REGRESSION NETWORKS: PRECISION AND UNCERTAINTY ESTIMATION

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Machine Learning in Particle Theory

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LECTURE PLAN

- I: THE PHYSICS PROBLEM
  - PARTON DISTRIBUTIONS AND THEIR DETERMINATION
  - THE PROBLEM OF PDF UNCERTAINTIES
- II: REGRESSION & UNCERTAINTY
  - MONTE CARLO UNCERTAINTIES
  - NEURAL NETWORK REGRESSION
- III: PROPER LEARNING
  - OVERLEARNING AND CROSS-VALIDATION
  - HYPEROPTIMIZATION AND GENERALIZATION
- IV: VALIDATION & TESTING
  - TESTING: DATA REGION AND EXTRAPOLATION REGION
  - THE MEANING OF CORRELATIONS
- V: UNDERSTANDING RESULTS
  - DISTRIBUTION OF RESULTS AND FAITHFULNESS
  - OUTLIERS AND GENERALIZATION

SOME GENERAL REFERENCES

REGRESSION AND STATISTICS

- C. M. Bishop, "Pattern recognition and machine learning", Springer, 2006-2009
- G. James, D. Witten, T. Hastie, R. Tibishrani, "An introduction to statistical learning", Springer, 2021

GENERAL MACHINE LEARNING

- I. Goodfellow, Y. Bengio, A. Courville, "Deep learning", MIT press, 2016
- A. Géron, "Hands-on machine learning with Scikit-Learn & TensorFlow", O'Reilly, 2017

PARTON DISTRIBUTIONS

- S. Forte, "Parton Distributions at the dawn of the LHC", Acta Phys. Pol. **B41** (2010) 2859, `arXiv:1011.5247`
- S. Forte and S. Carrazza, "Parton distribution functions", in "Artificial intelligence for High Energy Physics", P. Calafiura, D. Rousseau and K. Terao, eds., World Scientific 2022, pag 715, `arXiv:2008.12305`
- L. Del Debbio, T. Giani, T. Wilson, "Bayesian approach to inverse problems: an application to NNPDF closure testing", Eur. Phys. J. **C82** (2022) 33, `arXiv 2111.057887`

THE NNPDF CODE

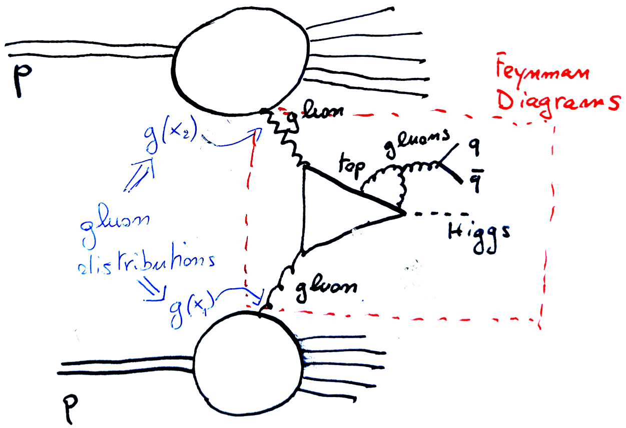
`https://nnpdf.mi.infn.it/nnpdf-open-source-code/`

I: THE PHYSICS PROBLEM

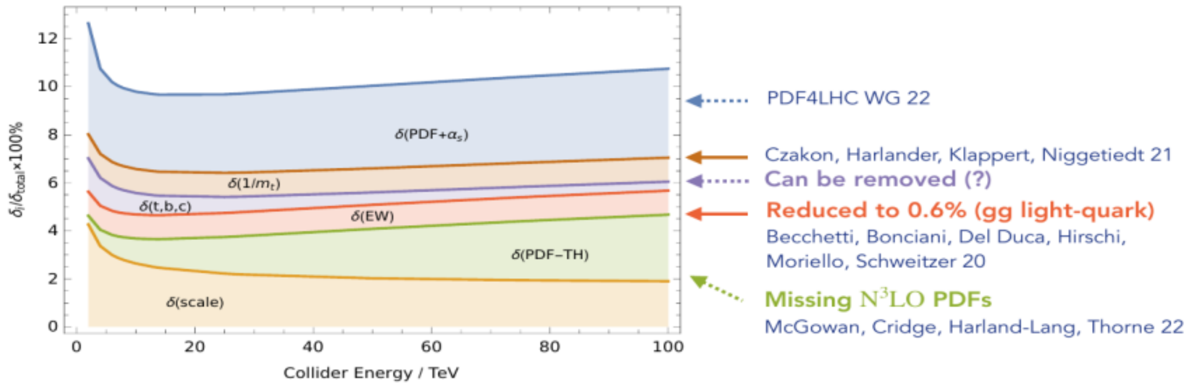
- FACTORIZATION AND PDFs
  - FACTORIZATION: LEPTONIC AND HADRONIC PROCESSES
  - PDFs AND THEIR PROPERTIES
- PDF DETERMINATION
  - FROM DATA TO PDFs
  - PHYSICAL PROCESSES
- UNCERTAINTIES
  - EXPERIMENTAL UNCERTAINTIES AND THEIR CORRELATIONS
  - MISSING HIGHER ORDERS AND THEORY UNCERTAINTIES
- THE PROBLEM OF MODEL UNCERTAINTIES
  - THE PROBLEM OF PDF UNCERTAINTIES
  - PLOTNOMIAL REGRESSION AND ITS PITFALLS

PDFs AND THEIR UNCERTAINTIES

QCD FACTORIZATION



UNCERTAINTIES: HIGGS IN GLUON FUSION



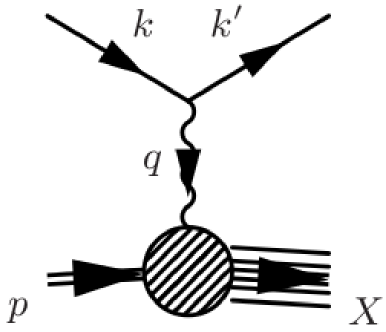
(R. Roentsch, Les Houches, June 2023)

- PDF ESPRESS THE "PROBABILITY" OF QUARKS OR GLUONS (PARTONS) TO ENTER A COLLISION
- THEIR KNOWLEDGE IS REQUIRED FOR THE COMPUTATION OF ANY PROCESS AT THE LHC
- THEIR KNOWLEDGE IS A DOMINANT SOURCE OF UNCERTAINTY

FACTORIZATION

FACTORIZATION IN DEEP-INELASTIC SCATTERING

STRUCTURE FUNCTIONS



Lepton fractional energy loss: $y = \frac{p\cdot q}{p\cdot k}$;
gauge boson virtuality: $q^2 = -Q^2$
Bjorken x: $x = \frac{Q^2}{2p\cdot q}$
lepton-nucleon CM energy: $s = \frac{Q^2}{xy}$;
virtual boson-nucleon CM energy $W^2 = Q^2\frac{1-x}{x}$;

$$\frac{d^2\sigma^{\lambda_p\lambda_\ell}(x,y,Q^2)}{dxdy} = \frac{G_F^2}{2\pi(1+Q^2/m_W^2)^2}\frac{Q^2}{xy}\left\{\left[-\lambda_\ell\, y\left(1-\frac{y}{2}\right)xF_3(x,Q^2) + (1-y)F_2(x,Q^2)\right.\right.$$

$$\left.\left.+y^2xF_1(x,Q^2)\right] - 2\lambda_p\left[-\lambda_\ell\, y(2-y)xg_1(x,Q^2) - (1-y)g_4(x,Q^2) - y^2xg_5(x,Q^2)\right]\right\}$$

$\lambda_l \to$ lepton helicity
$\lambda_p \to$ proton helicity

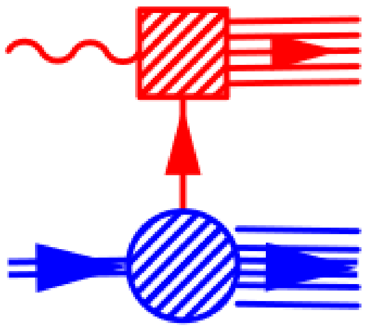
	PARITY CONS.	PARITY VIOL.
UNPOL.	F_1, F_2	F_3
POL.	g_1	g_4, g_5

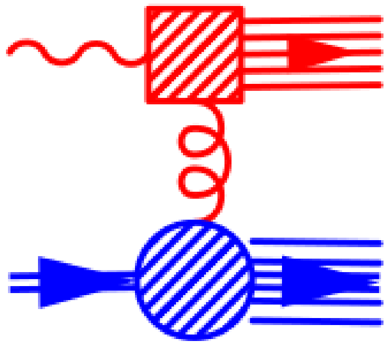
DEEP-INELASTIC SCATTERING

STRUCTURE FUNCTIONS AND PDFs

STRUCTURE FUNCTION=HARD COEFF. (PARTONIC STRUCTURE FUNCTION) $\otimes$PARTON DISTN.

