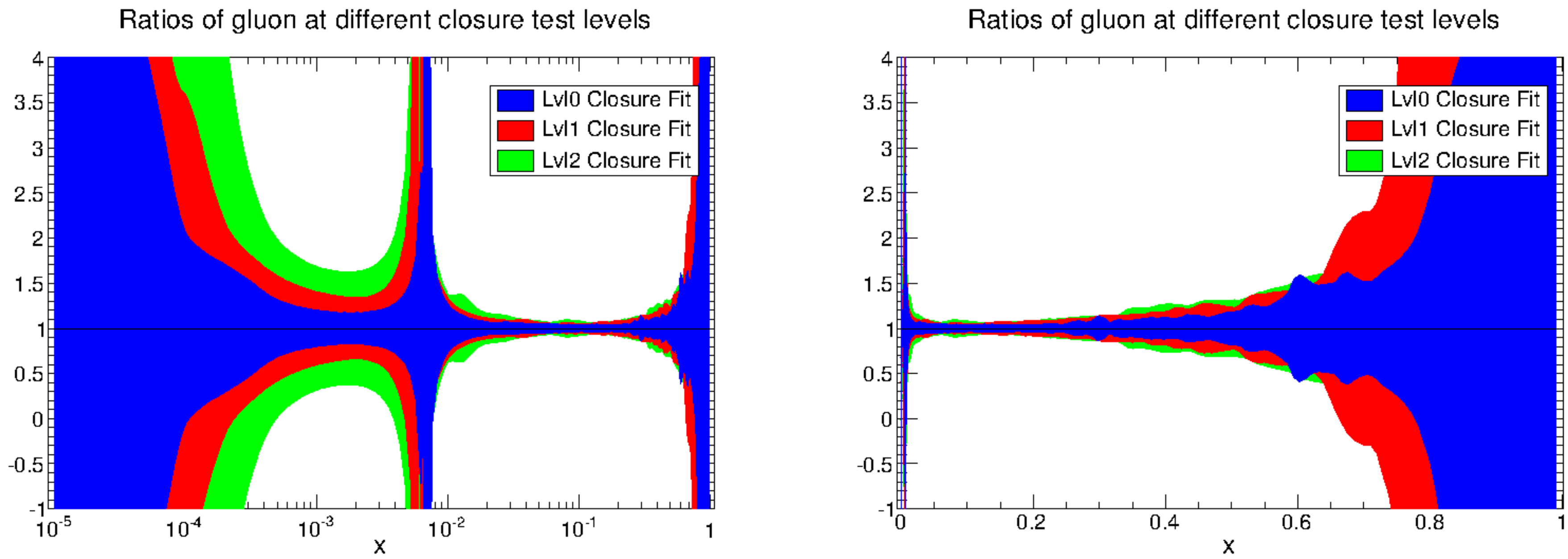




LEVEL-0, LEVEL-1 AND LEVEL-2

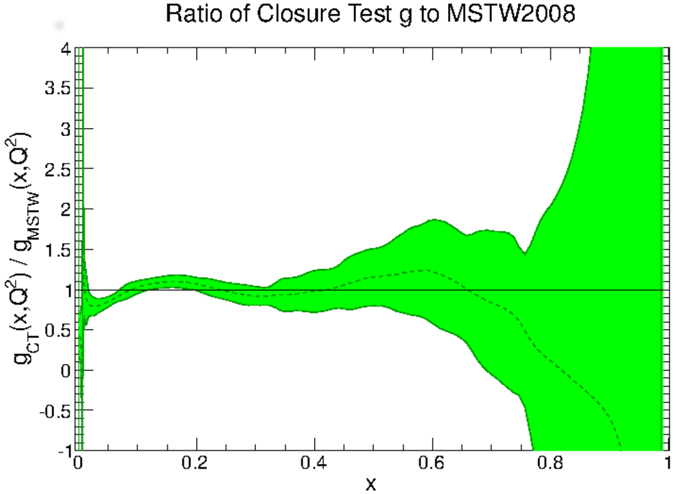
- LEVEL 0: FAKE DATA GENERATED WITH NO UNCERTAINTY
  $\rightarrow$ INTERPOLATION AND EXTRAPOLATION UNCERTAINTY
- LEVEL 1-2: FAKE DATA GENERATED WITH SAME UNCERTAINTY AS REAL DATA (INCLUDING CORRELATIONS)
- LEVEL 1: NO PSEUDODATA REPLICAS:
  $\Rightarrow$ REPLICAS FITTED TO SAME DATA OVER AND OVER AGAIN
  $\rightarrow$ FUNCTIONAL UNCERTAINTY DUE TO INFINITY OF EQUIVALENT MINIMA
- LEVEL 2: STANDARD NNPDF METHODOLOGY
  $\Rightarrow$ REPLICAS FITTED TO PSEUDODATA REPLICAS
  $\rightarrow$ DATA UNCERTAINTY
- THREE SOURCES OF UNCERTAINTY COMPARABLE IN DATA REGION

