Higher-order evolution of parton distributions

Andreas Vogt

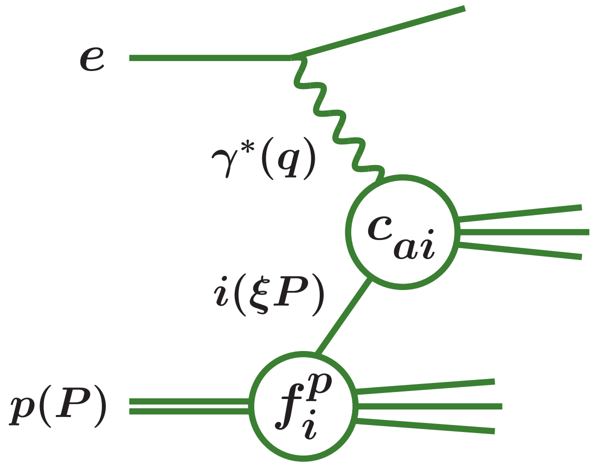
(University of Liverpool)

- DIS in pert. QCD, running α_s and partons, mass factorization
- Higher orders in the evolution equations, large-x/small-x limits
- Evolution in theory, emphasizing the symbolic N-space solution
- Evolution in practice: codes, benchmarks and a demonstration

Refs: hep-ph/0407321 (DIS 04), arXiv:0707.4106 (DIS 07), hep-ph/0408244 (Pegasus)

Parton densities and hard processes in pQCD

Example: inclusive photon-exchange deep-inelastic scattering (DIS)



Hard scale, Bjorken variable x

$$Q^2 = -q^2$$

$$x = Q^2/(2P\cdot q)$$

Order α_s^0, $m = 0$ quarks: $x = \xi$

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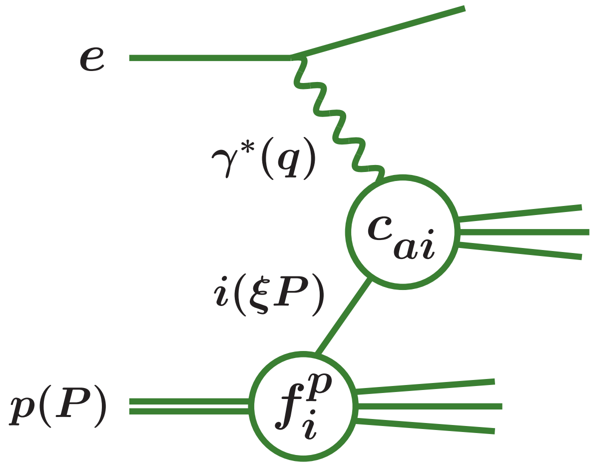

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Structure functions $F_{2,L}$ (at leading twist of operator-product exp.)

$$x^{-1} F_a^p(x, Q^2) = \sum_i \int_x^1 \frac{d\xi}{\xi}\, c_{a,i}\left(\frac{x}{\xi}, \alpha_s(\mu^2), \frac{\mu^2}{Q^2}\right) f_i^p(\xi, \mu^2)$$

Coefficient functions: scheme, scale $\mu = \mathcal{O}(Q)$, Mellin convolutions

$1/Q^2$ corrections ('higher twists'): extract or suppress by data cuts

Parton densities and hard processes in pQCD

Parton distributions f_i : renormalization-group evolution equations

$$\frac{d}{d\ln\mu^2} f_i(\xi,\mu^2) = \sum_k \left[P_{ik}(\alpha_s(\mu^2)) \otimes f_k(\mu^2)\right](\xi)$$

$\otimes$ **= Mellin convolution. Initial conditions incalculable in pert. QCD**

$\Rightarrow$ **predictions: fits of suitable reference processes, universality**

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Expansions in α_s: splitting functions P, coefficient functions c_a

$$P = \alpha_s P^{(0)} + \alpha_s^2 P^{(1)} + \alpha_s^3 P^{(2)} + \ldots$$

$$c_a = \underbrace{\alpha_s^{n_a}\Big[c_a^{(0)}}\, + \alpha_s c_a^{(1)} + \alpha_s^2 c_a^{(2)} + \ldots\Big]$$

LO: approximate shape, rough estimate of rate

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NLO: first real prediction of size of cross sections

