REGRESSION NETWORKS: PRECISION AND UNCERTAINTY ESTIMATION

STEFANO FORTE
UNIVERSITÀ DI MILANO & INFN

WITH TUTORIALS BY

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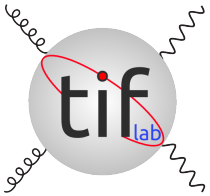
DIPARTIMENTO DI FISICA



MACHINE LEARNING IN PARTICLE THEORY

MITP, JULY 7, 2023

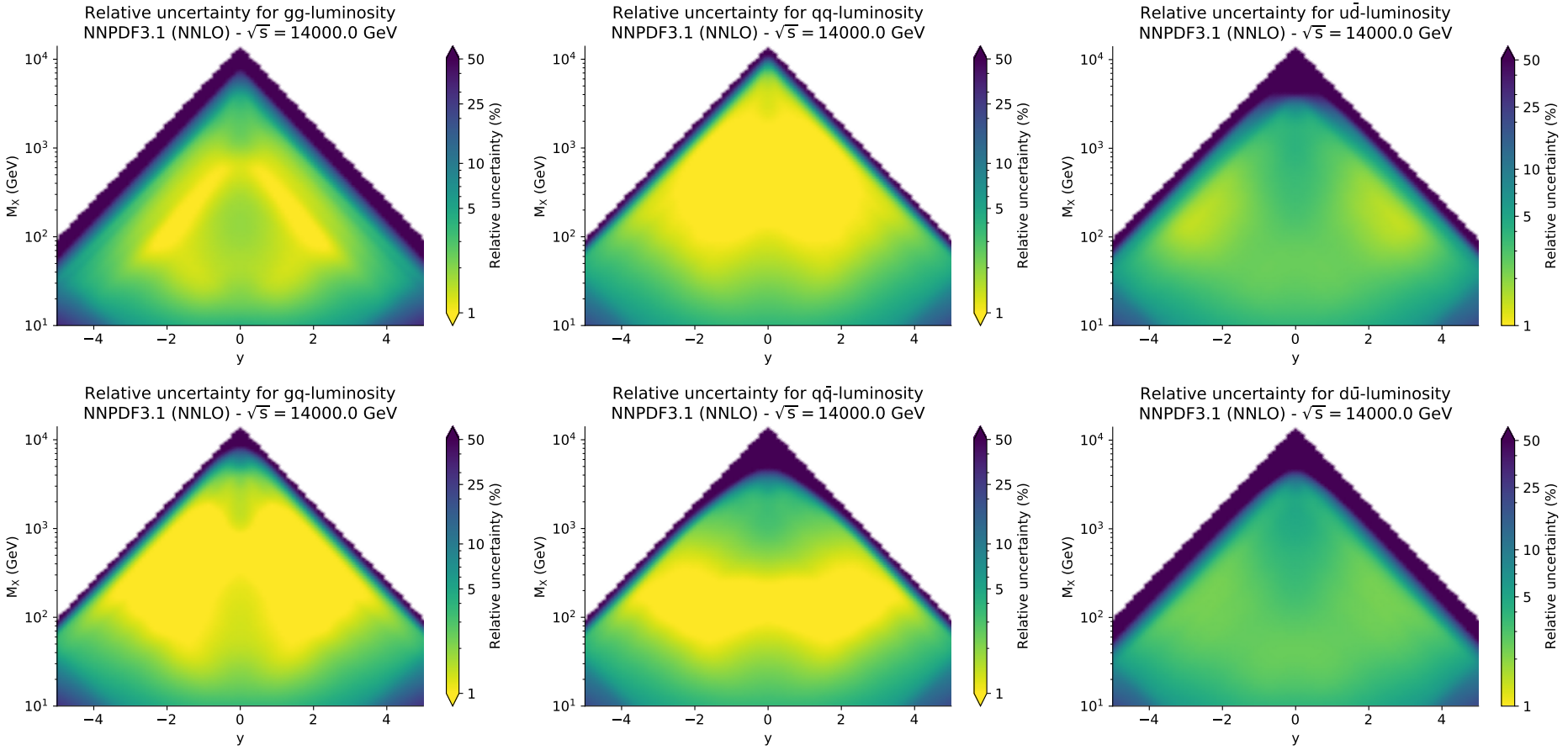
V: UNDERSTANDING RESULTS

- RESULT AND THEIR DISTRIBUTION
  - PDF UNCERTAINTIES: THE STATE OF THE ART
  - MODEL AND DATA UNCERTAINTIES
- THE LOSS DISTRIBUTION
  - LOSS QUALITY
  - CORRELATION TO FEATURES
- GENERALIZATION
  - OVERLEARNING
  - FEATURE LEARNING

