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## Parton distribution functions and $\alpha_S$

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In collaboration with A.D. Martin, W.J. Stirling and R.S. Thorne
[arXiv:0901.0002 ("MSTW 2008", 154 pages) and paper in preparation]
MSTW = MRST - R.G. Roberts (now retired) + G.W. (since 2006)
http://projects.hepforge.org/mstwpdf/

#### 

$$\sigma_{AB} = \sum_{a,b=q,g} f_{a/A}(x_a,\mu_F^2) \otimes f_{b/B}(x_b,\mu_F^2) \otimes \hat{\sigma}_{ab}$$



• Expand  $\hat{\sigma}_{ab}$ ,  $P_{aa'}$  and  $\beta$  as perturbative series in  $\alpha_S$  ( $\overline{\mathrm{MS}}$  scheme):

$$\hat{\sigma}_{ab} = \alpha_{S}^{r} \left[ \hat{\sigma}_{ab}^{\text{LO}} + \alpha_{S} \hat{\sigma}_{ab}^{\text{NLO}} + \alpha_{S}^{2} \hat{\sigma}_{ab}^{\text{NNLO}} \dots \right] \quad (r \ge 0)$$

$$\frac{\partial f_{a/A}}{\partial \ln Q^{2}} = \alpha_{S} \sum_{a'=q,g} \left[ P_{aa'}^{\text{LO}} + \alpha_{S} P_{aa'}^{\text{NLO}} + \alpha_{S}^{2} P_{aa'}^{\text{NNLO}} \dots \right] \otimes f_{a'/A}$$

$$\frac{\partial \alpha_{S}}{\partial \ln Q^{2}} = -\beta^{\text{LO}} \alpha_{S}^{2} - \beta^{\text{NLO}} \alpha_{S}^{3} - \beta^{\text{NNLO}} \alpha_{S}^{4} - \dots$$

• Need to extract input values  $f_{a/A}(x, Q_0^2)$  and  $\alpha_S(M_Z^2)$  from data.

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Data sets fitted in M	1STW 200	08 NLO analysis [a	rXiv:0901.0002
Data set           H1 MB 99 $e^+p$ NC           H1 MB 97 $e^+p$ NC           H1 low Q <sup>2</sup> 96–97 $e^+p$ NC           H1 high Q <sup>2</sup> 98–99 $e^-p$ NC           H1 high Q <sup>2</sup> 99–00 $e^+p$ NC           ZEUS SVX 95 $e^+p$ NC           ZEUS 96–97 $e^+p$ NC           ZEUS 98–99 $e^-p$ NC           ZEUS 99–00 $e^+p$ NC           ZEUS 99–00 $e^+p$ NC           ZEUS 99–00 $e^+p$ NC           H1 99–00 $e^+p$ CC           ZEUS 96–97 $e^+p$ incl. jets           ZEUS 96–97 $e^+p$ incl. jets	$\begin{array}{c c} \hline \chi^2 & / & N_{\rm pts.} \\ \hline 9 & / & 8 \\ \hline 42 & / & 64 \\ 44 & / & 80 \\ 122 & / & 126 \\ 131 & / & 147 \\ 35 & / & 30 \\ 86 & / & 144 \\ 54 & / & 92 \\ 63 & / & 90 \\ 29 & / & 28 \\ 38 & / & 30 \\ 107 & / & 83 \\ 19 & / & 24 \\ 30 & / & 30 \\ \end{array}$	$\begin{tabular}{ c c c c c } \hline \hline Data set \\ \hline \hline BCDMS $\mu p $F_2$ \\ BCDMS $\mu d $F_2$ \\ BCDMS $\mu d $F_2$ \\ NMC $\mu p $F_2$ \\ NMC $\mu n / \mu p$ \\ E665 $\mu p $F_2$ \\ E665 $\mu d $F_2$ \\ SLAC $ep $F_2$ \\ SLAC $ep $F_2$ \\ SLAC $ep $F_2$ \\ SLAC $ed $F_2$ \\ NMC/BCDMS/SLAC $F_L$ \\ \hline E866/NuSea $pp DY$ \\ \hline E866/NuSea $pd / pp DY$ \\ \hline \hline NuTeV $\nu N $F_2$ \\ \hline CHORUS $\nu N $F_2$ \\ \hline \end{tabular}$	$\begin{array}{r} \chi^2 \ / \ N_{\rm pts.} \\ \hline 182 \ / \ 163 \\ 190 \ / \ 151 \\ 121 \ / \ 123 \\ 102 \ / \ 123 \\ 130 \ / \ 148 \\ 57 \ / \ 53 \\ 53 \ / \ 53 \\ 30 \ / \ 37 \\ 30 \ / \ 38 \\ 38 \ / \ 31 \\ \hline 228 \ / \ 184 \\ 14 \ / \ 15 \\ \hline 49 \ / \ 53 \\ 26 \ / \ 42 \end{array}$
$\frac{2EUS 98-00 \ e^{\perp}p \text{ incl. jets}}{D\emptyset \text{ II } p\overline{p} \text{ incl. jets}}$		NuTeV $\nu N \times F_3$ CHORUS $\nu N \times F_3$	40 / 45 31 / 33
CDF II $p\bar{p}$ incl. jets CDF II $W \rightarrow l\nu$ asym. DØ II $W \rightarrow l\nu$ asym	56 / 76 29 / 22 25 / 10	$\begin{array}{c} CCFR \ \nu N \to \mu \mu X \\ NuTeV \ \nu N \to \mu \mu X \end{array}$	66 / 86 39 / 40
DØ II Z rap. CDF II Z rap.	19 / 28 49 / 29	All data sets	2543 / 2699