NNLO, $P^{(2)}$, $c_a^{(2)}$: first serious error estimate $\Leftrightarrow$ precision physics

The running coupling in perturbative QCD

$$d\alpha_s / d \ln \mu^2 = -\beta_0 \, \alpha_s^2 - \beta_1 \, \alpha_s^3 - \beta_2 \, \alpha_s^4 - \beta_3 \, \alpha_s^5 - \ldots \qquad (*)$$

N^{3}LO coefficient β_3 : van Ritbergen, Vermaseren, Larin (97); Czakon (04)

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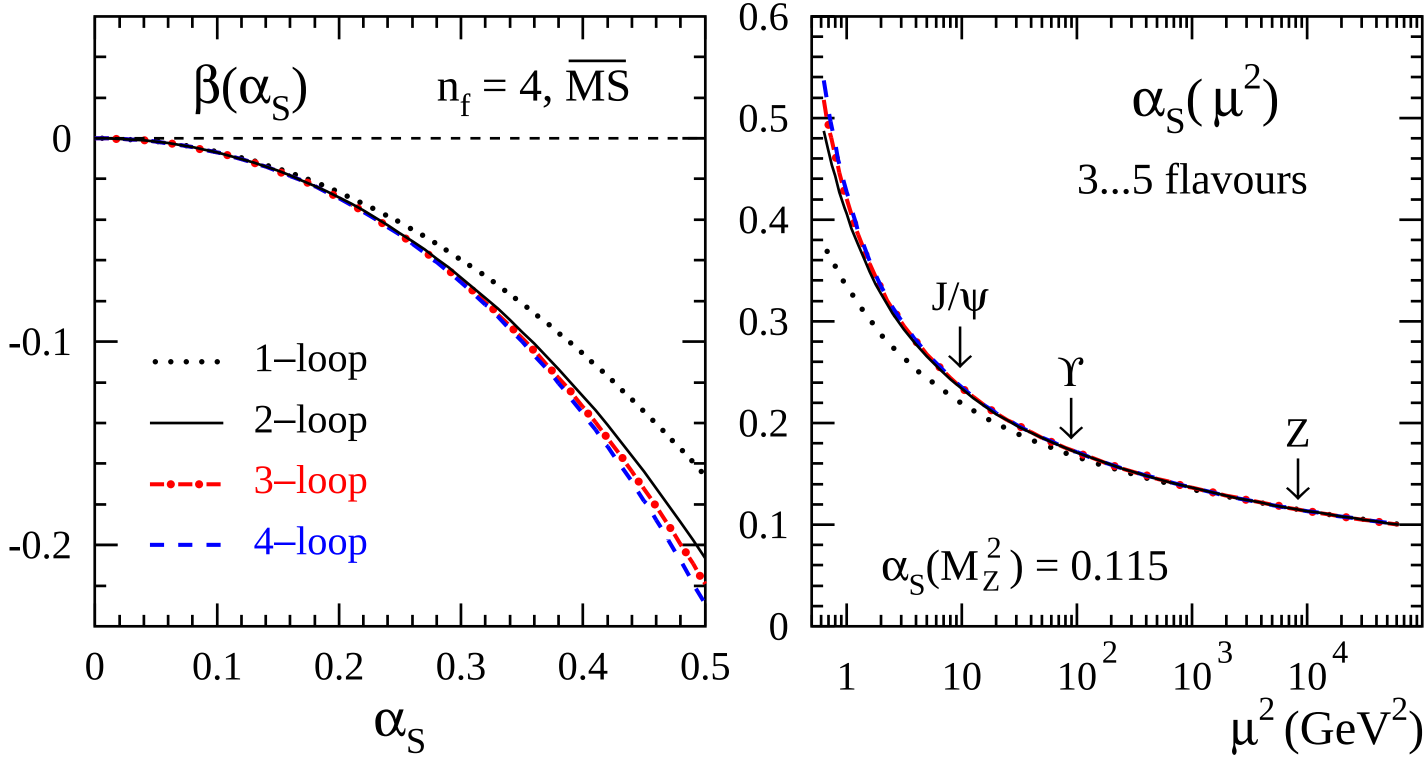