PDF UNCERTAINTIES NOW

UNCERTAINTIES 2016

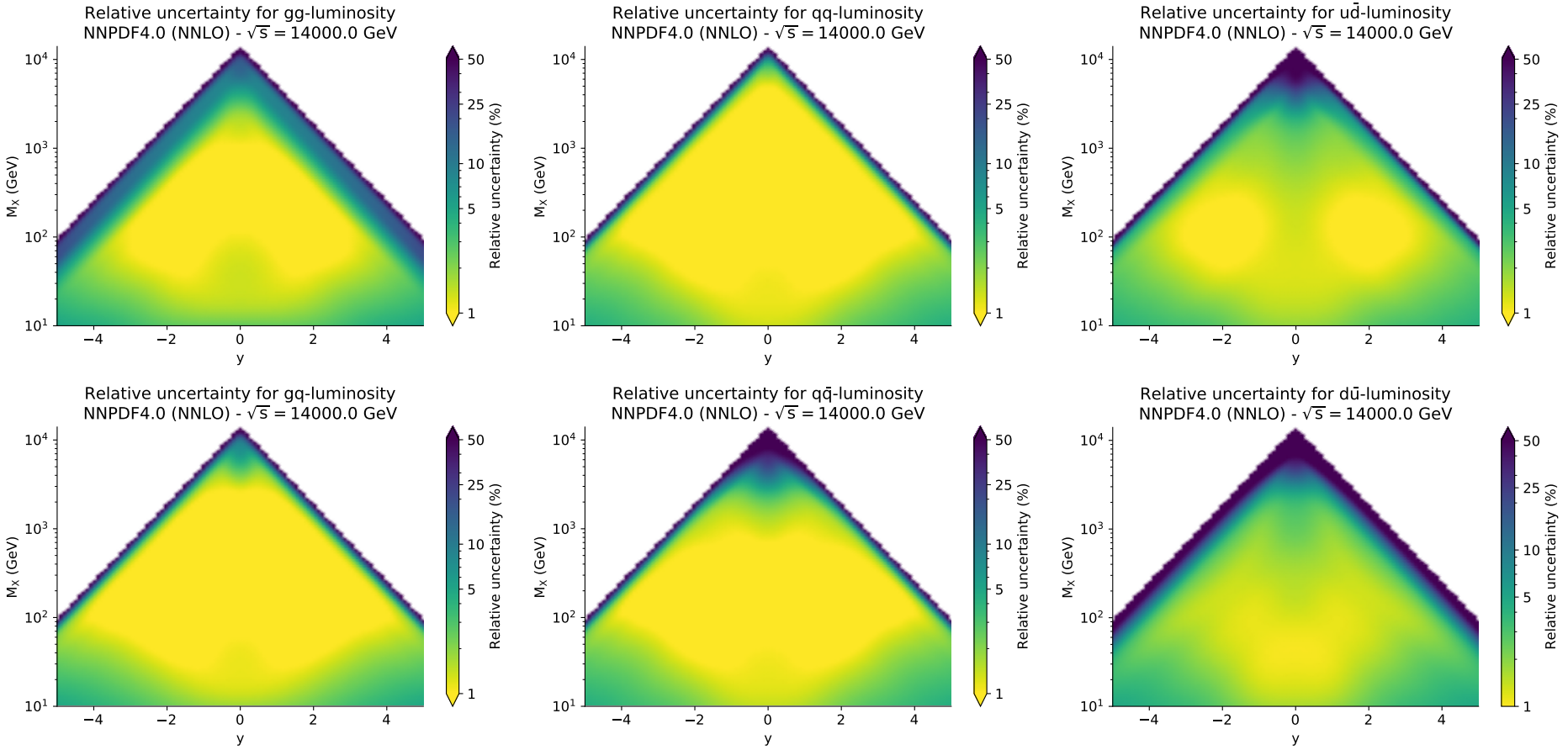
GLUON SINGLET FLAVORS



- 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 2022

GLUON SINGLET FLAVORS



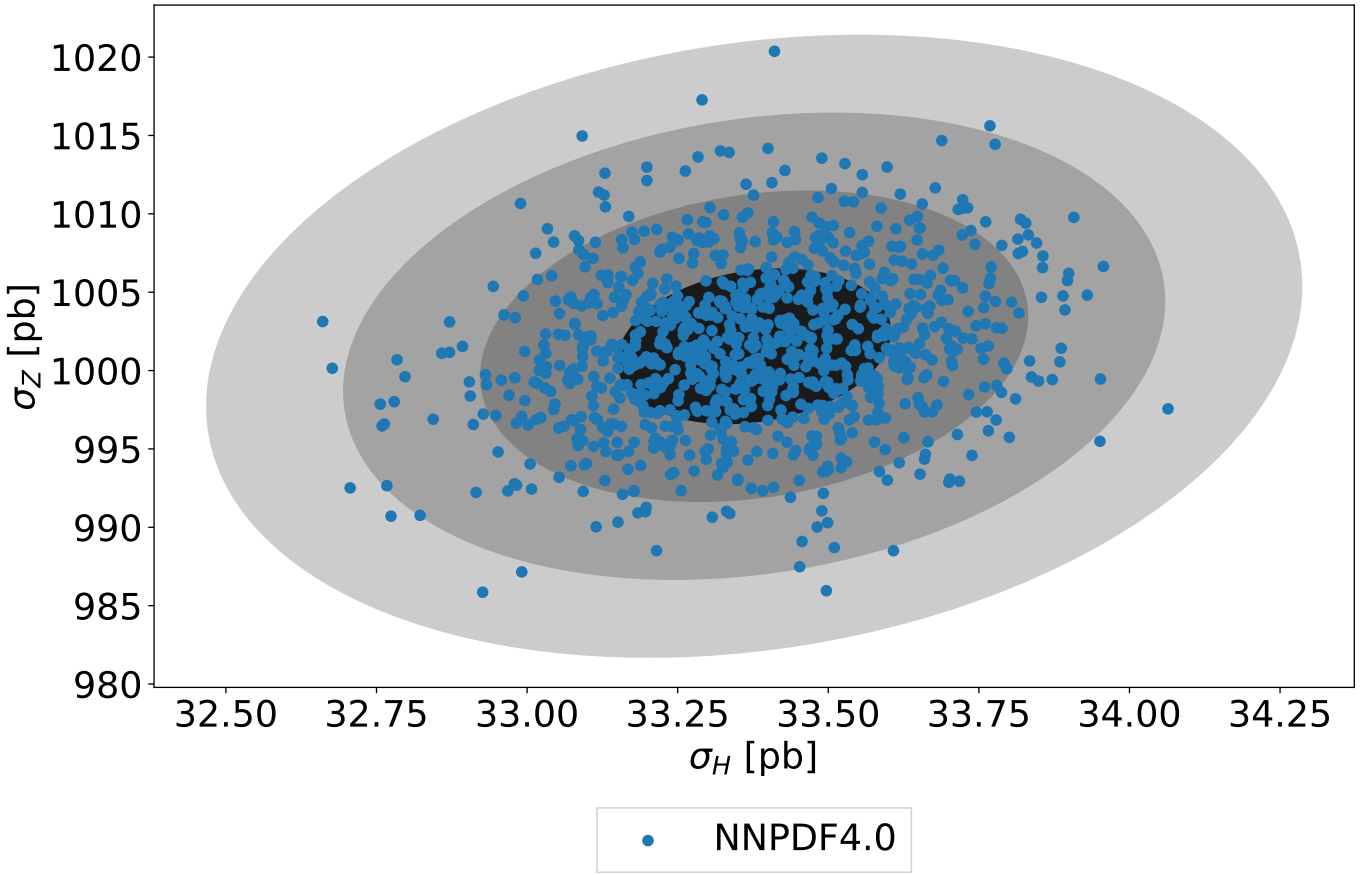
- TYPICAL UNCERTAINTIES IN DATA REGION: SINGLET $\sim 1\%$, NONSINGLET $\sim 2-3\%$
- DATA REGION: $10 \lesssim M_X \lesssim 3 \cdot 10^3$ TeV, $-4 \lesssim y \lesssim 4$