• Red = New w.r.t. MRST 2006 fit.

#### 

At input scale 
$$Q_0^2 = 1$$
 GeV<sup>2</sup> (notation:  $f_{a/p} \equiv a$ ):

$$\begin{aligned} xu_{v} &= A_{u} x^{\eta_{1}} (1-x)^{\eta_{2}} (1+\epsilon_{u} \sqrt{x} + \gamma_{u} x) \\ xd_{v} &= A_{d} x^{\eta_{3}} (1-x)^{\eta_{4}} (1+\epsilon_{d} \sqrt{x} + \gamma_{d} x) \\ xS &= A_{S} x^{\delta_{S}} (1-x)^{\eta_{S}} (1+\epsilon_{S} \sqrt{x} + \gamma_{S} x) \\ x(\bar{d} - \bar{u}) &= A_{\Delta} x^{\eta_{\Delta}} (1-x)^{\eta_{S}+2} (1+\gamma_{\Delta} x + \delta_{\Delta} x^{2}) \\ xg &= A_{g} x^{\delta_{g}} (1-x)^{\eta_{g}} (1+\epsilon_{g} \sqrt{x} + \gamma_{g} x) + A_{g'} x^{\delta_{g'}} (1-x)^{\eta_{g'}} \\ x(s+\bar{s}) &= A_{+} x^{\delta_{S}} (1-x)^{\eta_{+}} (1+\epsilon_{S} \sqrt{x} + \gamma_{S} x) \\ x(s-\bar{s}) &= A_{-} x^{\delta_{-}} (1-x)^{\eta_{-}} (1-x/x_{0}) \end{aligned}$$

- $A_u$ ,  $A_d$ ,  $A_g$  and  $x_0$  are determined from sum rules.
- 20 parameters allowed to go free for error propagation,
   cf. 15 for MRST error PDF sets (1 more for g, 4 more for s, s̄).



Fixed flavor number scheme

- No heavy quark PDF.
- Includes  $\mathcal{O}(m_H^2/Q^2)$  terms.
- No resummation of  $\alpha_{S} \ln(Q^{2}/m_{H}^{2})$  terms.

Zero-mass variable flavor number scheme

- Use heavy quark PDF.
- Mass dependence neglected.
- Resums  $\alpha_{S} \ln(Q^{2}/m_{H}^{2})$ terms similar to light quarks.