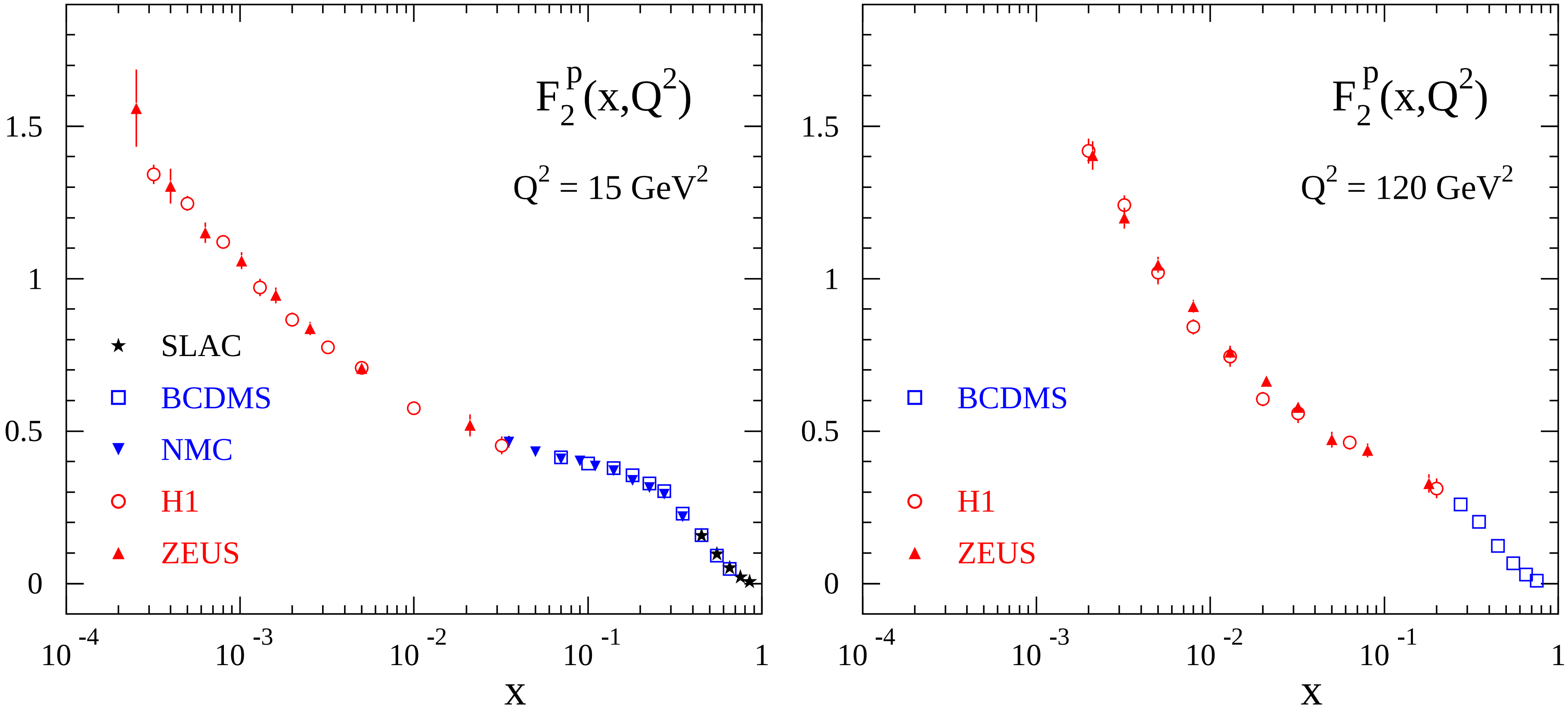
Perturbatively stable at $Q^2 > 1$ GeV^2. Boundary condition: exp. (+ lattice)

$(*)$ No (explicit) exact sol'n except LO. Use, e.g., 4$^{\text{th}}$-order Runge-Kutta (not PDG exp.)