THE GLUON: LEVEL 0, LEVEL 1 AND LEVEL 2



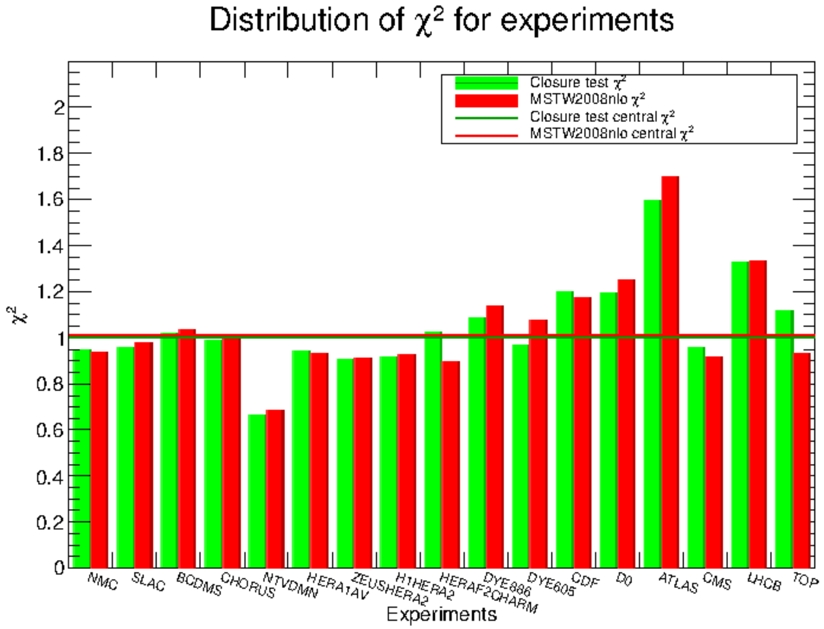
LEVEL-2: CENTRAL VALUES AND UNCERTAINTIES

THE GLUON: FITTED/"TRUE"

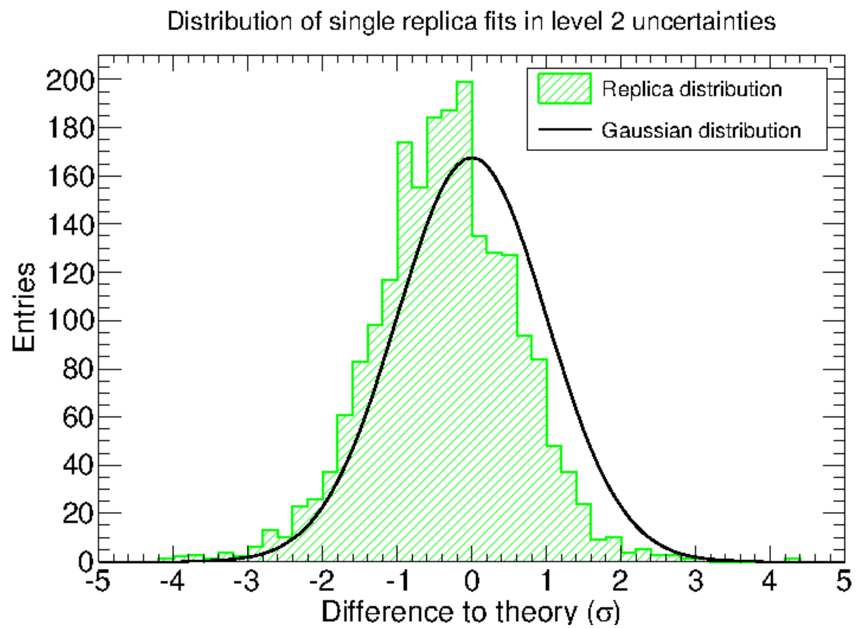


- CENTRAL VALUES:
  COMPARE FITTED VS. "TRUE" χ^2
  BOTH FOR INDIVIDUAL EXPERIMENTS
  & TOTAL DATASET
  FOR TOTAL $\Delta\chi^2 = 0.001 \pm 0.003$
- UNCERTAINTIES: DISTRIBUTION OF DEVIATIONS BETWEEN FITTED AND "TRUE" PDFs
  SAMPLED AT 20 POINTS BETWEEN 10^{-5} AND 1
  FIND 0.699% FOR ONE-SIGMA,
  0.948% FOR TWO-SIGMA C.L.