HARD COEFF.: XSECT FOR INCOMING PROTON MOMENTUM $p \Rightarrow$ INCOMING PARTON MOMENTUM $\hat{p} = xp$





$$F_2(x,Q^2) = x\sum_i \int_1^1 \frac{dy}{y} C_i\left(\alpha_s(Q^2), \frac{x}{y}\right)\left[q_i(y,Q^2)+\bar{q}_i(y,Q^2)\right] + C_g\left(\alpha_s(Q^2), \frac{x}{y}\right) g(y,Q^2)$$

q_i quark, $\bar{q}_i$ antiquark, g gluon

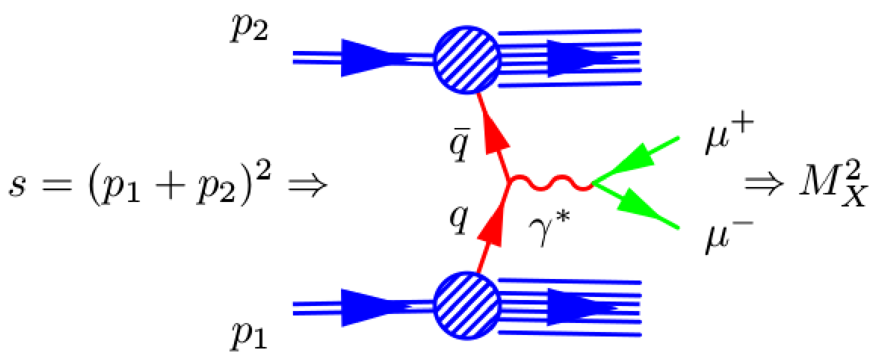
FACTORIZATION
HADRONIC PROCESSES
THE PARTON LUMINOSITY

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

$$\sigma_X(s, M^2) = \sigma_0 \sum_{a,b} \int_\tau^1 \frac{dx}{x} \mathcal{L}_{ab}\left(\frac{\tau}{x}\right) C\left(x, \alpha_s(M_H^2)\right)$$

- PARTON LUMINOSITY $\mathcal{L}_{ab}(\tau) = \int_\tau^1 \frac{dx}{x} f_{a/h_1}(x) f_{b/h_2}(\tau/x)$
- COEFFICIENT FUNCTION $\hat\sigma_{q_a q_b \to X}\left(x_1 x_2 s, M_X^2\right) = \sigma_0 C\left(\frac{M_X^2}{x_1 x_2 s}, \alpha_s(M_H^2)\right)$

EXAMPLE: THE DRELL-YAN PROCESS
AT LEADING ORDER



- Hadronic c.m. energy: $s = (p_1 + p_2)^2$
- Momentum fractions $x_{1,2} = \sqrt{\frac{\hat s}{s}} \exp \pm y$;
  Lead. Ord. $\hat s = M^2$
- Partonic c.m. energy: $\hat s = x_1 x_2 s$
- Invariant mass of final state X (dilepton, Higgs,…): $M_W^2 \Rightarrow$ scale of process
- Scaling variable $\tau = \frac{M_X^2}{s}$

$$\Rightarrow M^2 \frac{d\sigma}{dM^2} = \sigma_0 \mathcal{L}(\tau); \quad \sigma_0 = \frac{4}{9}\pi\alpha \frac{1}{s};$$

FACTORIZATION SUMMARY & MELLIN TRANSFORM

- x-SPACE FACTORIZED EXPRESSIONS:
  - LEPTON-HADRON
    $F(x,Q^2)=\sum_i \int_x^1 \frac{dy}{y} C_i\left(\alpha(Q^2),\frac{x}{y}\right) f_i(y,Q^2)=\left[C_i(\alpha(Q^2))\otimes f_i(Q^2)\right](x)$
  - HADRON-HADRON
    $\sigma(x,Q^2)=\sum_{ij}\int_x^1 \frac{dy}{y}\hat\sigma_{ij}\left(\alpha(Q^2),\frac{x}{y}\right)\mathcal{L}_{ij}=(y,Q^2)\left[\hat\sigma_{ij}(\alpha(Q^2))\otimes\mathcal{L}_{ij}(Q^2)\right](x)$
    $\hat\sigma_{ij}\left(\alpha(Q^2),x\right)=\sigma_0 C_{ij}\left(\alpha(Q^2),x\right);$
    $\mathcal{L}_{ij}(Q^2)(x)=\int_x^1\frac{dy}{y} f_i\left(\frac{x}{y}\right) f_j(y,Q^2)=\left[f_i\otimes f_j\right](x)$

- MELLIN TRANSFORM: $F(N)=\int_x^1 x^{N-1} f(x)\Leftrightarrow (x)=\int_{-i\infty}^{+i\infty} x^{-N} f(N)$
  $h(x)=\int_x^1\frac{dy}{y} f\left(\frac{x}{y}\right) g(y)=\left[f\otimes f\right](x)\Leftrightarrow H(N)=F(N)G(N)$

- N-SPACE FACTORIZED EXPRESSIONS:
  - LEPTON-HADRON $F(N,Q^2)=\sum_i C_i\left(\alpha(Q^2),N\right) f_i(N,Q^2)$
  - HADRON-HADRON $\sigma(x,N)=\sum_{ij}\hat\sigma_{ij}\left(\alpha(Q^2),N\right)\mathcal{L}_{ij}(N,Q^2)$
    $\mathcal{L}_{ij}(Q^2,N)=f_i(N)f_j(N)$

LARGE/SMALL x $\Leftrightarrow$ LARGE/SMALL N

THE SCALE DEPENDENCE OF PDFS
EVOLUTION EQUATIONS

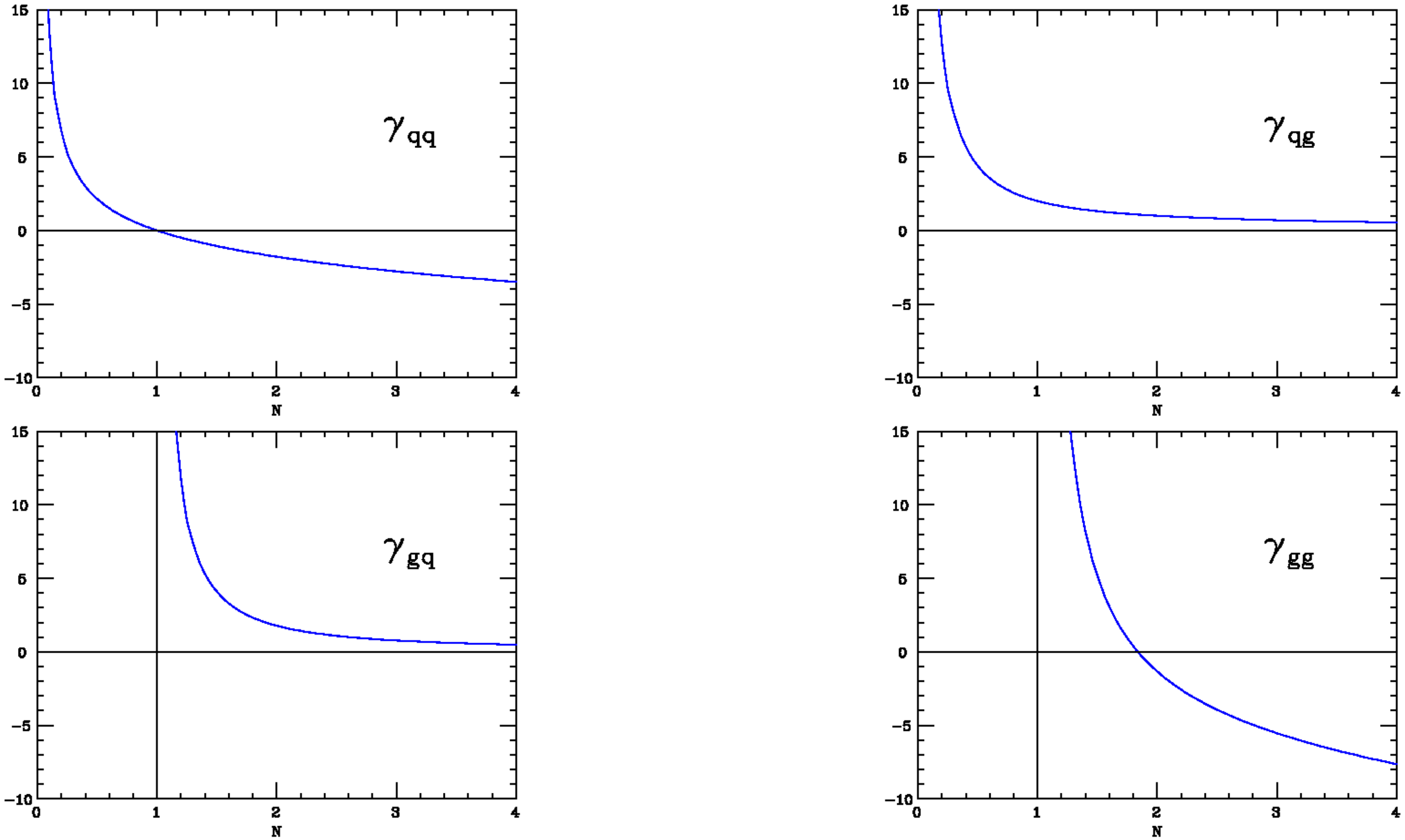
$$\frac{d}{dt} q_{NS}(N, Q^2) = \frac{\alpha_s(t)}{2\pi} \gamma_{qq}^{NS}(N, \alpha_s(t)) q_{NS}(N, Q^2),$$

$$\frac{d}{dt} \begin{pmatrix} \Sigma(N, Q^2) \\ g(N, Q^2) \end{pmatrix} = \frac{\alpha_s(t)}{2\pi} \begin{pmatrix} \gamma_{qq}^S(N, \alpha_s(t)) & 2n_f \gamma_{qg}^S(N, \alpha_s(t)) \\ \gamma_{gq}^S(N, \alpha_s(t)) & \gamma_{gg}^S(N, \alpha_s(t)) \end{pmatrix} \begin{pmatrix} \Sigma(N, Q^2) \\ g(N, Q^2) \end{pmatrix}.$$

- LOG SCALE $t = \ln \frac{Q^2}{\Lambda^2}$:
- ANOMALOUS DIMENSIONS VS. SPLITTING FUNCTIONS
  $\gamma(N, \alpha_s(t)) \equiv \int_0^1 dx\, x^{N-1} P(x, \alpha_s(t))$
- SINGLET $\Sigma(x, Q^2) = \sum_{i=1}^{n_f} \left(q_i(x, Q^2) + \bar{q}_i(x, Q^2) \right)$ VS.
  NONSINGLET $q^{NS}(x, Q^2) = q_i(x, Q^2) - q_j(x, Q^2)$
  COMBINATIONS OF QUARK PDFS
- PERTURBATIVE EXPANSION OF ANOMALOUS DIMENSION
  $\gamma_i(N, \alpha_s(t)) = \gamma_i^{(0)}(N) + \alpha_s(t) \gamma_i^{(1)}(N) + \ldots \Rightarrow$
  LOG RESUMMATION: LO $\Leftrightarrow$ LLQ^2; NLO $\Leftrightarrow$ LLQ^2, $\ldots$

SCALE DEPENDENCE:

ANOMALOUS DIMENSIONS (LEADING ORDER)



QUALITATIVE FEATURES

- AS Q^2 INCREASES, PDFS DECREASE AT LARGE x & INCREASE AT SMALL x DUE TO RADIATION
- GLUON SECTOR SINGULAR AT $N = 1 \Rightarrow$ GLUON GROWS MORE AT SMALL x
- $\gamma_{qq}(1) = 0 \Rightarrow$ NUMBER OF QUARKS CONSERVED

PARTON KINEMATICS VS. HADRON KINEMATICS

$$\sigma(\tau) = \int_\tau^1 \frac{dy}{y} \sum_{ij} \mathcal{L}_{ij}(y) \hat{\sigma}_{ij}\left(\frac{\tau}{z}\right); \quad \mathcal{L}_{ij}(y) \equiv \int_y^1 \frac{dx_1}{x_1} q_i(y) q_j\left(\frac{y}{x_1}\right)$$

- WHICH PARTON MOMENTUM FRACTIONS CONTRIBUTE TO A GIVEN HADRONIC PROCESS ?