Recent review by R. Thorne and W.-K. Tung [arXiv:0809.0714]

- Interpolate between two well-defined regions: FFNS for  $Q^2 \le m_H^2$ , ZM-VFNS for  $Q^2 \gg m_H^2$ .
- Define by demanding equivalence of the  $n_f = n$  (FFNS) and  $n_f = n + 1$  (VFNS) flavor descriptions above transition point:

$$\begin{aligned} F_{i}(x,Q^{2}) &= \sum_{k} C_{i,k}^{\mathrm{FF},n}(Q^{2}/m_{H}^{2}) \otimes f_{k}^{n}(Q^{2}) \\ &= \sum_{j} C_{i,j}^{\mathrm{VF},n+1}(Q^{2}/m_{H}^{2}) \otimes f_{j}^{n+1}(Q^{2}) \\ &\equiv \sum_{j,k} C_{i,j}^{\mathrm{VF},n+1}(Q^{2}/m_{H}^{2}) \otimes A_{jk}(Q^{2}/m_{H}^{2}) \otimes f_{k}^{n}(Q^{2}) \end{aligned}$$

$$\Rightarrow \quad C_{i,k}^{\text{FF},n}(Q^2/m_H^2) = \sum_j C_{i,j}^{\text{VF},n+1}(Q^2/m_H^2) \otimes A_{jk}(Q^2/m_H^2)$$

• But  $C_{i,j}^{VF,n_f,(m)}$  only uniquely defined in massless limit  $\Rightarrow$  ambiguous up to  $\mathcal{O}(m_H^2/Q^2)$  terms (can redistribute between orders).

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# Choice of GM-VFNS by MRST/MSTW

- MRST 1998–2004 used the Thorne–Roberts (TR) scheme [hep-ph/9709442]: demand  $\partial F_2^H / \partial \ln Q^2$  continuous.
- PDFs are discontinuous at NNLO in a VFNS [Buza et al. '96]:

$$f_{j/p}^{n_f+1}(x,m_H^2) = f_{j/p}^{n_f}(x,m_H^2) + \alpha_5^2 \sum_k A_{jk}(x) \otimes f_{k/p}^{n_f}(x,m_H^2),$$

but neglected in MRST 2001-2004 NNLO analyses.

- Structure functions at NNLO are then discontinuous in ZM-VFNS, but should be continuous in GM-VFNS. Original TR scheme technically difficult to implement at NNLO.
- Instead, R. Thorne [hep-ph/0601245] redefined simpler GM-VFNS (denoted TR') for use up to NNLO. Adopted elements of "ACOT(χ)" (→ talk by F. Olness):

$$C_{2,HH}^{VF,n_f,(m)}(z,Q^2/m_H^2) = C_{2,HH}^{ZM,n_f,(m)}(z/x_{max})$$





- Maintain continuity at  $Q^2 = m_H^2$  by freezing term with highest power of  $\alpha_S$  for  $Q^2 < m_H^2$  when moving above  $m_H^2$ .
- ACOT-type schemes instead use same order of  $\alpha_S$  for *n* and (n + 1)-flavors, e.g.  $F_2^H = 0$  at LO for  $Q^2 < m_H^2$ .





- Massive  $\mathcal{O}(\alpha_S^3)$  NC coefficient functions unknown, but needed for GM-VFNS at NNLO.
- Model [Thorne '06] using known leading threshold logarithms [Laenen, Moch '99] and leading ln(1/x) terms [Catani, Ciafaloni, Hautmann '91]. Variation in free parameters does not lead to a large change.
- Massive  $\mathcal{O}(\alpha_{S}^{2})$  CC coefficient functions unknown, but needed for GM-VFNS at NLO (important for  $s, \bar{s}$  determination from CCFR/NuTeV  $\nu N \rightarrow \mu^{+}\mu^{-}X$  data).
- Model by modifying O(α<sub>5</sub><sup>2</sup>) NC contributions for different threshold behaviour. More sophisticated modeling in MSTW 2008. No attempt made to model O(α<sub>5</sub><sup>3</sup>) CC contribution needed at NNLO.



## Impact of consistent GM-VFNS at NNLO



## MRST 2006 NNLO [arXiv:0706.0459]

- First implementation of TR' scheme.
- Increase in low-x PDFs when discontinuities included.
- σ<sub>W,Z</sub> at the LHC sensitive to light sea-quark PDFs at x ~ 0.006 (for y = 0) ⇒ σ<sub>W,Z</sub> increase by 6%. A correction, not an *uncertainty*.
- From CTEQ6.1 NLO (ZM-VFNS) to CTEQ6.5 NLO (GM-VFNS): 8% increase in σ<sub>W,Z</sub> at LHC. A correction, not an *uncertainty*.