LEVEL-2 FITTED χ^2 VS "TRUE"



NORM. DISTRIBUTION OF DEVIATIONS



LEVEL-2 STABILITY TESTS

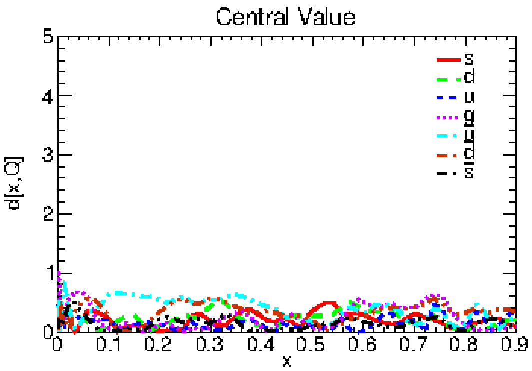
- INCREASE MAXIMUM GA TRAINING LENGTH TO 80K
  TESTS EFFICIENCY OF CROSS-VALIDATION
- INCREASE NN ARCHITECTURE TO 2-20-15-1
  NUMBER OF FREE PARAMETRES INCREASE BY MORE THAT $10\times$
- CHANGE PDF PARAMETRIZATION BASIS
  OLD: ISOTRIPLET, $\bar{u} - \bar{d}$, $s + \bar{s}$, $s - \bar{s}$;
  NEW: ISOTRIPLET, SU(3)-OCTET, BOTH TOTAL $(q + \bar{q})$ & VALENCE $(q - \bar{q})$

STATISTICAL EQUIVALENCE!

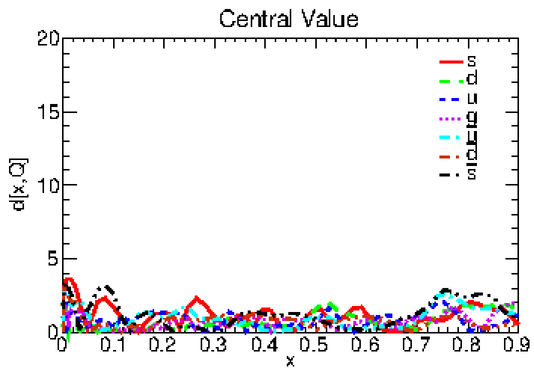
DISTANCES BETWEEN REF. AND NEW FIT:

difference in units of standard deviation of the mean

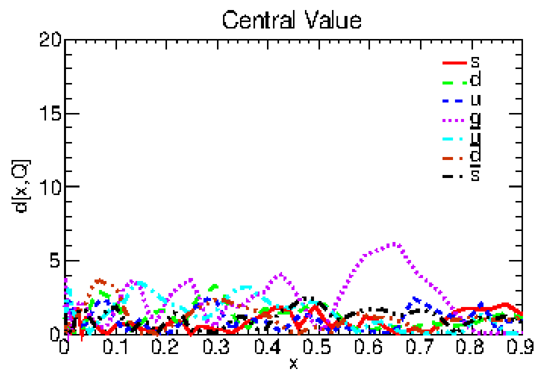
30K GENS VS 80K GENS



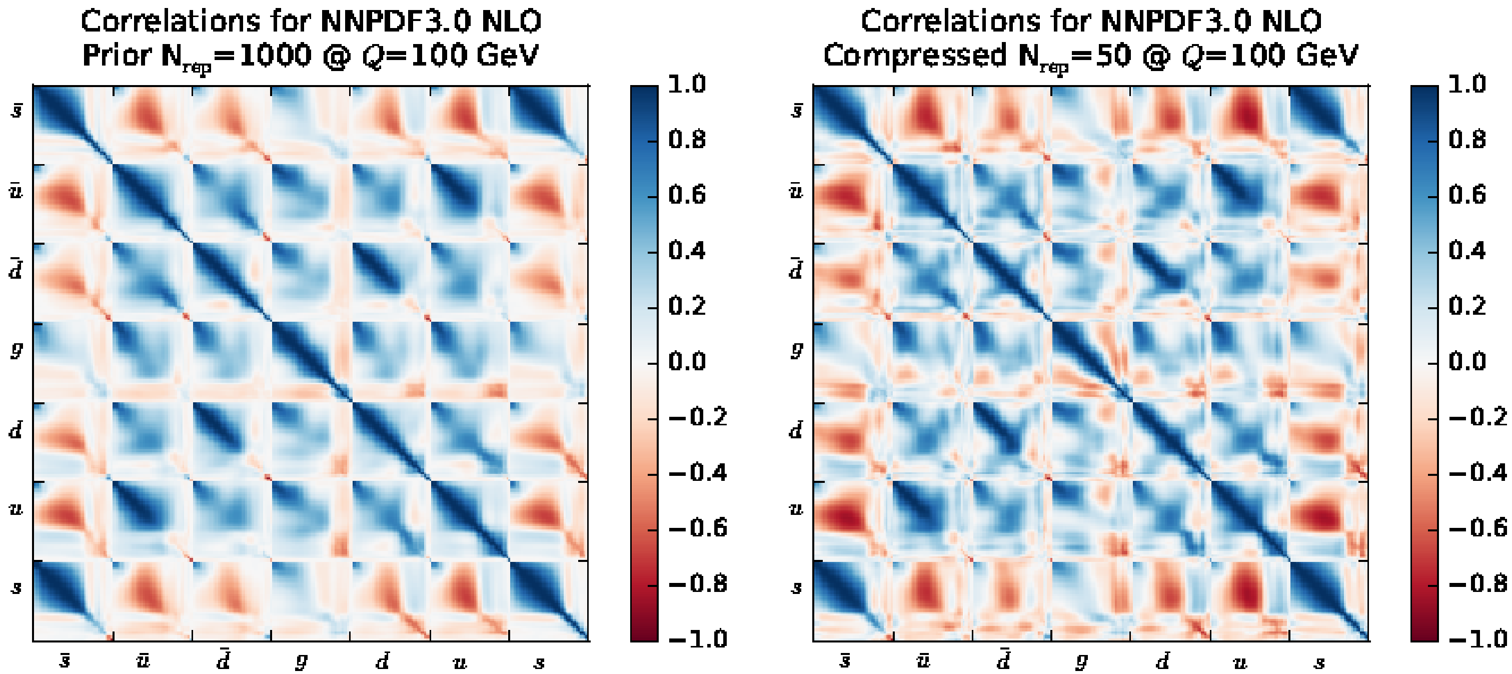
2.3 BASIS VS 3.0 BASIS



300 VS 37 PARMS



OPTIMIZATION I
MONTECARLO COMPRESSION

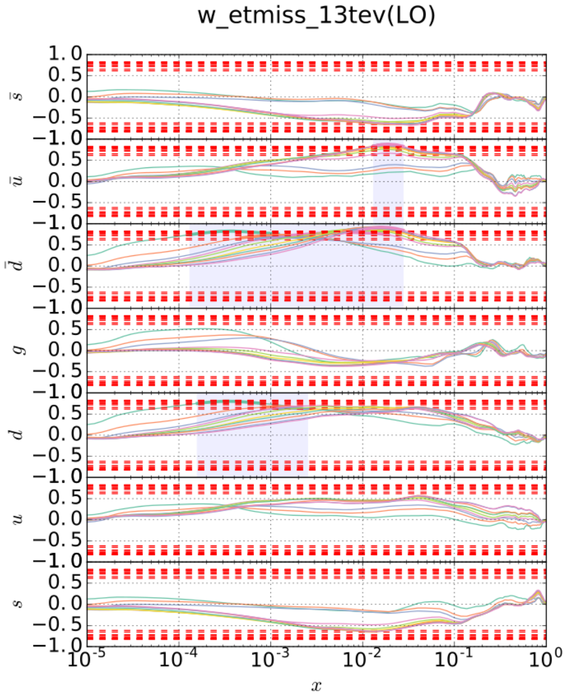


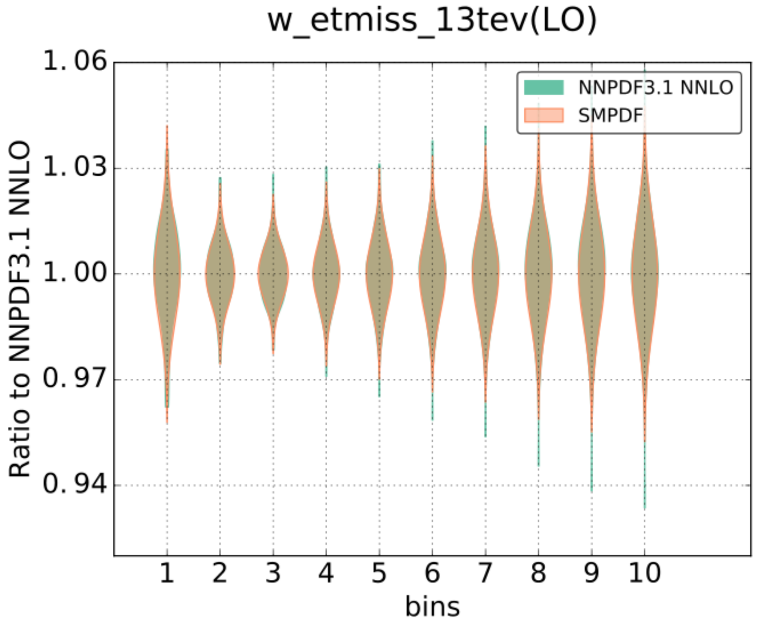
(Carrazza, Latorre, Kassabov, Rojo, 2015)

- CONSTRUCT A VERY LARGE REPLICA SAMPLE
- SELECT (BY GENETIC ALGORITHM) A SUBSET OF REPLICAS WHOSE STATISTICAL FEATURES ARE AS CLOSE AS POSSIBLE TO THOSE OF THE PRIOR
- $\Rightarrow$ FOR ALL PDFs ON A GRID OF POINTS
MINIMIZE DIFFERENCE OF: FIRST FOUR MOMENTS, CORRELATIONS; OUTPUT OF KOLMOGOROV-SMIRNOV TEST (NUMBER OF REPLICAS BETWEEN MEAN AND σ, 2σ, INFINITY)
- 50 COMPRESSED REPLICA REPRODUCE 1000 REPLICA SET TO PRECENT ACCURACY