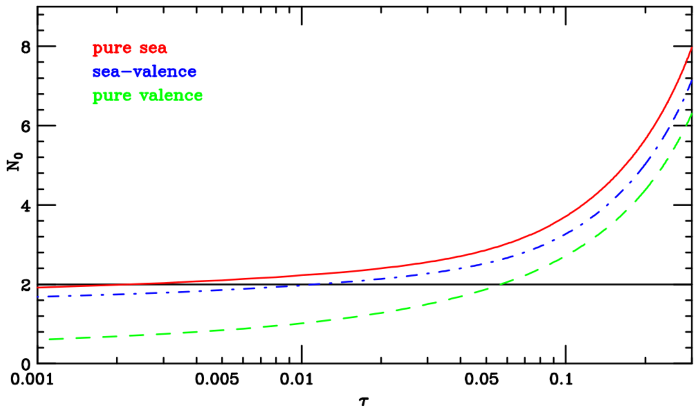
INVERSION OF MELLIN TRANSFORMS

$$f_n = \int_x^1 x^{n-1} f(x) \Leftrightarrow F(x) = \int_{-i\infty}^{+i\infty} x^{-n} f_n$$

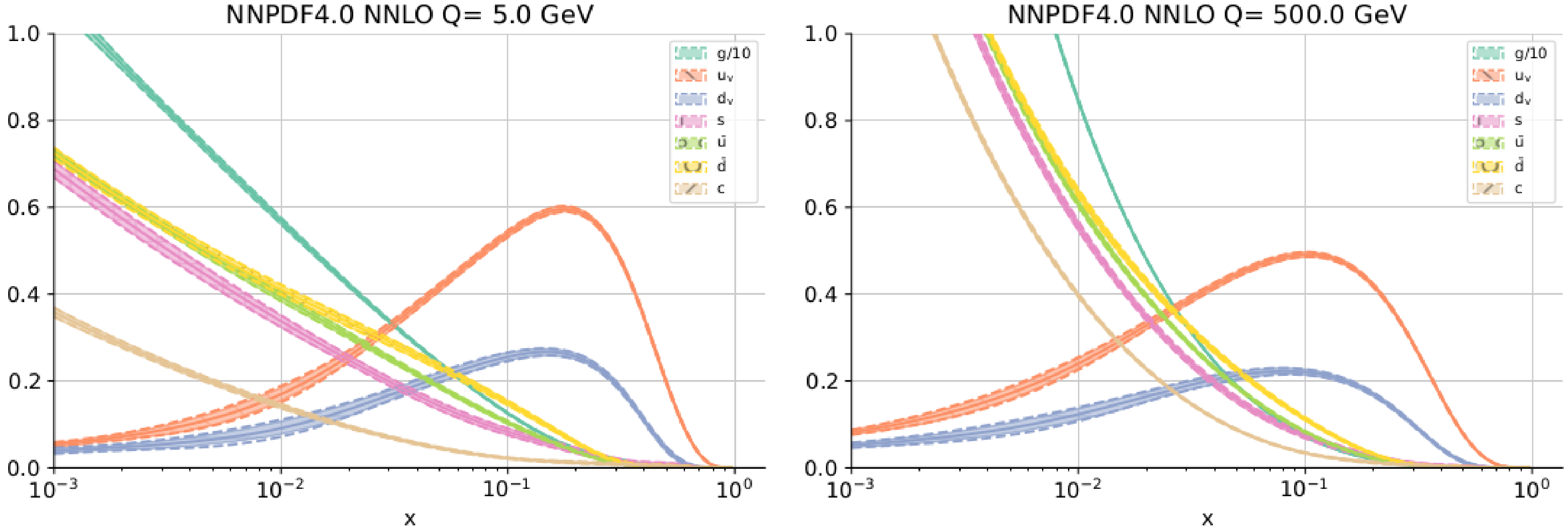
integrate to the right of convergence abscissa

- MELLIN INVERSION DOMINATED BY SADDLE POINT
- POSITION OF SADDLE DEPENDS ON HADRONIC KINEMATICS, CONTROLLED BY PARTON LUMINOSITY DEPENDENCE ON x OF $\mathcal{L}$ POWERLIKE, OF $\hat{\sigma}$ LOGARITHMIC
- PDF PEAKED AT SMALL x ("SEA" $\bar{q}$ VS. "VALENCE" $q - \bar{q}$) $\Rightarrow$ LUMI PEAKS AT SMALL N

SADDLE VS $\tau = Q^2/s$



PDFs: QUALITATIVE FEATURES



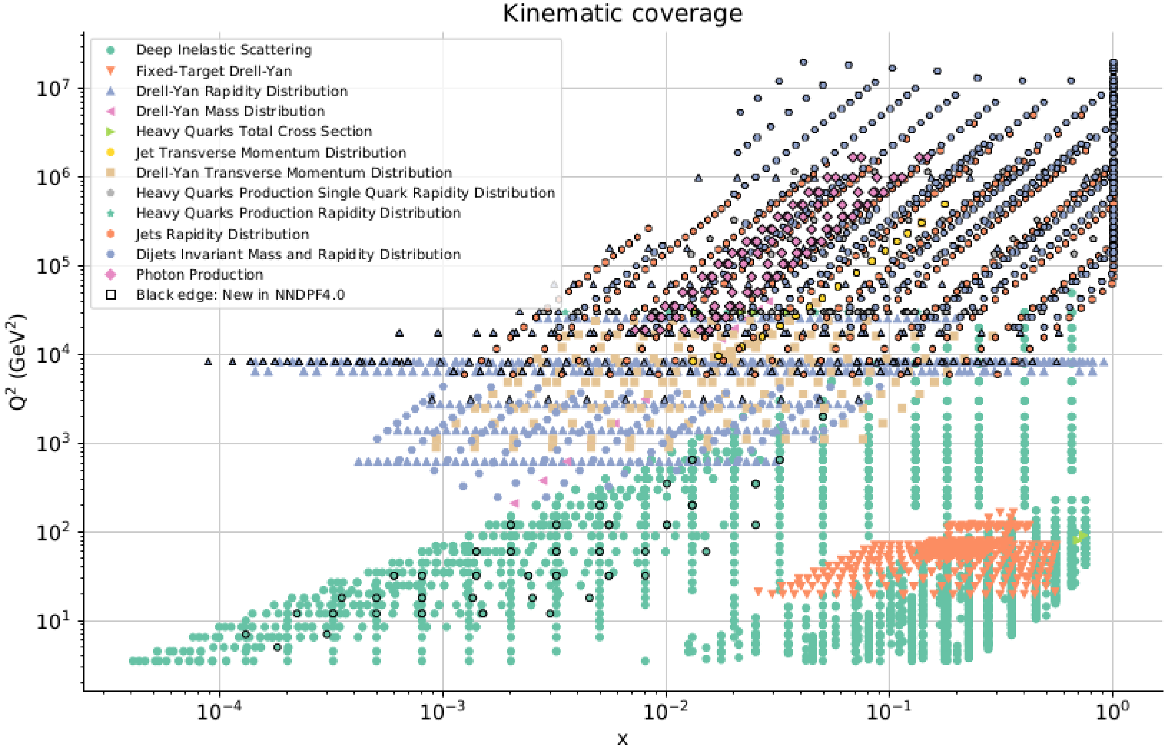
- THE MOMENTUM PROBABILITY DENSITY $xf_i(x)$ IS SHOWN AT TWO DIFFERENT SCALES (LEFT $\Rightarrow$ LOW SCALE; RIGHT $\Rightarrow$ HIGH SCALE)
- AS $x \geq 1$ KINEMATIC CONSTRAINT $f_i(x) = 0$
- "VALENCE" UP AND DOWN: PEAKED AT $x \sim 0.3$; EXPECT $f_x(x) \underset{x\to 1}{\sim} (1-x)_i^\beta$
- "SEA" ANTIQUARK AND GLUON GROW AT SMALL x
- "SINGLET" AND GLUON MIX $\Rightarrow$ ALL PDFs LOOK THE SAME AS $x \to 0$

PDF DETERMINATION

PDF DETERMINATION

DATA → PARTON DISTRIBUTIONS

Experimental data in NNPDF4.0



More than 4000 datapoints!