THE MC DISTRIBUTION: UNCERTAINTIES

DISTRIBUTION OF RESULTS

HOW DOES IT LOOK LIKE?

- PLOT RESULTS IN (σ_H, σ_Z) PREDICTION SPACE
- DISTRIBUTION OF REPLICAS $\Rightarrow$ OPTIMAL IMPORTANCE SAMPLING

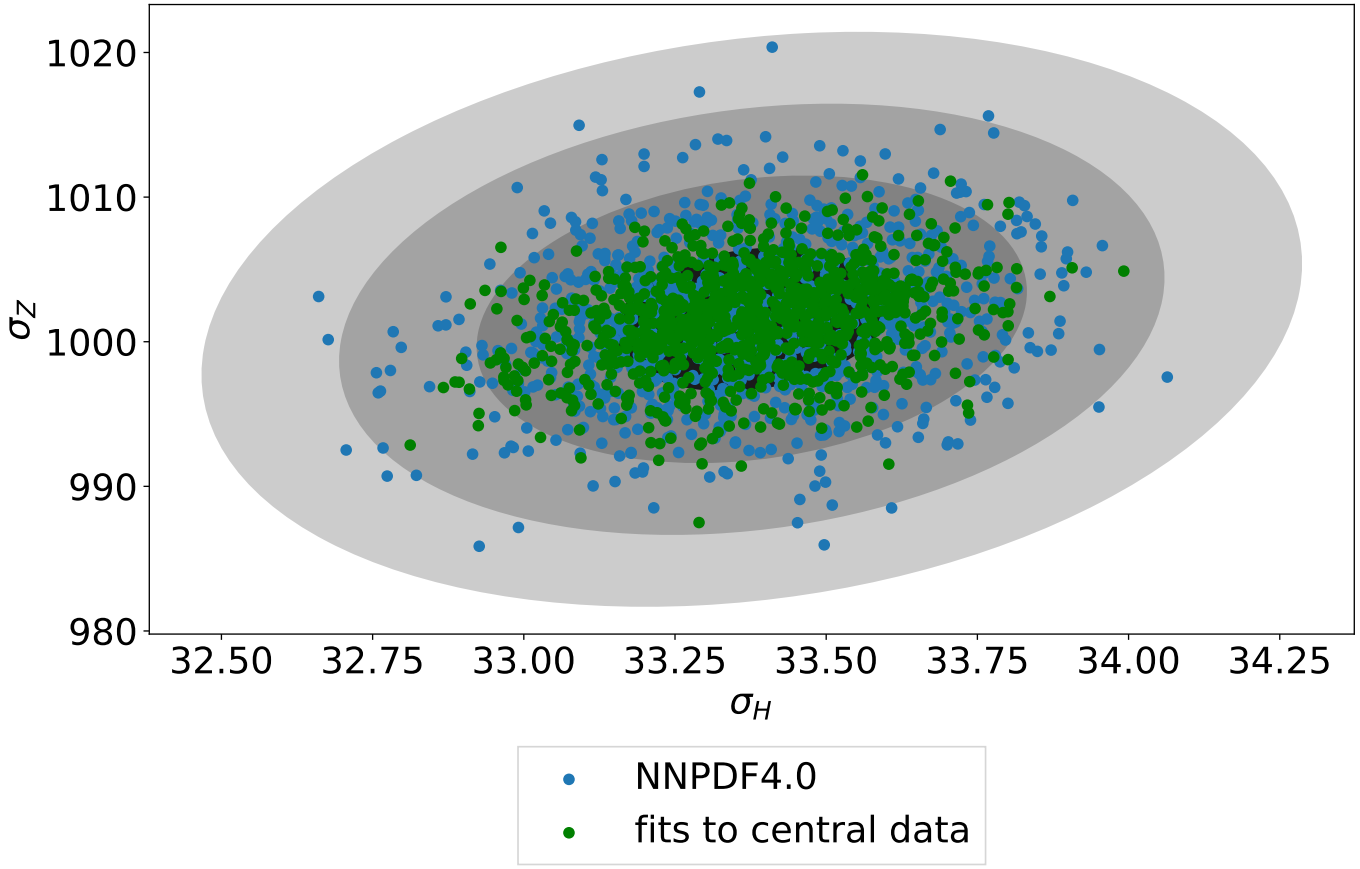


DISTRIBUTION OF REPLICAS DRIVEN BY

- DATA UNCERTAINTIES $\Rightarrow$ DATA REPLICA FLUCTUATION
- INTERPOLATION, EXTRAPOLATION AND FUNCTIONAL UNCERTAINTIES $\Rightarrow$ BEST FIT DEGENERACY

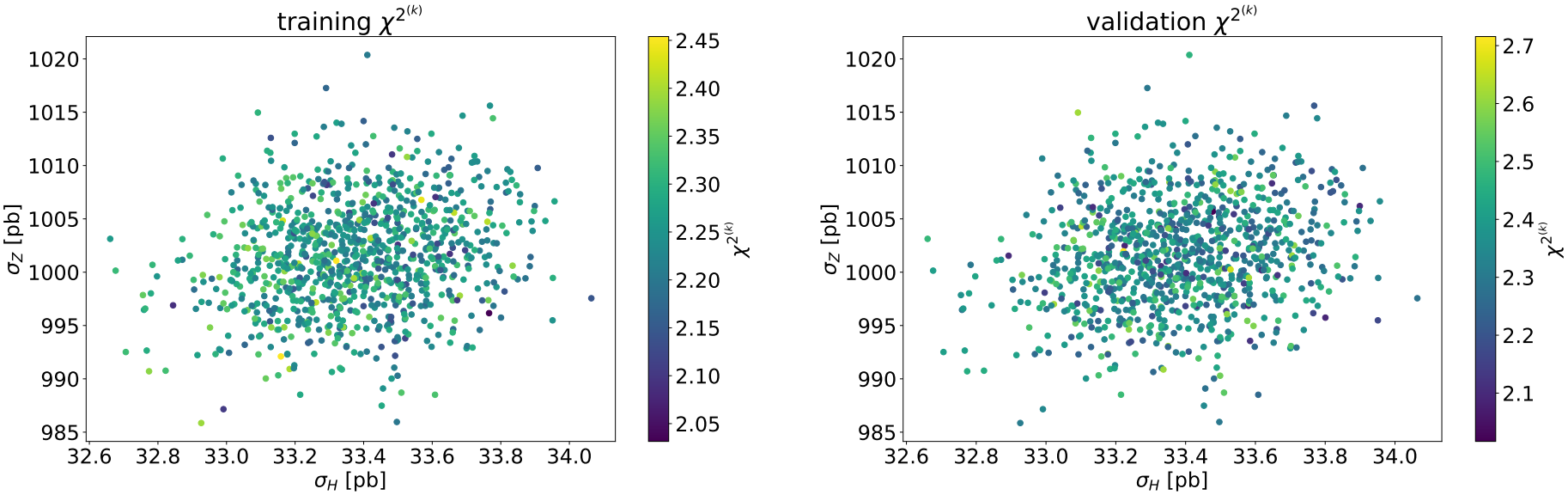
LEVEL-1 vs FULL UNCERTAINTIES

- REPLICA FLUCTUATION $\Rightarrow$ DATA UNCERTAINTIES
- NO REPLICA FLUCTUATION $\Rightarrow$ MODEL UNCERTAINTY



THE REPLICA DISTRIBUTION

LOSS QUALITY



- COMPARE TRAINING AND VALIDATION LOSS FOR EACH REPLICA
- NO CORRELATION BETWEEN FIT QUALITY AND POSITION IN THE (σ_H, σ_Z) PLANE
- UNIFORM QUALITY