OPTIMIZATION II
SMPDF COMPRESSION

- SELECT SUBSET OF THE COVARIANCE MATRIX CORRELATED TO A GIVEN SET OF PROCESSES
- PERFORM SVD ON THE REDUCED COVARIANCE MATRIX, SELECT DOMINANT EIGENVECTOR, PROJECT OUT ORTHOGONAL SUBSPACE
- ITERATE UNTIL DESIRED ACCURACY REACHED
- COMPRESSED HESSIAN REPRESENTATION OF PROBABILITY DISTN.
- CAN ADD PROCESSES TO GIVEN SET; CAN COMBINE DIFFERENT OPTIMIZED SETS
- WEB INTERFACE AVAILABLE





(Carrazza, SF, Kassabov, Rojo, 2016)

- EG ggH, $Hb\bar{b}$, $W\ E_T^{\rm miss} \Rightarrow 11$ EIGENVECTORS
- STUDY CORRELATIONS OF PDFS TO DATA AND AMONG THEMSELVES!

ALL IS WELL?

CAN WE DO BETTER?

- ARCHITECTURE: DO WE NEED SEVEN NNs?
- PREPROCESSING: ARE RESULTS TRULY INDEPENDENT OF IT?
- MINIMIZATION: IS THE GA OPTIMIZED?
- STOPPING: OVER/UNDERLEARNING?

UNCERTAINTIES ARE FAITHFUL, BUT

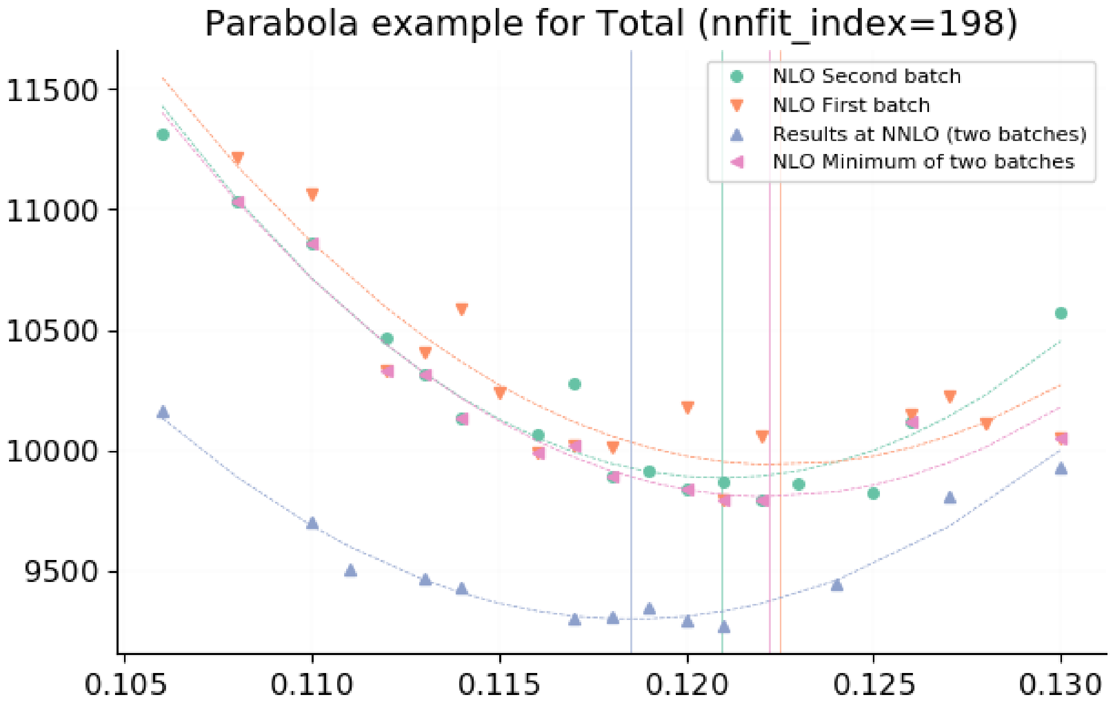
ARE THEY THE SMALLEST WITH GIVEN DATA?

IS THERE NO INFORMATION LOSS?

EXTRAS

MORE EFFICIENT MINIMIZATION?

- LOOK AT α_s DEPENDENCE (CORRELATED REPLICAS)
- SIGNIFICANT FLUCTUATIONS ABOUT PARABOLIC SHAPE
  NOT DUE TO FINITE-SIZE MONTE CARLO SAMPLE