New processes:

- direct photon
- single top
- dijets
- W+jet
- DIS jet

ISSUES AND TASKS:

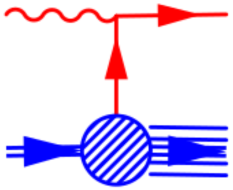
- FROM PHYSICAL OBSERVABLES TO PDFS: SOLVE EVOLUTION EQUATIONS, CONVOLUTE WITH PARTON-LEVEL CROSS-SECTIONS
- DISENTANGLING PDFS: CHOOSE A BASIS OF PDFS ($2N_f$ QUARKS + 1 GLUON) & A SET OF SUITABLE PHYSICAL PROCESSES TO DETERMINE THEM ALL
- PROBABILITY IN THE SPACE OF FUNCTIONS: CHOOSE A STATISTICAL APPROACH (MULTIGAUSSIAN, MONTE CARLO, . . .)
- UNCERTAINTY ON FUNCTIONS: CHOOSE A REGRESSION MODEL

DISENTANGLING PDFs

- CC F_1 AND F_3 IN PRINCIPLE PROVIDE FOUR COMBINATIONS, AND NC F_1 TWO MORE $\Rightarrow$ ALL LIGHT FLAVORS
- $W^\pm$ AND Z PRODUCTION (INCLUDING DOUBLE DIFFERENTIAL: MASS AND RAPIDITY) PROVIDE INDEPENDENT COMBINATIONS
- WHEN PRODUCING ELECTROWEAK FINAL STATES, THE GLUON CAN ONLY BE ACCESSED FROM SCALE DEPENDENCE OR HIGHER ORDERS (DIFFERENTIAL DISTRIBUTIONS)
  …EXCEPT IN HIGGS PRODUCTION!
- JET PRODUCTION GIVES A DIRECT HANDLE ON THE GLUON

FLAVOR SEPARATION (DIS & DY)
LEADING ORDER PARTON CONTENT

DEEP-INELASTIC SCATTERING



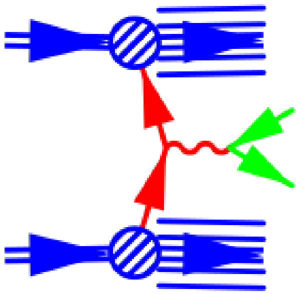
NC	${F_1}^{\gamma} = \sum_i e_i^2\,(q_i + \bar{q}_i)$
NC	${F_1}^{Z,\,\mathrm{int.}} = \sum_i B_i\,(q_i + \bar{q}_i)$
NC	${F_3}^{Z,\,\mathrm{int.}} = \sum_i D_i\,(q_i + \bar{q}_i)$
CC	$F_1^{W^+} = \bar{u} + d + s + \bar{c}$
CC	$-F_3^{W^+}/2 = \bar{u} - d - s + \bar{c}$

ℓ	e	V	A
u,c,t	$+2/3$	$(+1/2 - 4/3\sin^2\theta_W)$	$+1/2$
d,s,b	-1/3	$(-1/2 + 2/3\sin^2\theta_W)$	-1/2
ν	0	$+1/2$	$+1/2$
e,μ, τ	-1	$(-1/2 + 2\sin^2\theta_W)$	-1/2

$B_q(Q^2) = -2e_q V_\ell V_q P_Z + (V_\ell^2 + A_\ell^2)(V_q^2 + A_q^2)P_Z^2;\ D_q(Q^2) = -2e_q A_\ell A_q P_Z + 4V_\ell A_\ell V_q A_q P_Z^2;\ P_Z = Q^2/(Q^2 + M_Z^2)$

$$W^+ \to W^- \Rightarrow u \leftrightarrow d,\ c \leftrightarrow s;\ p \to n \Rightarrow u \leftrightarrow d$$

DRELL-YAN



$$L^{ij}(x_1, x_2) \equiv q_i(x_1, M^2)\bar{q}_j(x_2, M^2)$$

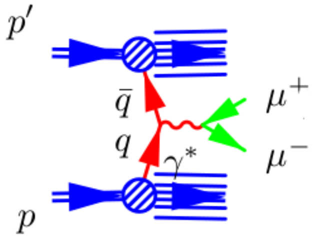
γ	$\frac{d\sigma}{dM^2 dy}(M^2, y) = \frac{4\pi\alpha^2}{9M^2 s}\sum_i e_i^2 L^{ii}(x_1, x_2)$
W	$\frac{d\sigma}{dy} = \frac{\pi G_F M_V^2 \sqrt{2}}{3s}\sum_{i,j}\lvert V_{ij}^{\mathrm{CKM}}\rvert L^{ij}(x_1, x_2)$
Z	$\frac{d\sigma}{dy} = \frac{\pi G_F M_V^2 \sqrt{2}}{3s}\sum_i \left(V_i^2 + A_i^2\right) L^{ij}(x_1, x_2)$

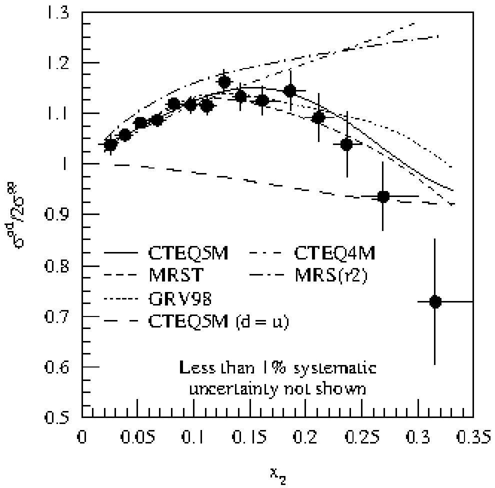
$V_{ij}^{\mathrm{CKM}} \to$ CKM MATRIX ($i = u,\ c\,t,\ j = d,\ s\,b$), $V_{ij}^{\mathrm{CKM}} = 1 + O(\lambda)$; $\lambda = \sin\theta_C \approx 0.22$

FIXED-TARGET DRELL-YAN (TEVATRON)
QUARKS AND ANTIQUARK SEPARATION

BY CHARGE CONJUGATION $\bar{q}_{\bar{P}} = q_p$

DRELL-YAN p/d ASYMMETRY

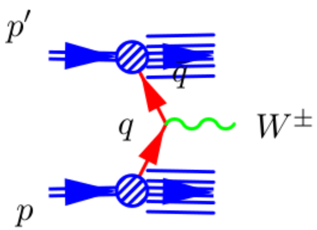


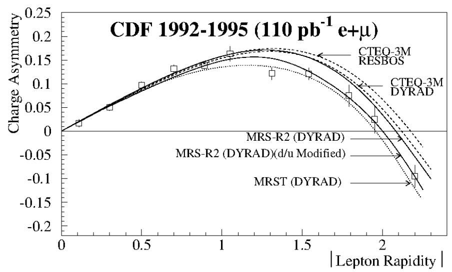


$$\frac{\sigma^{pn}}{\sigma^{pp}} \sim \left.\frac{\frac{4}{9}u^p\bar{d}^p+\frac{1}{9}d^p\bar{u}^p}{\frac{4}{9}u^p\bar{u}^p+\frac{1}{9}d^p\bar{d}^p}\right|_{\text{large } x} \approx \frac{\bar{d}}{\bar{u}}$$

E866 (2001)

$W^{\pm}$ ASYMMETRY





$$\frac{\sigma^{p\bar{p}}_{W+}}{\sigma^{p\bar{p}}_{W-}} = \frac{u^p(x_1)d^p(x_2)+\bar{d}^p(x_1)\bar{u}^p(x_2)}{d^p(x_1)u^p(x_2)+\bar{u}^p(x_1)\bar{d}^p(x_2)} \sim \frac{u^p d^p}{d^p u^p}$$

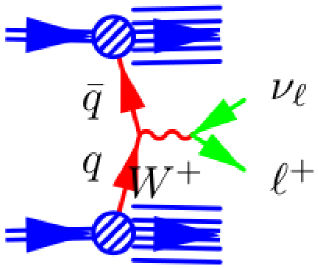
if x_1, x_2 in valence region,
neglecting HQ & Cabibbo suppr.

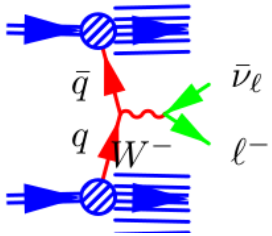
CDF (1998)

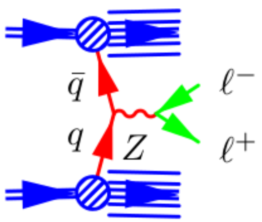
COLLIDER DRELL-YAN (LHC)

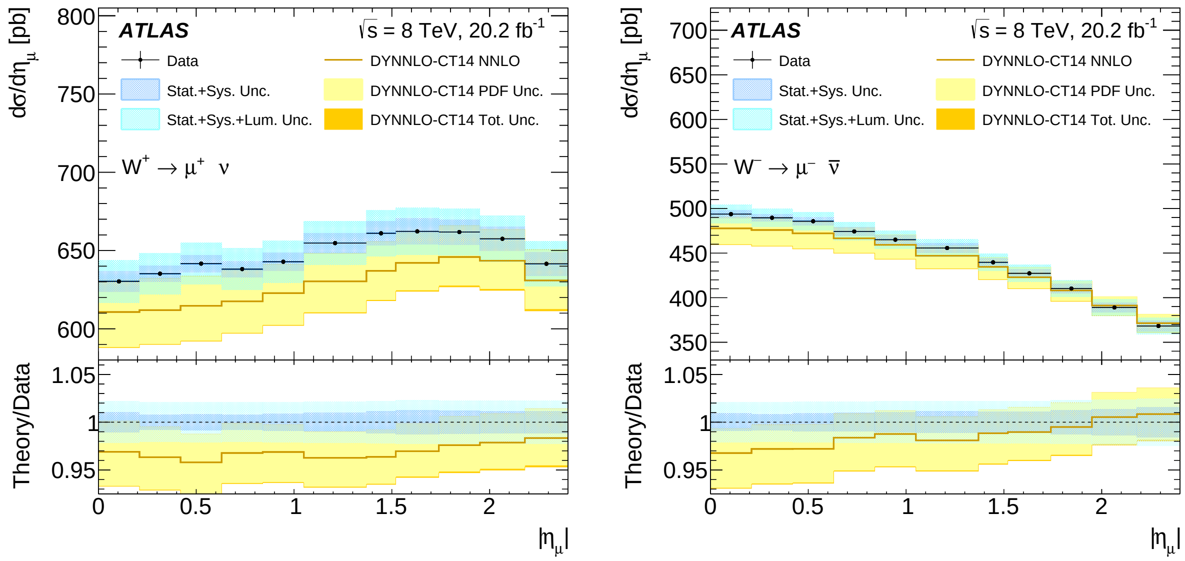
$W^{\pm}$ AND Z PRODUCTION

W AND Z CROSS SECTIONS





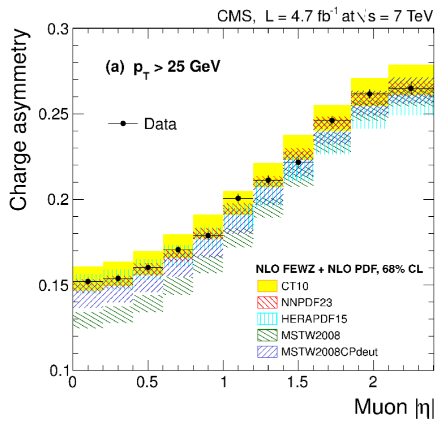




ATLAS (2019)