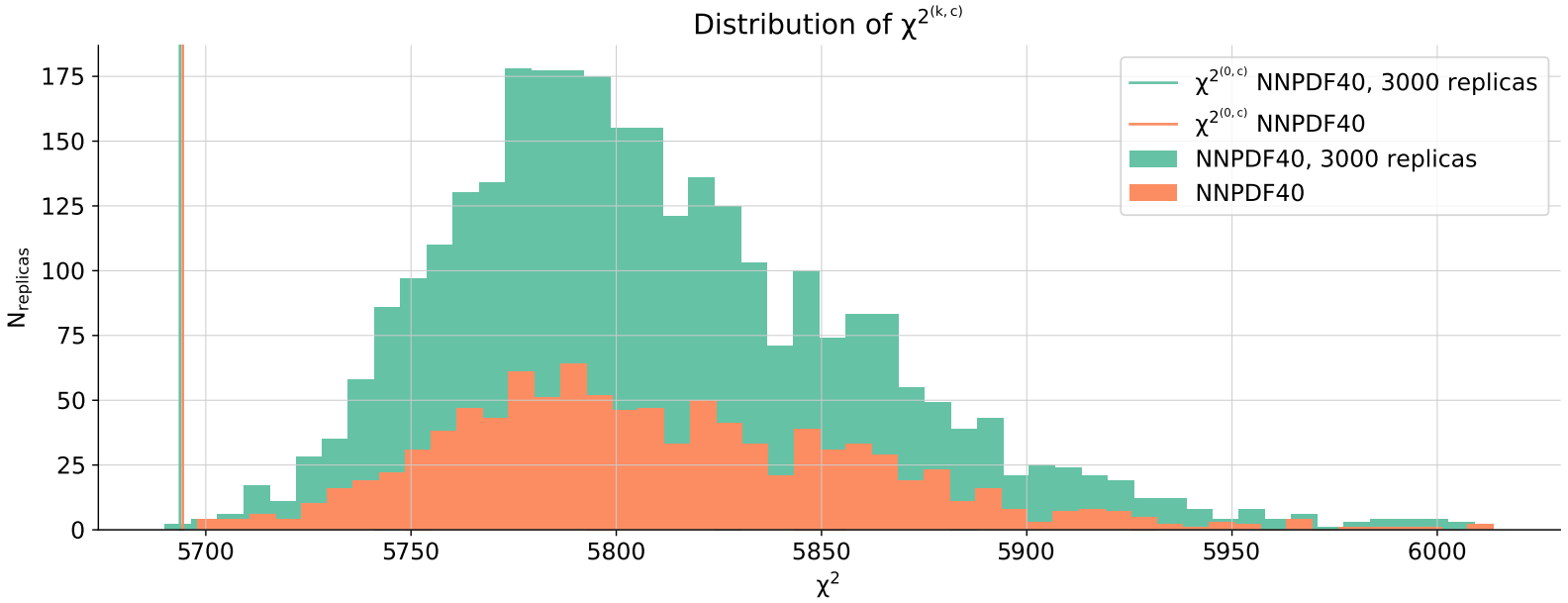
METRICS IN REPLICA SPACE

REPLICA LOSS DISTRIBUTION

COMPARISON TO CENTRAL DATA

- EACH PDF REPLICA FITTED TO A DATA REPLICA
- LOSS COMPUTED TO CENTRAL DATA STATISTICALLY DISTRIBUTED

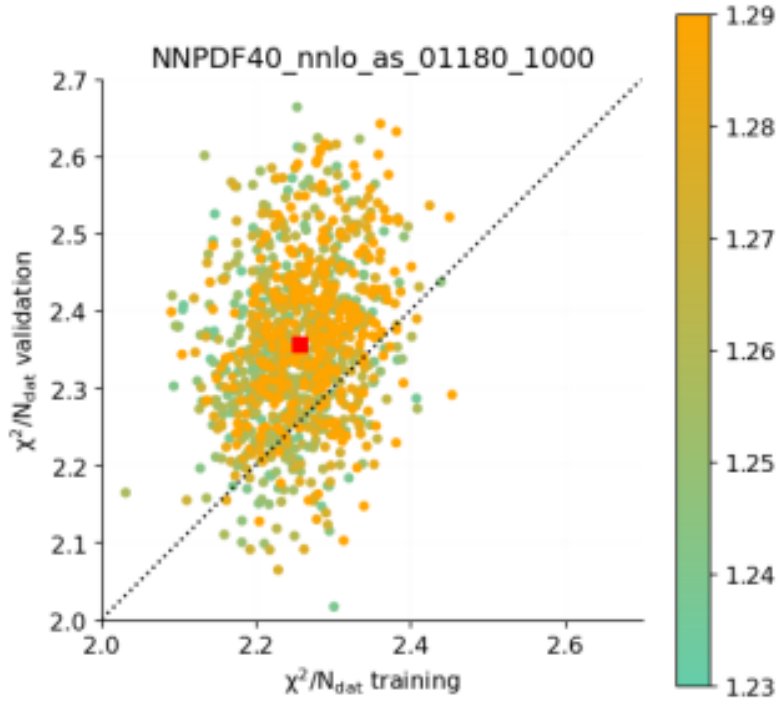