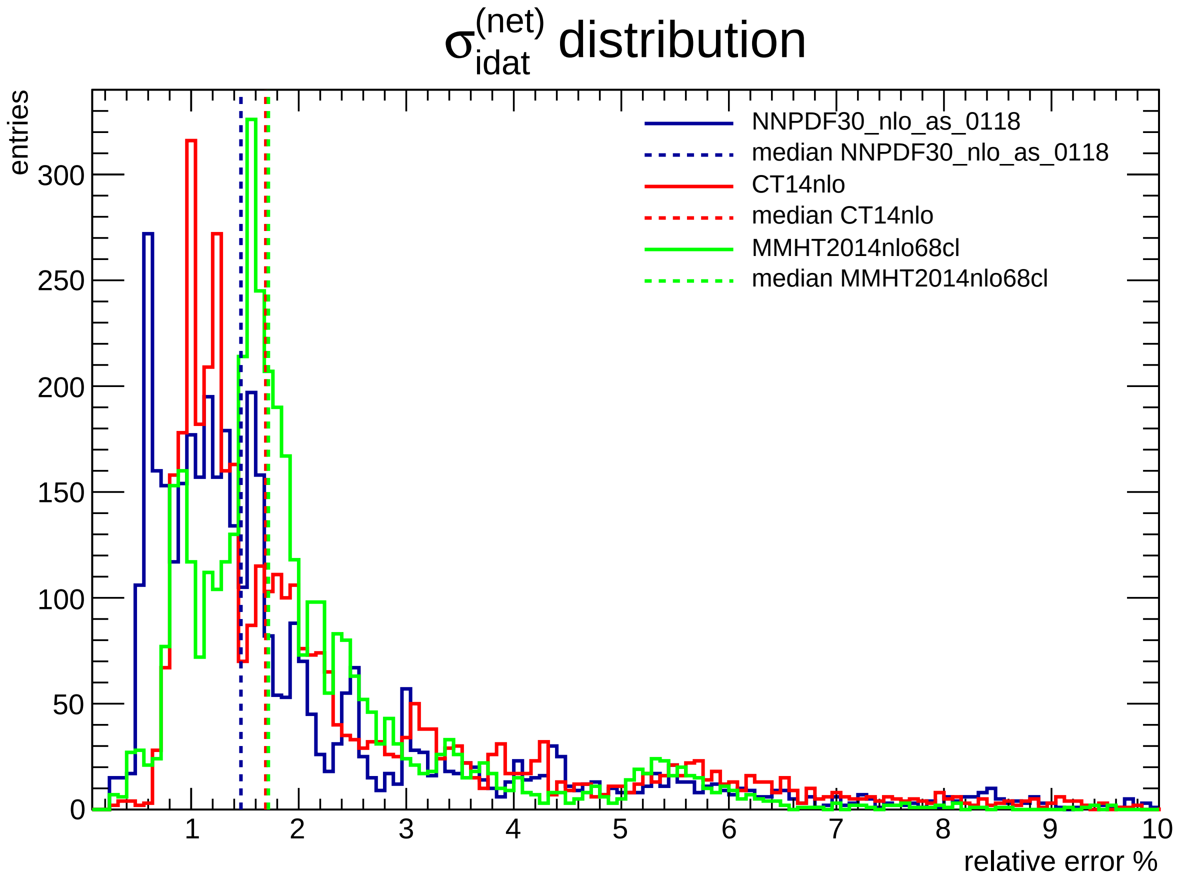
BATCH MINIMIZATION

- MINIMIZE EACH REPLICA MORE THEN ONCE & KEEP BEST RESULTS
- SIGNIFICANT STABILIZATION

PDF UNCERTAINTIES: HOW MUCH DO THEY VARY?

- COMPUTE PERCENTAGE PDF UNCERTAINTY ON ALL DATA INCLUDED IN GLOBAL FIT
- COMPARE GLOBAL FITS

PERCENTAGE PDF UNCERTAINTY ON PREDICTIONS



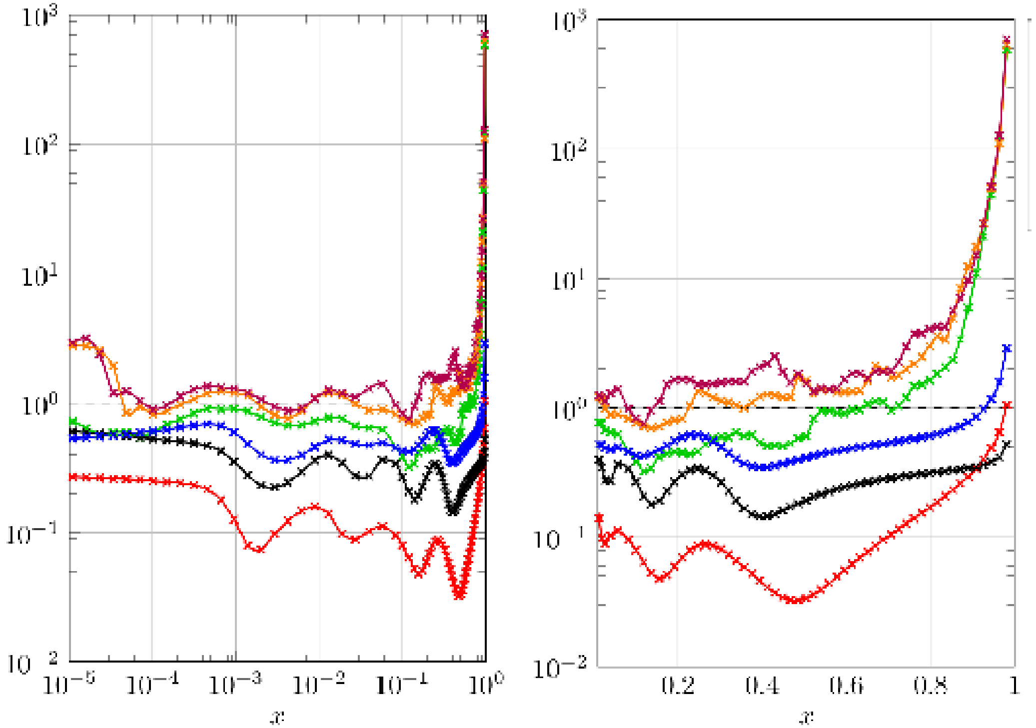
- MEDIAN SIMILAR
- DISTRIBUTION VERY DIFFERENT!
- NNPDF: SMALLER MODE, BUT FAT TAIL ⇔ GREATER FLEXIBILITY