$\sigma^{p\bar{p}}_{W^+} = u\bar{d} + c\bar{s}$; $\sigma^{p\bar{p}}_{Z} = u\bar{u} + d\bar{d} + s\bar{s}$: STRANGENESS DETERMINED BY COMPARISON

W MUON ASYMMETRY



CMS (2013)

$$\frac{\sigma^{p\bar{p}}_{W^+}}{\sigma^{p\bar{p}}_{W^-}} = \frac{u(x_1)\bar{d}(x_2)+\bar{d}(x_1)u(x_2)}{d(x_1)\bar{u}(x_2)+\bar{u}(x_1)d(x_2)}$$

"VALENCE" $x \Rightarrow$ NEGLECT STRANGENESS

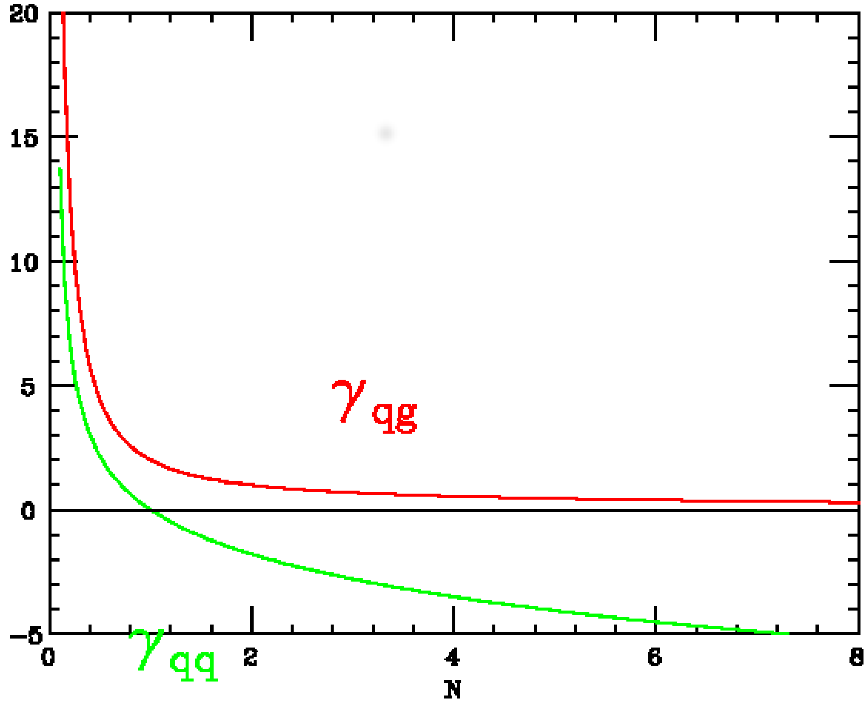
$\Rightarrow$ DETERMINE $\bar{u} - \bar{d}$

THE GLUON FROM DIS

SCALE DEPENDENCE OF FLAVOR SINGLET STRUCTURE FUNCTIONS

$$\frac{d}{dt}F_2^s(N,Q^2) = \frac{\alpha_s(Q^2)}{2\pi}\left[\gamma_{qq}(N)F_2^s + 2\,n_f\gamma_{qg}(N)g(N,Q^2)\right] + O(\alpha_s^2)$$

ANOMALOUS DIMENSIONS



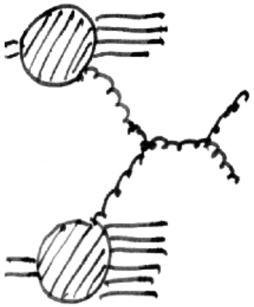
LARGE x GLUON DIFFICULT TO DETERMINE FROM DEEP-INELASTIC SCATTERING

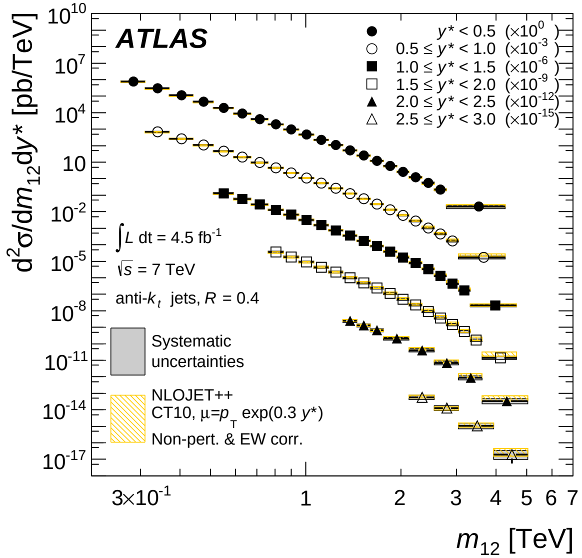
THE GLUON IN HADRONIC COLLISIONS

THE GLUON ONLY INTERACTS THROUGH QCD

JETS

GLUON



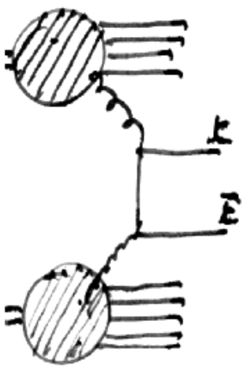


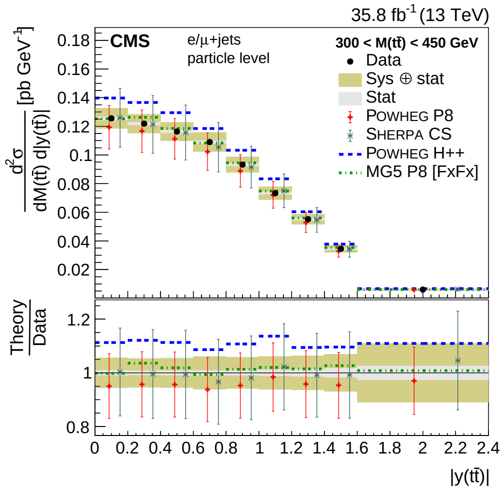
- ONE-JET/DIJET INCLUSIVE USED TO CONSTRAIN THE LARGE x GLUON SINCE TEVATRON
- WIDE KINEMATIC REGION AT LHC

ATLAS (2014)

TOP

GLUON





- WIDE RAPIDITY RANGE: CAN ACCESS WIDE x REGION

CMS (2018)

UNCERTAINTIES

DATA UNCERTAINTIES: COVARIANCE MATRIX

PREDICTIONS VS. DATA: LOSS

$$\chi^2 = \sum_{i,j}^{N_{\rm pt}} (T_i - D_i)(\text{cov}^{-1})_{ij}(T_j - D_j)$$

THE COVARIANCE MATRIX

$$\text{cov}_{ij} = \delta_{ij} s_i^2 + \sum_{\alpha=1}^{N_c} \sigma_{i,\alpha}^{(c)} \sigma_{j,\alpha}^{(c)} + \left(\sum_{\alpha=1}^{N_{\mathcal{L}}} \sigma_{i,\alpha}^{(\mathcal{L})} \sigma_{j,\alpha}^{(\mathcal{L})} \right) D_i D_j$$

- D_i: DATA; T_i: PREDICTION
- s_i: UNCORRELATED STATISTICAL UNCERTAINTY FOR i-TH DATAPOINT
- $\sigma_{i,\alpha}^{(c)}$: α-TH CORRELATED ADDITIVE SYSTEMATICS FOR i-TH DATAPOINT
- $\sigma_{i,\alpha}^{(\mathcal{L})}$: α-TH CORRELATED MULTIPLICATIVE SYSTEMATICS FOR i-TH DATAPOINT

DATA UNCERTAINTIES: NUISANCE PARAMETERS

THE PARAMETERS

$$\chi^2(\{a\},\{\lambda\}) = \sum_{k=1}^{N_{\rm pt}} \frac{1}{s_k^2}\left(D_k - T_k - \sum_{\alpha=1}^{N_\lambda}\beta_{k,\alpha}\lambda_\alpha\right)^2 + \sum_{\alpha=1}^{N_\lambda}\lambda_\alpha^2$$

SYSTEMATIC UNCERTAINTIES

$\beta_{i,\alpha} = \sigma_{i,\alpha}^{(c)}$ for $\alpha = 1,\ldots,N_c$; $\beta_{i,\alpha} = \sigma_{j,\alpha}^{(\mathcal{L})}D_i$ for $\alpha = N_c+1,\ldots,N_{\mathcal{L}}$

BEST-FIT VALUES

$$\lambda_{0\alpha} = \sum_{i=1}^{N_{\rm pt}} \frac{D_i - T_i}{s_i}\sum_{\delta=1}^{N_\lambda}\mathcal{A}^{-1}_{\alpha\delta}\frac{\beta_{i,\delta}}{s_i}$$