- Change  $TR \rightarrow TR'$  allows study of scheme dependence at NLO.
- MRST 2004 (TR) and MRST 2006 (TR') fits use same data.



- Nearly 3% increase in σ<sub>W,Z</sub> at the LHC at NLO. Genuine theory uncertainty: should decrease going to higher orders.
- An uncertainty, not a correction at NLO.

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MRST 2001/2002 : approximate NNLO splitting [van Neerven, Vogt '00]. MRST 2004 : exact NNLO splitting [Moch, Vermaseren, Vogt '04]. MRST 2006 : added discontinuities at  $Q^2 = m_H^2$  [Buza *et al.* '96]:

$$f_{j/p}^{n_f+1}(x,m_H^2) = f_{j/p}^{n_f}(x,m_H^2) + \alpha_S^2 \sum_k A_{jk}(x) \otimes f_{k/p}^{n_f}(x,m_H^2),$$

with TR' GM-VFNS for structure functions [Thorne '06]. MSTW 2008 : minor refinements to NNLO evolution code:

- added perturbative NNLO generation of  $q \neq \bar{q}$  (very small).
- improved definition of  $\alpha_s$  (MRST form unconventional).
- evolution checked against public PEGASUS [Vogt '04] and HOPPET [Salam, Rojo '08] codes for fitted input PDFs.

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 Treatment of jet data in MRST/MSTW analyses

## MRST 2001–2006

- Fit six "pseudogluon" points at Q<sup>2</sup> = 2000 GeV<sup>2</sup> inferred from Tevatron Run I inclusive jet data.
- Comparison to actual jet data, calculated at LO with a K-factor, only made *after* the fit.

## **MSTW 2008**

- Fit to Tevatron Run II and HERA DIS inclusive jet data.
- Complete treatment of correlated systematic errors.
- Use FASTNLO code [Kluge, Rabbertz, Wobisch '06] to calculate NLO cross sections exactly during the fit.
- Full NNLO  $\hat{\sigma}_{ab}$  not yet known: include 2-loop threshold corrections [Kidonakis, Owens '00] for Tevatron jet data at NNLO and exclude HERA DIS jet data.





[Data: hep-ex/0701051]

CDF Run II inclusive jet data,  $\chi^2$  = 56 for 76 pts.

 $D \oslash$  Run II inclusive jet data (cone, R = 0.7) MSTW 2008 NLO PDF fit ( $\mu_{R} = \mu_{F} = p_{T}^{\text{JET}}$ ),  $\chi^{2} = 114$  for 110 pts.



[Data: arXiv:0802.2400]





• Run II jet data prefer smaller gluon distribution at high x.



**Highlighted** numbers indicate  $\chi^2$  values for data sets explicitly included in various NLO global fits:

CDFI	DØI	$CDFII(k_T)$	DØII	$\Delta \chi^2_{\rm non-jet}$	$\alpha_{S}(M_{Z}^{2})$
(33 pts.)	(90 pts.)	(76 pts.)	(110 pts.)	(2513 pts.)	
53	119	64	117	0	0.1197
51	48	132	180	9	0.1214
56	110	56	114	2	0.1202
53	85	<b>68</b>	117	1	0.1204

- Fit to Run I jets  $\Rightarrow$  description of Run II jets bad.
- Fit to Run II jets  $\Rightarrow$  description of Run I jets bad.
- Fit neither  $\Rightarrow$  similar description as fitting Run II only.
- **Summary**: Some inconsistency between Run I and Run II jets. Run II jets slightly more consistent with rest of data.





• Smaller high-x gluon than previous MRST and CTEQ fits.





 Data favor less gluon at high x (MSTW 2008 over CTEQ6.6).