1000 REPLICAS VS. 3000 REPLICAS



- AVERAGE $\Rightarrow$ CXENTRAL PREDICTION PDF $\Rightarrow$ LOW LOSS
- NOT NECESSARILY LOWEST

REPLICA LOSS DISTRIBUTION
TRAINING AND VALIDATION

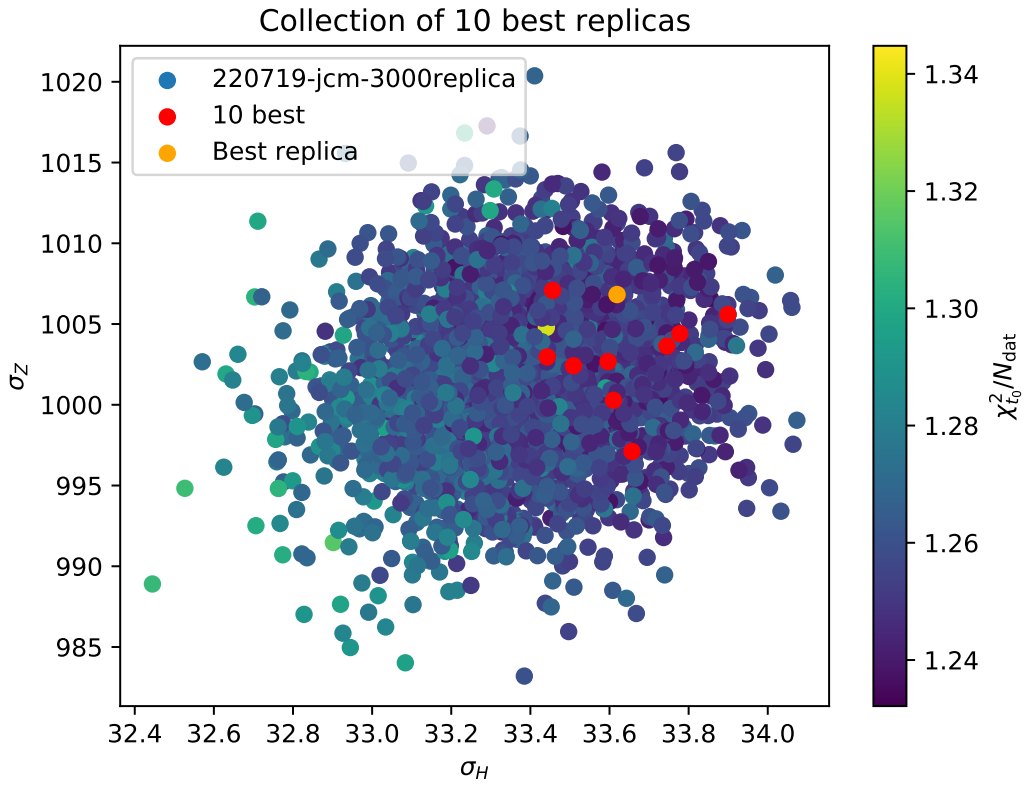
- ARE FITS WITH HIGH LOSS TO CENTRAL DATA POOR (UNDERLEARNT)?