From structure functions to parton densities

Exp.: SLAC (e, 30 GeV), CERN (μ, 300 GeV), DESY ($e^{\pm}$, 30$\times$800 GeV)

Selected data on the proton structure function F_2



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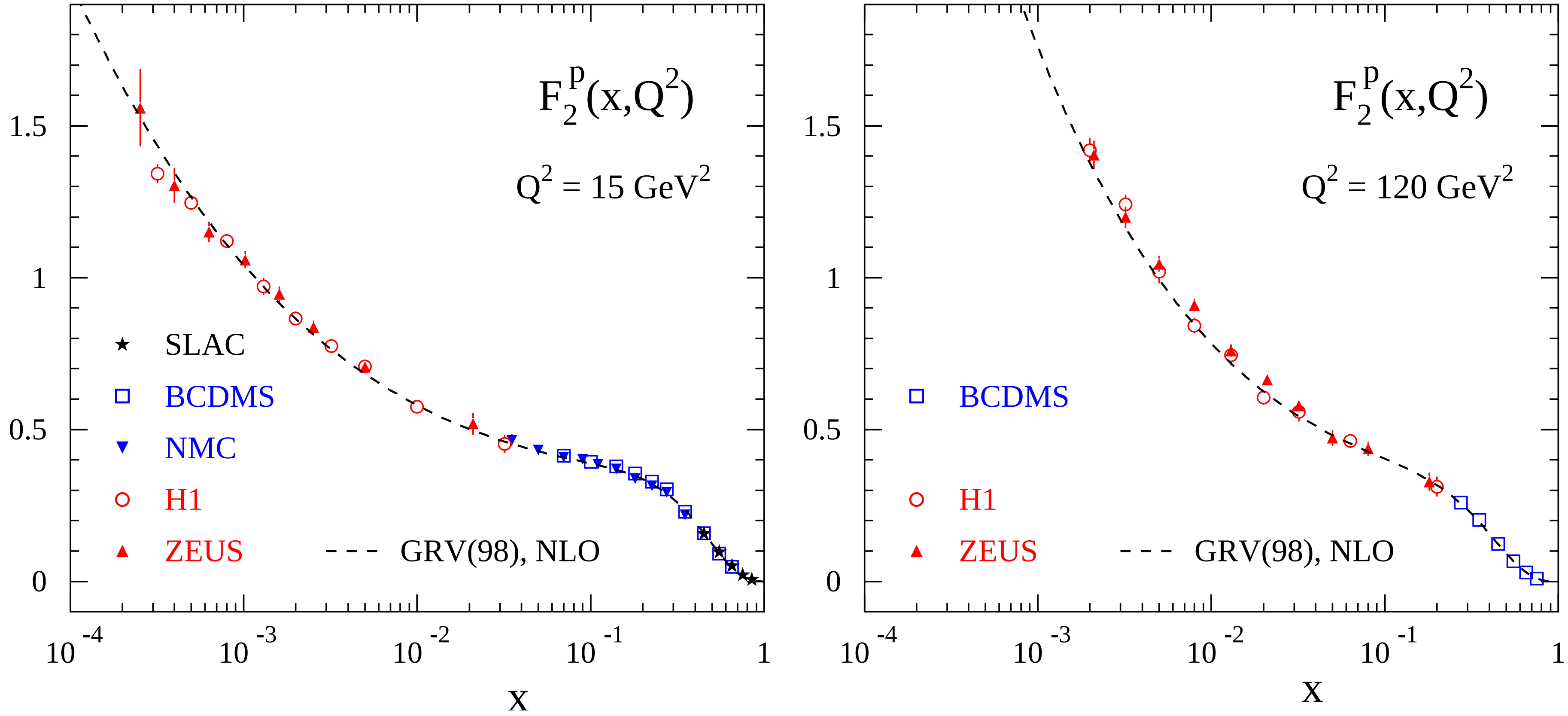
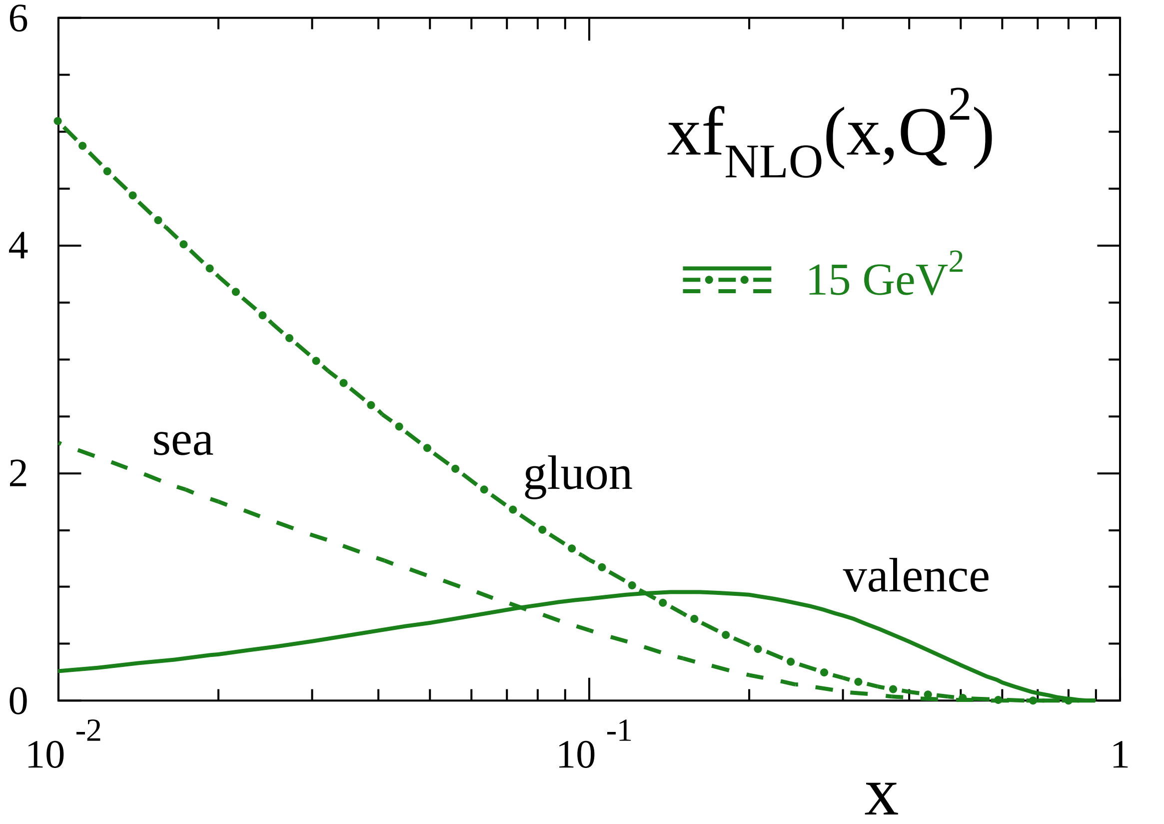