REDUCED COVARIANCE MATRIX

$$\mathcal{A}_{\alpha\beta} = \delta_{\alpha\beta} + \sum_{k=1}^{N_{\rm pt}}\frac{\beta_{k,\alpha}\beta_{k,\beta}}{s_k^2}$$

CONSTRUCTION OF THE COVARIANCE MATRIX: INVERSE

$$({\rm cov})^{-1}_{ij} = \left[\frac{\delta_{ij}}{s_i^2} - \sum_{\alpha,\beta=1}^{N_\lambda}\frac{\beta_{i,\alpha}}{s_i^2}\mathcal{A}^{-1}_{\alpha\beta}\frac{\beta_{j,\beta}}{s_j^2}\right],$$

THE COVARIANCE MATRIX

$$({\rm cov})_{ij} \equiv s_i^2\delta_{ij} + \sum_{\alpha=1}^{N_\lambda}\beta_{i,\alpha}\beta_{j,\alpha}$$

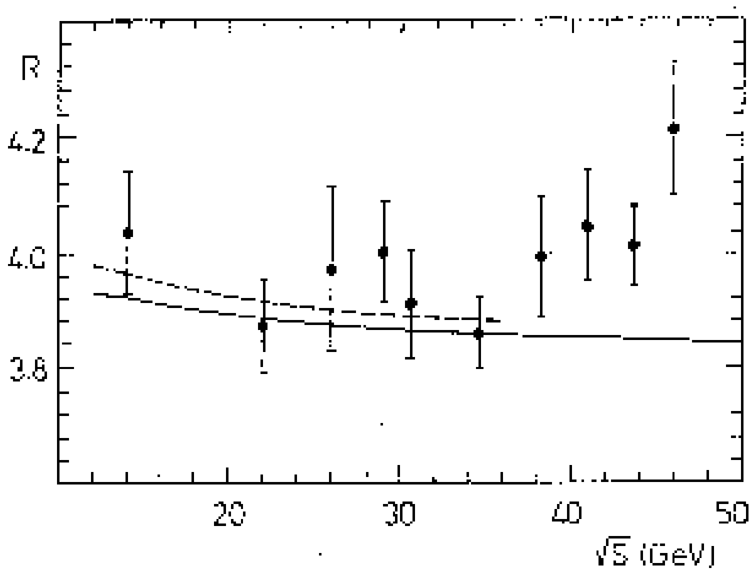
MULTIPLICATIVE UNCERTAINTIES

THE D'AGOSTINI BIAS

- NORMALIZATION UNCERTAINTIES IN COVARIANCE MATRIX
  $(\mathrm{cov})_{ij} = \sigma_{i,n}\sigma_{j,n} D_i D_j$
  $\Rightarrow$ MAXIMUM-LIKELIHOOD RESULT BIASED (d'Agostini, 1994)

- EQUIVALENT TO RESCALING DATA BUT NOT UNCERTAINTIES

$$R = \frac{e^+e^- \to \mathrm{hadrons}}{e^+e^- \to \mu^+\mu^-}$$

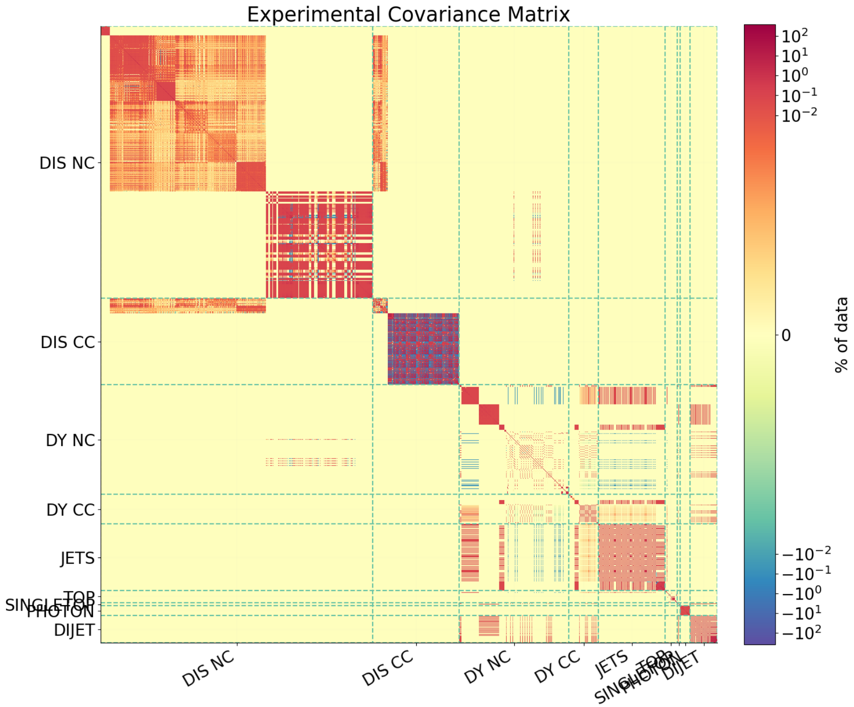


(CELLO collab., 1987)

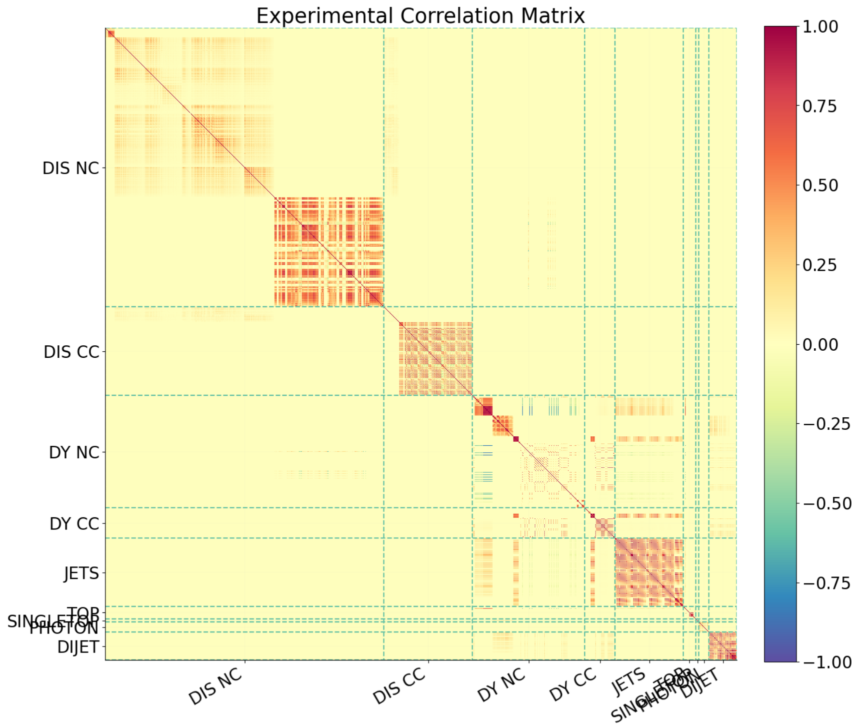
- MUST COMPUTE UNCERTAINTY FROM PREVIOUS THEORY PREDICTION
  RESULT OF PREVIOUS FIT: $(\mathrm{cov})_{ij} = \sigma_{i,n}\sigma_{j,n} T_i^{(0)} T_j^{(0)}$

A LOOK AT THE COVARIANCE MATRIX

COVARIANCE



CORRELATION



MISSING HIGHER ORDER (THEORY) UNCERTAINTIES

- 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

- 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 $P(t) = \delta(t - t^{\text{exact}})$
- IN ACTUAL FACT ONLY SOME PERTURBATIVE RESULT t_p IS EXACTLY KNOWN SO $t^{\text{exact}} = t_p + \Delta_p$, 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 MINIMZATION
- CAN COMPUTE PDF UNCERTAINTY GIVEN MHOU

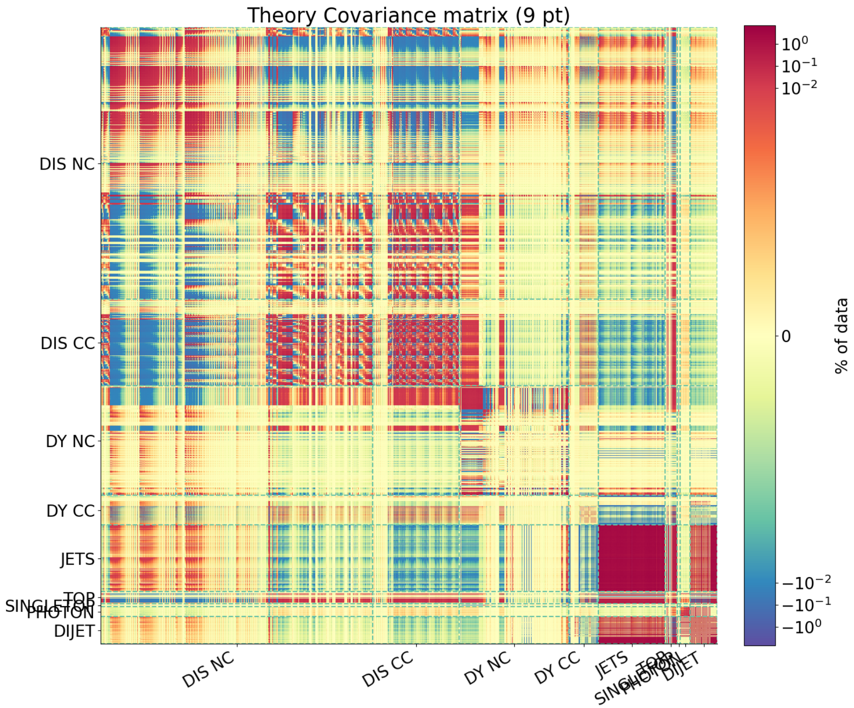
THEORY COVARIANCE MATRICES

THEORY COVARIANCE MATRIX: processes i, j, scale choice $\{\mu^{(k)}\}$, default $\{\mu_0\}$