THE $\Delta\chi^2$ PROBLEM

- TOLERANCE MIGHT COMPENSATE FOR MISSING FUNCTIONAL UNCERTAINTY
- BUT WHAT IS $\Delta\chi^2$ FOR AN NNPDF FIT?
- CAN ANSWER USING HESSIAN CONVERSION! $\Delta\chi^2 = 16 \pm 15$
  - NON-PARABOLIC BEHAVIOUR NEAR MINIMUM ON SCALE OF UNCERTAINTIES?
  - INEFFICIENCY OF THE MINIMIZATION PROCEDURE?

CLOSURE-TESTING: THE PARAMETRIZATION DEPENDENCE

GLUON PDF UNCERTAINTY NORMALIZED TO MSTW08



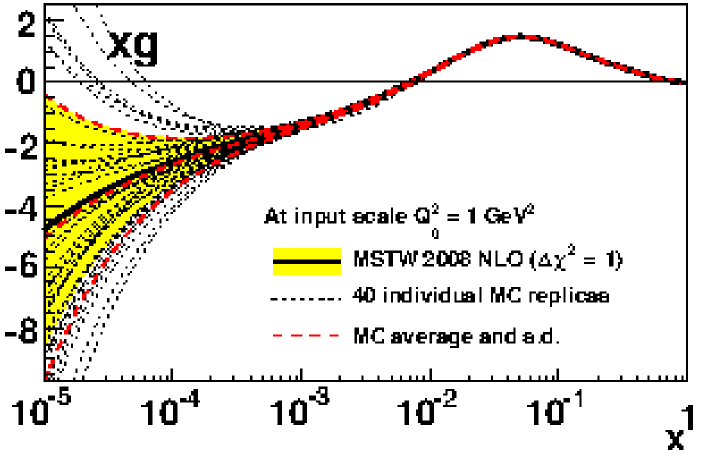
(C. Mascaretti, 2016)

- CLOSURE TEST PERFORMED WITH DATA GENERATED BASED ON MST08 FUNCTIONAL FORM
- REFITTED EITHER WITH NNPDF OR MSTW-CT FUNCTIONAL FORM
- LEVEL 0: VANISHING DATA UNCERTAINTY
  - MSTW-CT: FIT HAS ZERO UNCERTAINTY
  - NNPDF: ABOUT HALF OF TOTAL UNCERTAINTY
- LEVEL 1: NOMINAL DATA UNCERTAINTY, BUT REPLICAS FITTED W/O PSEUDODATA
  - MSTW-CT: FIT HAS SMALL UNCERTAINTY
  - NNPDF: ABOUT 2/3 OF FINAL UNCERTAINTY
- LEVEL 2
  - NNPDF UNCERTAINTY LARGER THAN MSTW-CT
  - NNPDF UNCERTAINTY SIMILAR TO MSTW WITH TOLERANCE

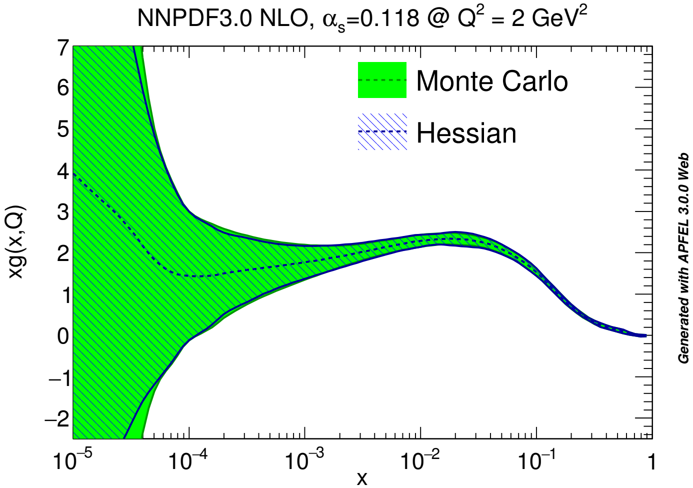
"STANDARD" PARAMETRIZATION MISSES INTERPOLATION & FUNCTIONAL UNCERTAINTY?