- NNLO trend similar to NLO: smaller 2008 gluon at high x, larger 2008 gluon at low x (momentum sum rule).
- $\alpha_S(M_Z^2) = 0.1191 (2006)$  $\rightarrow 0.1171 (MSTW 2008)$



 Higgs cross sections smaller at Tevatron with 2008 PDFs (→ talk by D. de Florian). 
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## Uncertainties in global PDF analysis

## "Theoretical" errors

- *Examples:* input parameterisation form, neglected higher-order and higher-twist QCD corrections, electroweak corrections, choice of cuts, nuclear corrections, heavy flavor treatment.
- Difficult to quantify *a priori*. Often correction only known after an improved treatment/calculation is available.

#### "Experimental" errors

- If all the above sources of "theoretical" errors are fixed, how do we propagate the experimental uncertainties on the fitted data points through to the PDF uncertainties?
- Generally use the Hessian method [Pumplin et al. '01]: diagonalize covariance matrix from the fit and produce ± eigenvector PDF sets displaced from best-fit PDF set.



#### Parameter-fitting criterion

- $T^2 = 1$  for 68% (1- $\sigma$ ) C.L.,  $T^2 = 2.71$  for 90% C.L.
- In practice: minor inconsistencies between fitted data sets, and unknown experimental and theoretical uncertainties, so not appropriate for global PDF analysis.

#### Hypothesis-testing criterion (proposed by CTEQ)

- Much weaker: treat PDF sets obtained from eigenvectors of covariance matrix as alternative hypotheses.
- Determine  $T^2$  from the criterion that each data set should be described within its 90% C.L. limit. Very roughly, a "good" fit has  $\chi^2 \simeq N_{\rm pts.} \pm \sqrt{2N_{\rm pts.}}$  for each data set.
- CTEQ:  $T^2 = 100$  for 90% C.L. limit, MRST:  $T^2 = 50$ .

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- Tolerance in "+" direction provided by E866/NuSea pp DY data.
- Tolerance in "-" direction provided by NuTeV  $\nu N xF_3$  data.



#### MSTW 2008 NLO PDF fit



**Eigenvector number** 





- Fit to reduced dataset comprising 589 DIS data points, cf. 2699 data points in global fit.
- Errors given by T<sup>2</sup> = 1 don't overlap ⇒ inconsistent data sets included in global fit.
- Dynamic tolerance  $T^2 > 1$ accommodates mildly inconsistent data sets.



## Uncertainties on $\alpha_S$ in global PDF analysis

#### [MSTW, in preparation]

- PDFs (including uncertainty sets) are determined for a fixed value of α<sub>S</sub> ⇒ use same value in cross section calculations.
- In MRST/MSTW analyses, α<sub>S</sub> is fitted, then **fixed** at the best-fit value for final error propagation.

## Problems:

- **1** What is the (experimental) error on  $\alpha_s$ ?
- 2 How to include this error in cross section calculations?

## Solutions:

- **1** Apply same method used to determine the tolerance for each eigenvector to determine the experimental error on  $\alpha_S(M_Z^2)$ .
- 2 Then generate best-fit and eigenvector PDF sets for different fixed  $\alpha_S$  values for use in calculations of cross sections.



• Lower limit on  $\alpha_s(M_Z^2)$  provided by SLAC  $F_2^{ed}$  data.



- Additional theory uncertainty ( $\sim |\rm NNLO-NLO|=\pm 0.003).$
- cf. PDG world average value of  $\alpha_S(M_Z^2) = 0.1176 \pm 0.002$ .





- Correlation at low x, anticorrelation at high x.
- PDF uncertainties smaller when  $\alpha_S$  shifted to limits.



• Two effects: (i) correlation of quark distributions with  $\alpha_S$  at LHC (less correlation at Tevatron), (ii) higher-order corrections.

Parton distribution functions and  $\alpha_S$ 





- Anticorrelation at low x: HERA ∂F<sub>2</sub>/∂ ln Q<sup>2</sup> ~ α<sub>5</sub> g.
- Correlation at high x to maintain momentum sum rule.







 Anticorrelation of gg luminosity with α<sub>S</sub> at LHC cancels out (almost exactly) correlation due to higher-order corrections.



6

4 2

0

-2 -4 -6

-8

-10<sup>l</sup>

100

68% C.L. uncertainties

150

200

250

M<sub>u</sub> (GeV)

300

PDF +  $\alpha_{s}$ 

• Enhanced "PDF+ $\alpha_{s}$ " uncertainty compared to "PDF only" uncertainty, particularly at the LHC.