F_2 $\longrightarrow$ quark distributions, scale dependence $\longrightarrow$ gluon distribution

The proton's parton densities, qualitatively

Valence: $q - \bar{q}$ $\leftrightarrow$ additive quantum numbers. Quark sea: $q = \bar{q}$ parts

Large x ($\stackrel{\text{now}}{\equiv} \xi$): valence $\gg$ glue $\gg$ sea. Small x: glue $>$ sea $\gg$ valence



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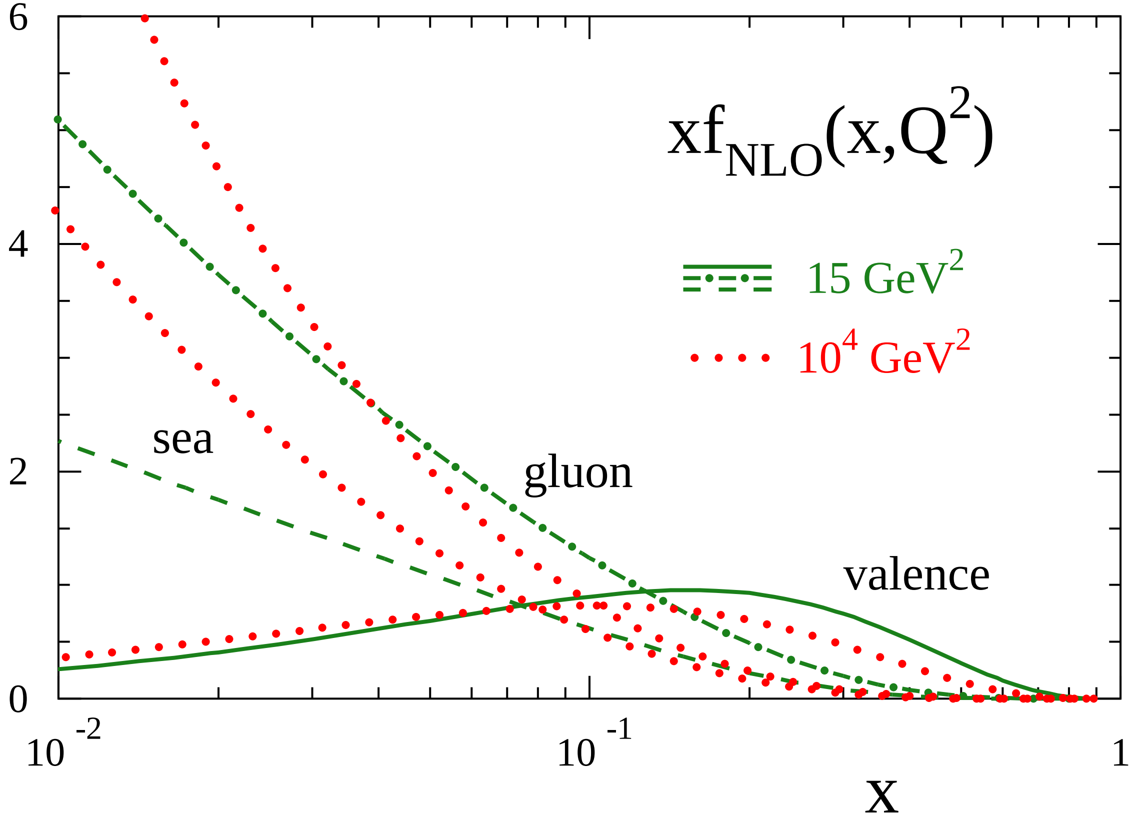
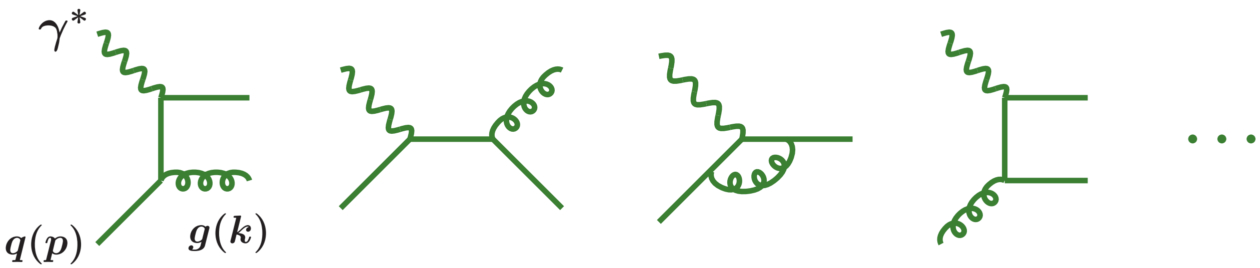


HERA $\longrightarrow$ LHC: need evolution from few GeV to TeV scales, and momentum fractions down to at least $x \simeq 10^{-4}$ (for particles with $M \simeq$ 100 GeV)

From mass singularities to splitting functions

First-order DIS:
(inclusive, $\int d^4k$)



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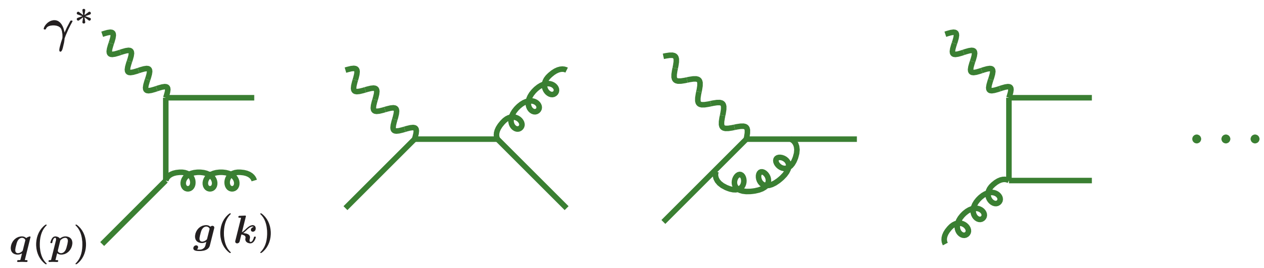

Emissions collinear to the incoming partons ($m_{\mathrm{q,g}} = 0$): denominators

$$(p-k)^2 \ = \ -2|\vec{p}\,||\vec{k}|(1-\cos\vartheta) \ \xrightarrow{\vartheta\to 0} \ -|\vec{p}\,||\vec{k}|\,\vartheta^2 \quad \stackrel{\int d\vartheta}{\Rightarrow} \quad \text{mass singularities}$$