MC ⇔ HESSIAN

- TO CONVERT HESSIAN INTO MONTECARLO GENERATE MULTIGAUSSIAN REPLICAS IN PARAMETER SPACE
- ACCURATE WHEN NUMBER OF REPLICAS SIMILAR TO THAT WHICH REPRODUCES DATA



(Thorne, Watt, 2012)



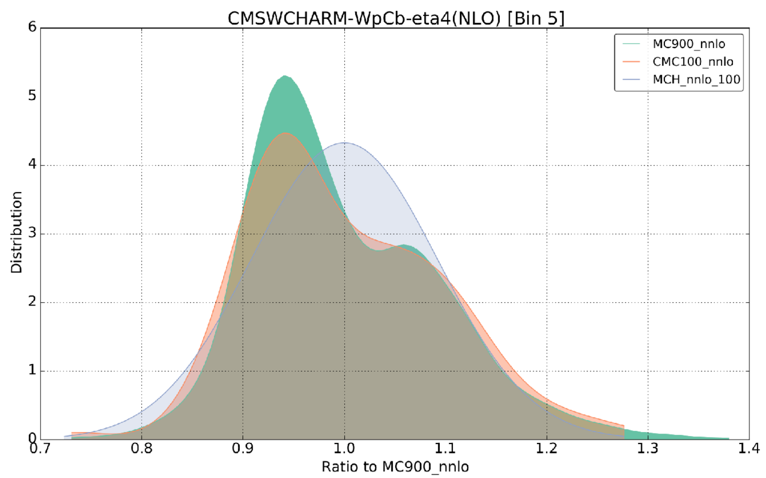
(Carrazza, SF, Kassabov, Rojo, 2015)

- TO CONVERT MONTE CARLO INTO HESSIAN, SAMPLE THE REPLICAS $f_i(x)$ AT A DISCRETE SET OF POINTS & CONSTRUCT THE ENSUING COVARIANCE MATRIX
- EIGENVECTORS OF THE COVARIANCE MATRIX AS A BASIS IN THE VECTOR SPACE SPANNED BY THE REPLICAS BY SINGULAR-VALUE DECOMPOSITION
- NUMBER OF DOMINANT EIGENVECTORS SIMILAR TO NUMBER OF REPLICAS ⇒ ACCURATE REPRESENTATION

NONGAUSSIAN BEHAVIOUR

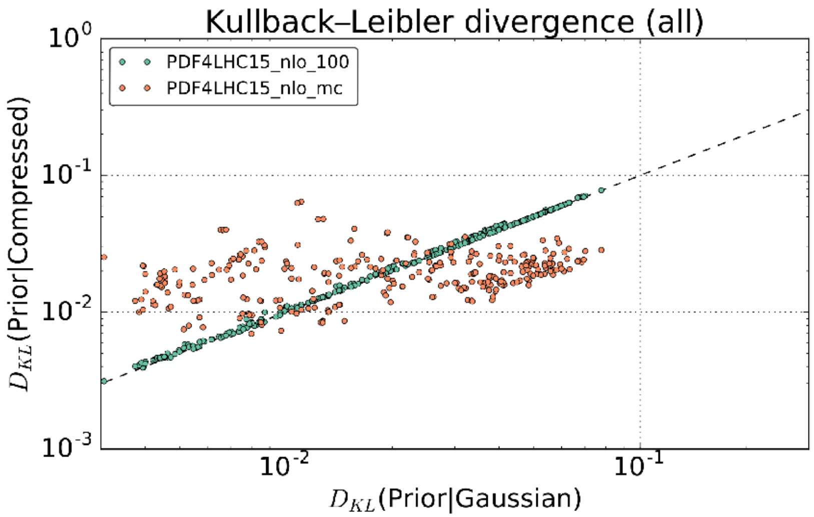
MONTE CARLO COMPARED TO HESSIAN

CMS $W + c$ production



- DEVIATION FROM GAUSSIANITY E.G. AT LARGE x DUE TO LARGE UNCERTAINTY + POSITIVITY BOUNDS
$\Rightarrow$ RELEVANT FOR SEARCHES
- CANNOT BE REPRODUCED IN HESSIAN FRAMEWORK
- WELL REPRODUCED BY COMPRESSED MC

- DEFINE KULLBACK-LEIBLER DIVERGENCE
$D_{\rm KL} = \int_{-\infty}^{\infty} P(x) \frac{\ln P(x)}{\ln Q(x)}\, dx$
BETWEEN A PRIOR P AND ITS REPRESENTATION Q
- $D_{\rm KL}$ BETWEEN PRIOR AND HESSIAN DEPENDS ON DEGREE OF GAUSSIANITY
- $D_{\rm KL}$ BETWEEN PRIOR AND COMPRESSED MC DOES NOT



CAN (A) GAUGE WHEN MC IS MORE ADVANTAGEOUS THAN HESSIAN;
(B) ASSESS THE ACCURACY OF COMPRESSION