- NO CORRELATION BETWEEN LOSS TO CENTRAL DATA AND TRAINING, VALIDATION LOSS
- UNIFORM FIT QUALITY
- DISPERSION DUE
  - DATA REPLICA FLUCTUATION $\Rightarrow$ DATA UNCERTAINTIES
  - MODEL UNCERTAINTIES
    $\Rightarrow$ INTERPOLATION, EXTRAPOLATION AND FUNCTIONAL UNCERTAINTIES

REPLICA LOSS DISTRIBUTION

CORRELATION TO FEATURES



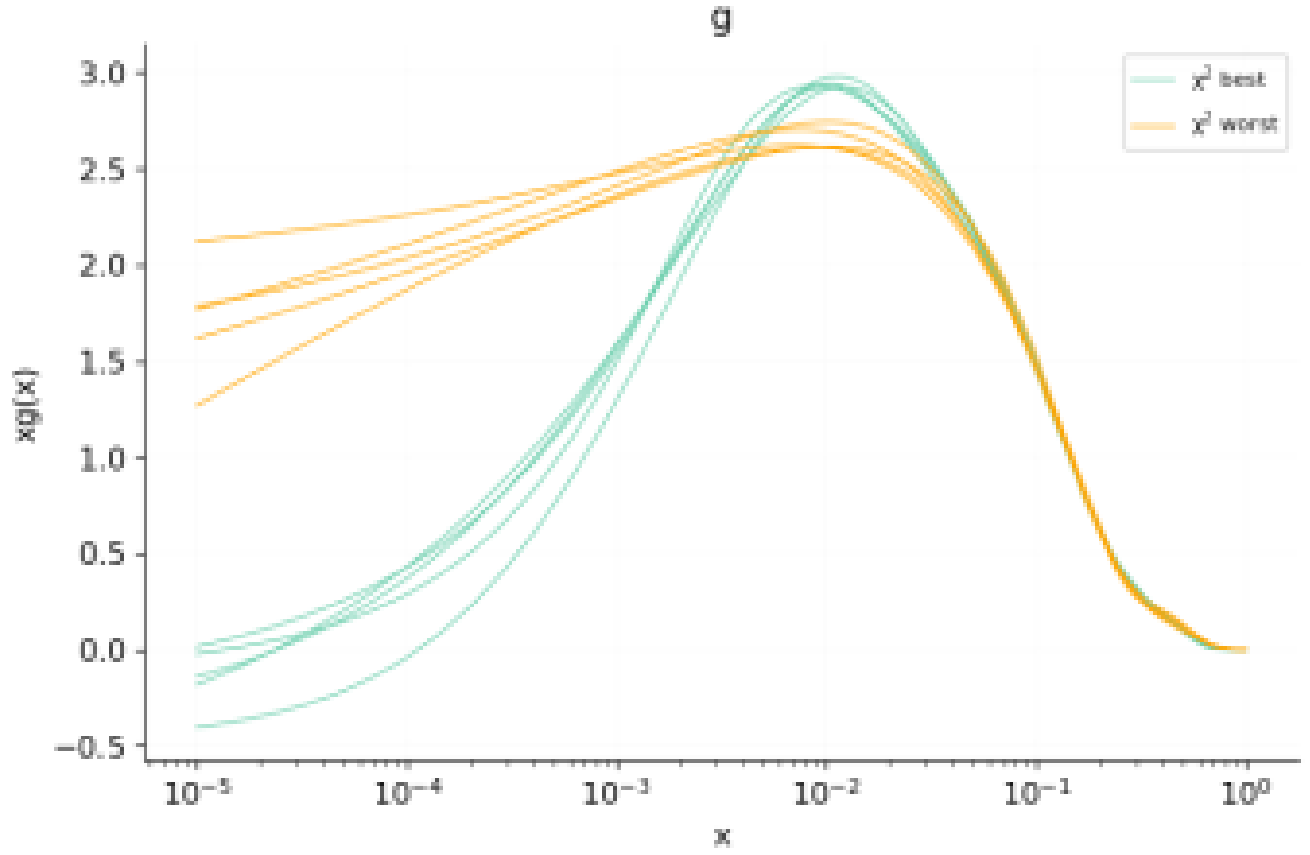
LOSS TO CENTRAL DATA

- CORRELATED TO POSITION IN (σ_H, σ_z) PLANE
- CORRELATED TO A FEATURE?