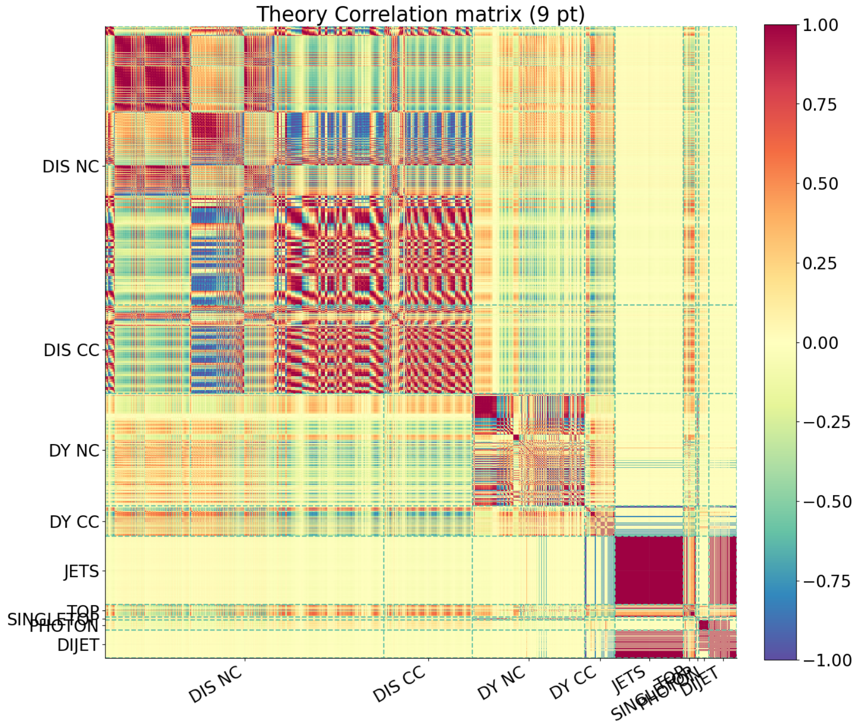
$$\sigma_{i,j} = \frac{1}{N} \sum_k \left(\sigma_i[\{\mu^{(k)}\}] - \sigma_i[\{\mu_0\}] \right) \left(\sigma_j[\{\mu^{(k)}\}] - \sigma_j[\{\mu_0\}] \right)$$

- SINGLE PROCESS: k RUNS OVER COMMON SET OF SCALE CHOICES
- MANY PROCESSES:
  - UNCORRELATED RENORMALIZATION: DIFFERENT FOR DIFFERENT HARD PROCESSES
  - CORRELATED FACTORIZATION: MHOU OF PERTURBATIVE EVOLUTION UNIVERSAL

COVARIANCE



CORRELATION



MODEL-DEPENDENT REGRESSION

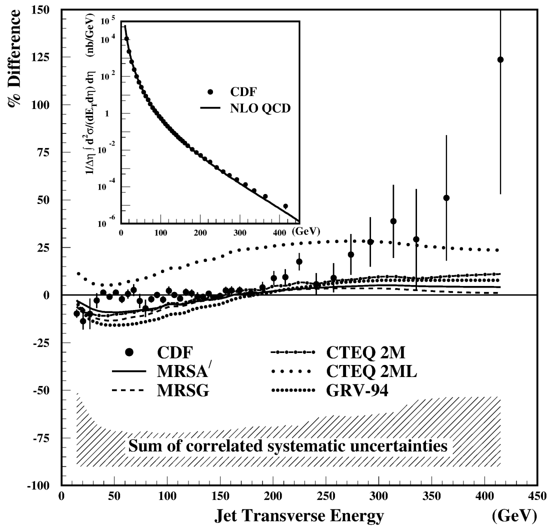
A MODEL-DEPENDENT (HESSIAN) APPROACH

- CHOOSE A FIXED FUNCTIONAL FORM
  - SINCE 1973, PHYSICALLY MOTIVATED ANSATZ $f_i(x, Q_0^2) = x^\alpha (1-x)^\beta g_i(x)$;
    $g_i(x)$ POLYNOMIAL IN x OR $\sqrt{x}$
  - MMHT 2015:
    * BASIS FUNCTIONS g; $u_v = u - \bar{u}$; $d_v = d - \bar{d}$; $S = 2(\bar{u} + \bar{d}) + s + \bar{s}$; $s_+ = s + \bar{s}$; $\Delta = \bar{d} - \bar{u}$;
      $s_- = s - \bar{s}$.
    * FOR ALL BUT Δ s_-, $g \Rightarrow xf_i(x, Q_0^2) = Ax^\alpha(1-x)^\beta \left(1 + \sum_{i=1}^4 a_i T_i(y(x))\right)$;
      T_i CHEBYSHEV POLYNOMIALS, $y = 1 - 2\sqrt{x} \leftrightarrow$ MUST MAP $x = [0,1]$ INTO $y = [-1,1]$;
      $T_i(-1) = T_i(1) = 1$
    * GLUON $xg(x, Q_0^2) = Ax^\alpha(1-x)^\beta \left(1 + \sum_{i=1}^2 a_i T_i(y(x))\right) + A' xT\alpha'(1-x)^{\beta'}$
    * SEA ASYMMETRY $x\Delta(x, Q_0^2) = Ax^\alpha(1-x)^\beta(1 + \gamma x + \epsilon x^2)$
    * STRANGENESS ASYMMETRY $x\Delta(x, Q_0^2) = Ax^\alpha(1-x)^\beta(1 - x/x_0)$
    * 41 PARAMETERS, 4 FIXED BY SUM RULES
    * 12 PARMS FIXED AT BEST FIT, REMAINING 25 USED FOR COVARIANCE MATRIX
      $\Rightarrow$ INCREASED TO 30 IN MSHT 2019
- EVOLVE TO DESIRED SCALE & COMPUTE PHYSICAL OBSERVABLES
- DETERMINE BEST-FIT VALUES OF PARAMETERS
- DETERMINE ERROR BY PROPAGATION OF ERROR ON PARMS. $\Delta\chi^2 = 1$('HESSIAN METHOD');
  PARM. SCANS ALSO POSSIBLE ('LAGR. MULTIPLIER METHOD')

THE PROBLEM OF MODEL DEPENDENCE:

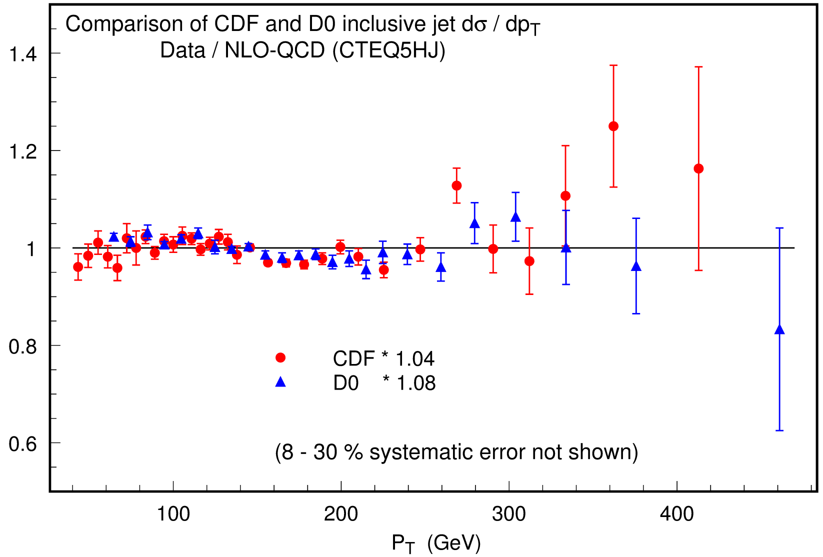
A DISCOVERY THAT WASN'T

- DISCREPANCY BETWEEN QCD CALCULATION AND CDF JET DATA (1995)
- EVIDENCE FOR QUARK COMPOSITENESS?
- RESULT STRONGLY DEPENDS ON GLUON AT $x \gtrsim 0.1$
- PDF MUST VANISH AT $x = 0$, BUT (THEN) NO DATA FOR $x \gtrsim 0.05$!



DISCREPANCY REMOVED IF JET DATA USED FOR GLUON DETERMINATION

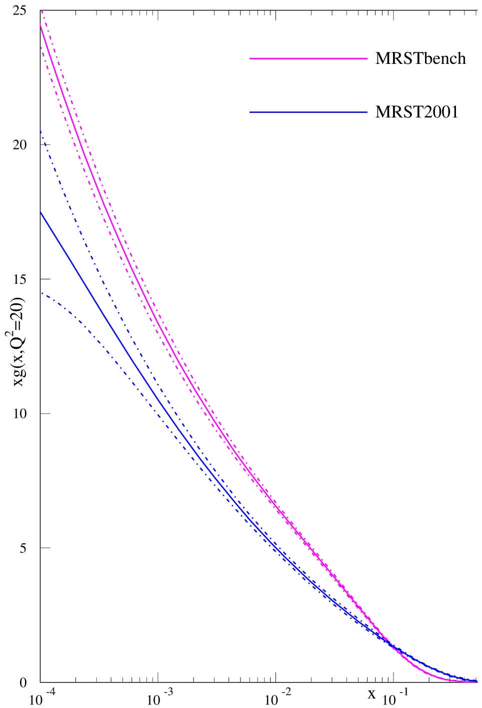
NEW CTEQ GLUON (1998)