6

2 0

-2

-6

-8

-10<sup>L</sup>

100

150

200

250

M<sub>L</sub> (GeV)

300





- Mostly gluon-initiated at low  $p_T \Rightarrow$  correlated with  $\alpha_S$ .
- Mostly quark-initiated at high  $p_T \Rightarrow$  anticorrelated with  $\alpha_S$ .

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Summary	<i>'</i>				

- MSTW 2008 (LO, NLO, NNLO) PDF fits [arXiv:0901.0002] are the most comprehensive to date: supersede MRST sets.
- Pre-2006 MRST *NNLO* PDF sets should be considered obsolete due to incomplete heavy flavor treatment.
- Almost all necessary NNLO processes are now known. Exceptions: inclusive jets, massive  $\mathcal{O}(\alpha_5^3)$  NC and  $\mathcal{O}(\alpha_5^2)$  CC DIS.
- **Tevatron Run II jets** prefer smaller high-x gluon than Run I: impact on Higgs cross sections at Tevatron.
- **Improved** "dynamic tolerance" controlling propagation of experimental errors through to PDF uncertainties.
- Now possible to consistently calculate combined "PDF+α<sub>S</sub>" uncertainty on cross sections: additional sets public soon.

#### Backup •00000

# Comparison to CTEQ6.6 NLO



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# Comparison to MRST 2006 NNLO



# Alternative approach: NNPDF Collaboration

**NNPDF Collaboration:** R. Ball, L. Del Debbio, S. Forte, A. Guffanti, J. Latorre, A. Piccione, J. Rojo, M. Ubiali

#### MSTW approach [arXiv:0901.0002]

Parametrization Minimisation Error propagation Application  $xf_{a/p} \sim A_a x^{\Delta_a}(1-x)^{\eta_a}(1+\epsilon_a\sqrt{x}+\gamma_a x)$ Non-linear least-squares (Marquardt method) Hessian method with dynamical tolerance Use best-fit and 40 eigenvector PDF sets

#### NNPDF approach [arXiv:0808.1231]

Parametrization Minimisation Error propagation Application Neural network (37 free parameters per PDF) Genetic algorithm (stop before overlearning) Generate  $N_{\rm rep} \sim O(1000)$  MC data replicas Calculate average and s.d. over  $N_{\rm rep}$  PDF sets

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# First results from NNPDF1.0 [arXiv:0808.1231]

- Fit restricted set of only DIS structure function data (SLAC, BCDMS, NMC, H1, ZEUS, CHORUS).
- Inadequate treatment of heavy quarks (ZM-VFNS).



• Up valence: relative data set normalizations fitted by MSTW.

• Up antiquark: NNPDF1.0 negative by  $\sim$  2- $\sigma$ , no Drell–Yan.

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## Uncertainties for MSTW 2008 and NNPDF1.0



• NNPDF1.0 has fixed  $s = \overline{s} = (\overline{u} + \overline{d})/4$  at  $Q_0^2 = 2 \text{ GeV}^2$ .

- NNPDF1.1 [arXiv:0811.2288]: free strangeness but no νN dimuon data to constrain, so huge PDF uncertainties.
- Conclusion: NNPDF approach looks promising, but PDFs not yet directly comparable to those from standard approach.

## Backup

## Parametrization dependence of low-x gluon

- PDFs lose probabilistic interpretation beyond LO.
- Negative small-x gluon distribution preferred at low scales.
- MRST/MSTW parametrize as:

$$\begin{aligned} xg(x, Q_0^2) &= xg_1(x, Q_0^2) + xg_2(x, Q_0^2) \sim A_g \, x^{\delta_g} + A_{g'} \, x^{\delta_{g'}} \\ \Rightarrow \Delta g(x, Q_0^2) \sim \pm g_1(x, Q_0^2) \, \Delta \delta_g \, \ln(1/x) \pm g_2(x, Q_0^2) \, \Delta \delta_{g'} \, \ln(1/x) \end{aligned}$$



• Other groups (CTEQ, Alekhin) parametrize with a valence-like  $xg(x, Q_0^2) \sim x^{\delta_g}$ : less freedom at small x.