FEATURE CORRELATION

REPLICAS WITH LOWEST & HIGHEST LOSS TO CENTRAL DATA

THE GLUON



- REPLICAS CLOSER TO CENTRAL DATA $\Rightarrow$ MORE STRUCTURE

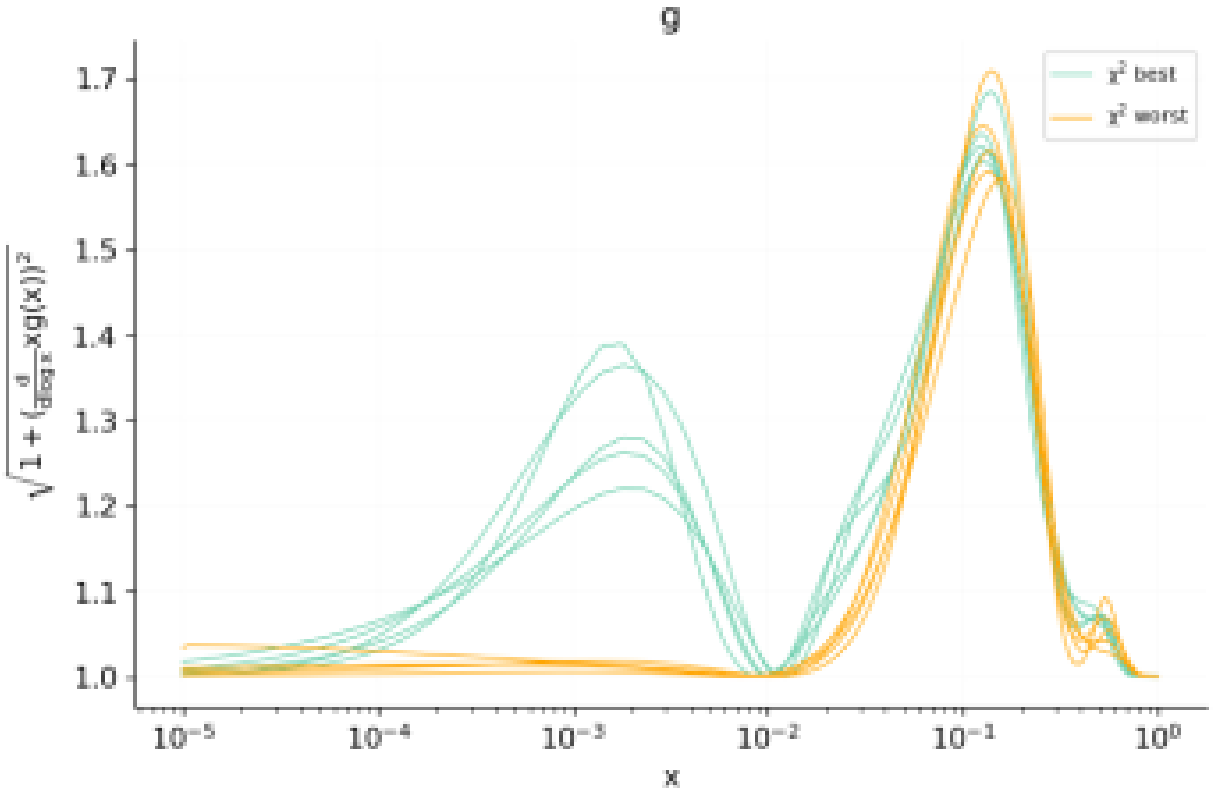
THE PDF KINETIC ENERGY

REPLICAS WITH LOWEST & HIGHEST LOSS TO CENTRAL DATA

$$\mathrm{KE} = \sqrt{1 + \left(\frac{d}{d\ln x} x f(x, Q^2)\right)^2}$$

ARCLENGTH OF THE NN OUTPUT IN TERMS OF INPUT

THE GLUON



- REPLICAS CLOSER TO CENTRAL DATA $\Rightarrow$ MORE STRUCTURE
- HIGHER KINETIC ENERGY

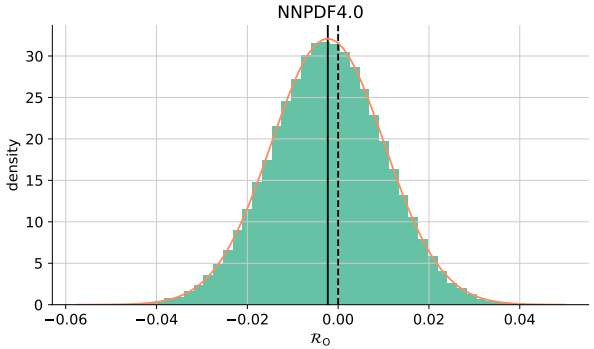
GENERALIZATION

OVERLEARNING

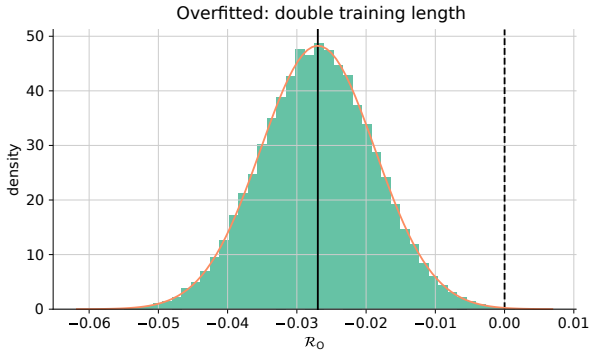
- INDUCE OVERLEARING: DOUBLE TRAINING LENGTH