MODEL-DEPENDENT UNCERTAINTIES
THE HERA-LHC BENCHMARK PUZZLE

- RESTRICTED AND VERY CONSISTENT DATASET USED
- RESULTS COMPARED TO THEN-BEST RESULT FROM FULL DATASET

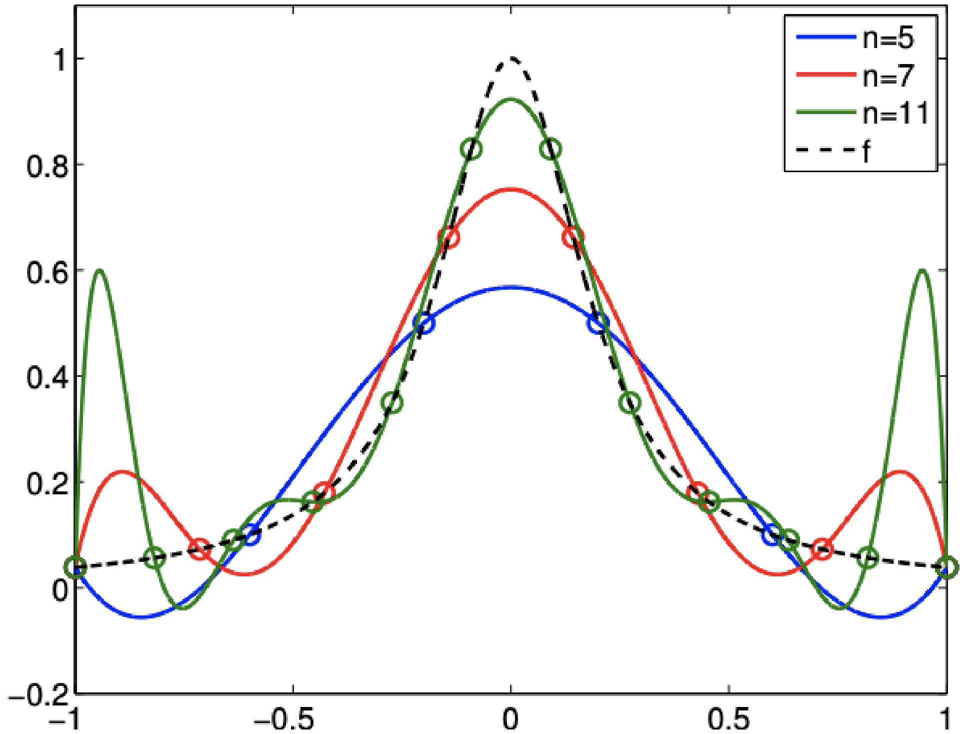
BENCHMARK VS DEFAULT GLUON



"...the partons extracted using a very limited data set are completely incompatible, even allowing for the uncertainties, with those obtained from a global fit with an identical treatment of errors...The comparison illustrates the problems in determining the true uncertainty on parton distributions." (R.Thorne, HERALHC, 2005)

REGRESSION THROUGH POLYNOMIALS

THE RUNGE PHENOMENON

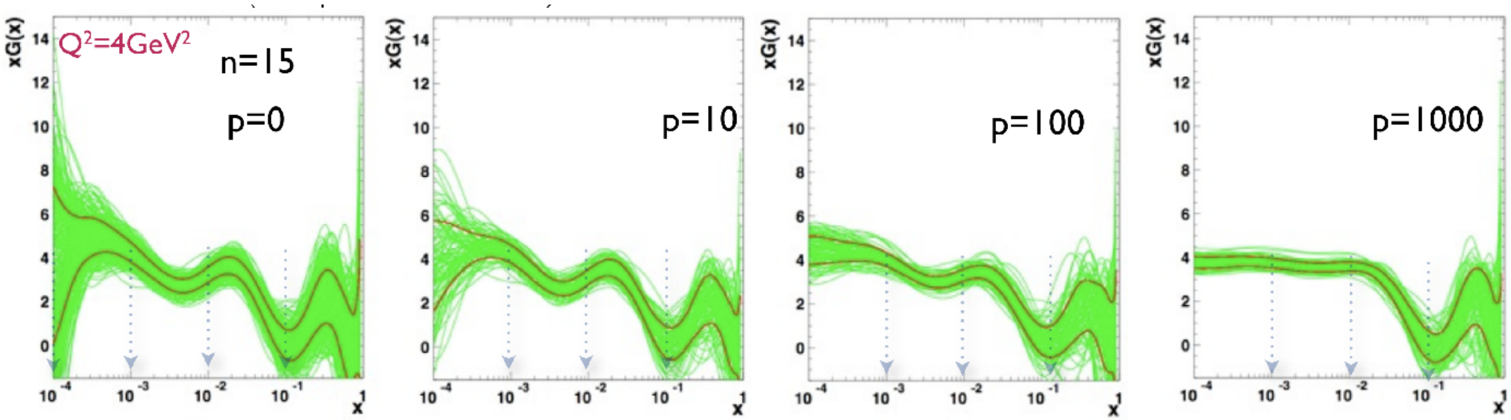


- INTERPOLATE WITH A POLYNOMIAL A FUNCTION SAMPLED AT EQUALLY SPACED POINTS
- RUNGE/AGNESI FUNCTION: $\frac{1}{1+x^2}$ SAMPLED AT $x_i = \frac{2i}{n} - 1,\ i = 1, \ldots, n$
- OSCILLATIONS INCREASE AS THE DEGREE OF THE POLYNOMIAL INCREASES
- ALLEVIATED WITH SUITABLE CHOICE OF POLYNOMIALS AND SAMPLING POINTS (CHEBYSHEV NODES)

REGRESSION THROUGH POLYNOMIALS

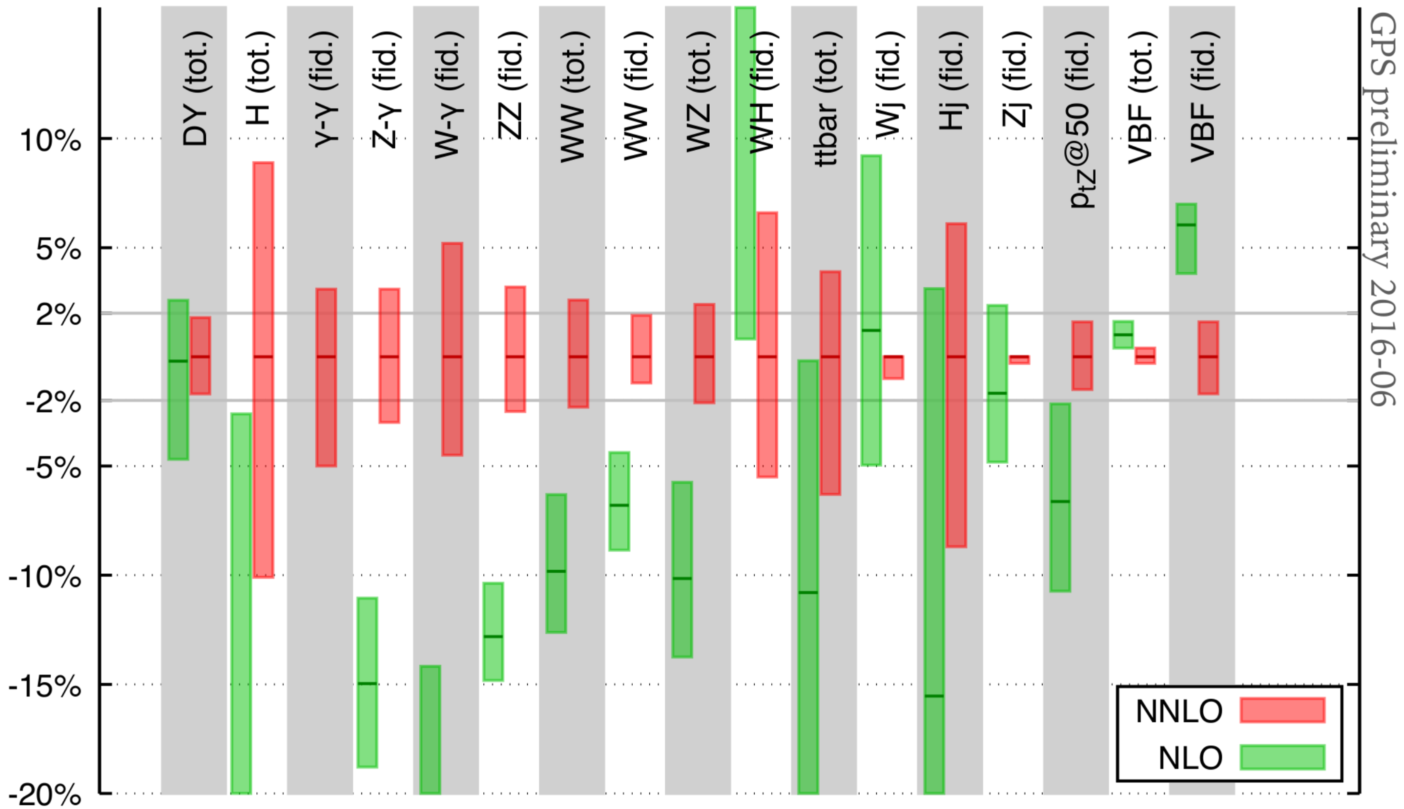
CHEBYSHEV AND LENGTH PENALTY

- OLD IDEA FOR PDF MODELING (PARISI, SOURLAS, 1978):
  EXPAND PDFS OVER BASIS OF ORTHOGONAL POLYNOMIALS
- GLAZOV, RADESCU, 2009: SYSTEMATIC MONTE CARLO APPROACH
- LENGTH PENALTY STABILIZATION:
  CONTRIBUTION TO χ^2 PROPORTIONAL TO THE ARCLENGTH WITH WEIGHT p
- RESULTS STRONGLY DEPENDENT ON ARBITRARY CHOICE OF p



EXTRAS

VALIDATION OF THEORY UNCERTAINTIES
NLO SCALE VARIATION VS ACTUAL NNLO CORRECTION



(G. Salam, 2016)

- SCALE VARIATION CANNOT PREDICT OPENING OF NEW CHANNELS OR RESUMMATION
- ISSUE KNOWN IN MOST CASES

VALIDATION OF THEORY UNCERTAINTIES

NLO SCALE VARIATION VS ACTUAL NNLO CORRECTION

OBSERVABLES INCLUDED IN NNPDF4.0 PDF DETERMINATION