THE OVERFIT METRIC

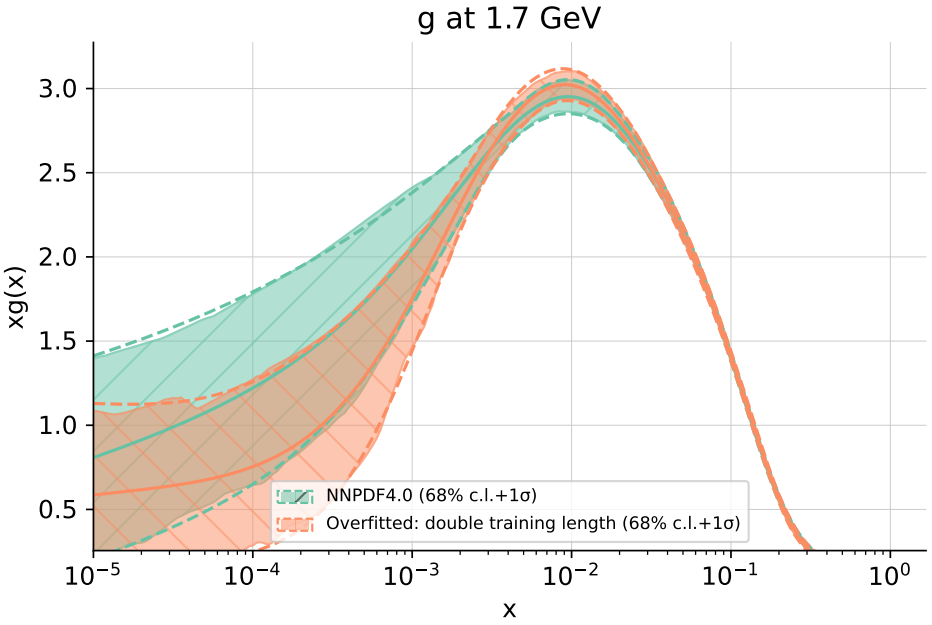
DEFAULT NNPDF4.0



OVERFIT VARIANT



THE GLUON



- LOOK AT THE OUTPUT $\Rightarrow$ MORE STRUCTURE IN GLUON

A PUZZLE

- BEST FIT TO CENTRAL DATA CORRELATED TO HIGH ARCLENGTH
- HIGH ARCLENGTH CORRELATED TO OVERLEARNING
- TRAINING/VALIDATION LOSS

  UNCORRELATED TO QUALITY OF FIT TO CENTRAL DATA

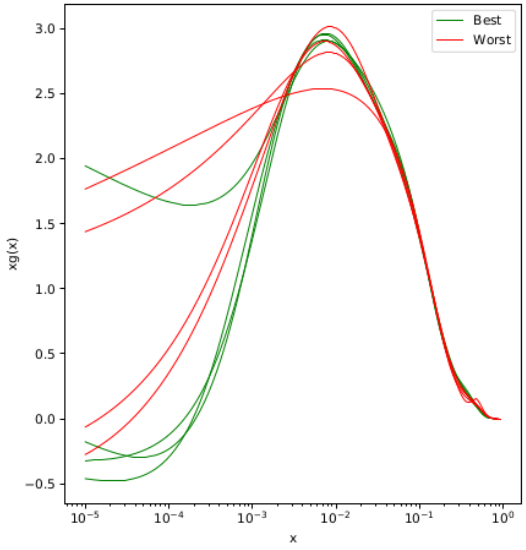
EXPLANATION

GENERALIZATION

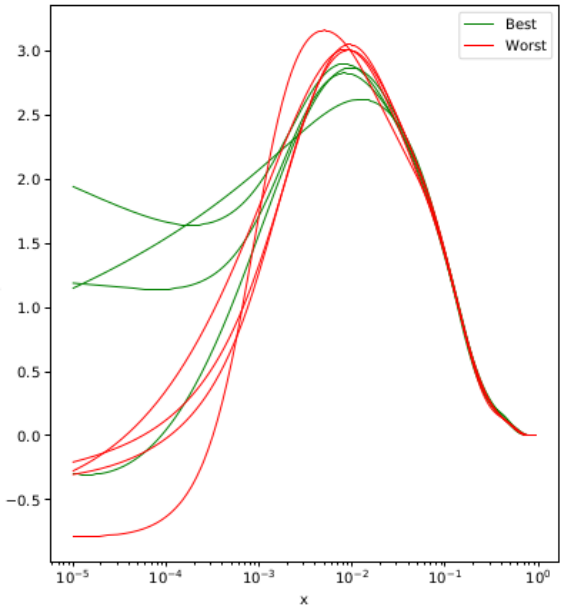
- OVERFITTING CAN MEAN POOR GENERALIZATION
- KEPT IN CHECK BY K-FOLDING (NOT CROSS-VALIDATION)
- LOOK AT BEST LOSS TO FITTED VS. EXCLUDED FOLDS

THE GLUON

FITTED FOLDS



EXCLUDED FOLD



- BEST VS WORST REVERSED
- HIGH K.E. SOLUTIONS DO NOT GENERALIZE

NO EFFECT THAT REQUIRES MORE THAN 10% ACCURACY IN MEASUREMENT IS WORTH INVESTIGATING

Walther Nernst

~~NO EFFECT THAT REQUIRES MORE THAN 10% ACCURACY IN MEASUREMENT IS WORTH INVESTIGATING~~
Walther Nernst

ACCURACY OF OBSERVATION IS THE EQUIVALENT OF ACCURACY OF THINKING
Wallace Stevens