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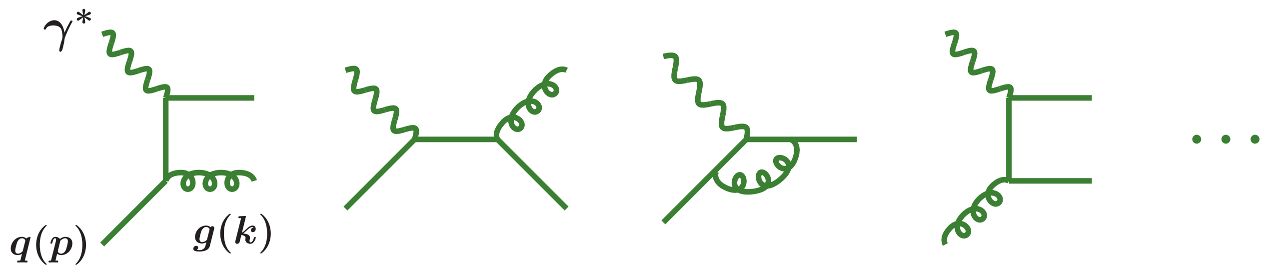

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Regularization (dim. $= 4-2\varepsilon$, singularities $\sim 1/\varepsilon$) and mass factorization

$$F_a(Q^2) \;=\; \hat{F}_{a,k}(\alpha_s(Q^2),\varepsilon) \otimes \hat{f}_k \;=\; C_{a,i}(\alpha_s(Q^2)) \otimes \Gamma_{ik}(\alpha_s(Q^2),\varepsilon) \otimes \hat{f}_k$$

$C_{a,i}$: **coefficient functions of observable a**

Γ_{ik} : **universal $1/\varepsilon$ - poles + . . . (fact. scheme). Usual: $\overline{\text{MS}}$**

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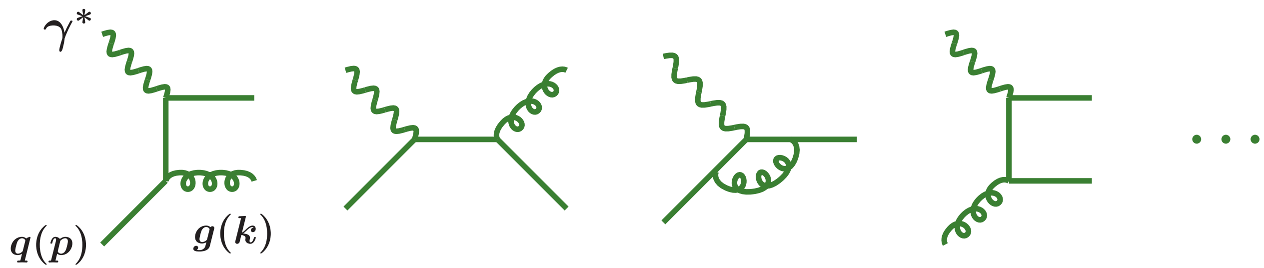

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Renormalized parton distributions f_i : splitting functions P_{ij}

$$\frac{\partial}{\partial\ln Q^2}\,f_i \;=\; \frac{\partial\,\Gamma_{ik}}{\partial\ln Q^2}\otimes\hat{f}_k \;=\; \frac{\partial\,\Gamma_{ik}}{\partial\ln Q^2}\otimes\Gamma^{-1}_{kj}\otimes f_j \;\equiv\; P_{ij}\otimes f_j$$

The general evolution equations

Previous page: 'simplified version for the general public'. $\varepsilon^{n>0}$ parts, scales

Q^2: physical hard scale(s)

$\mu_{\rm r}^2$: renormalization scale, argument of $\alpha_{\rm s}$

$\mu_{\rm f}^2\ (= \mu^2)$: mass factorization scale, argument of parton densities

Coefficient functions: Q^2, $\mu_{\rm r}^2$, $\mu_{\rm f}^2$. PDFs, splitting functions: $\mu_{\rm r}^2$, $\mu_{\rm f}^2$

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Evolution for $\mu_{\rm r} \neq \mu_{\rm f}$: Taylor-expand $\alpha_{\rm s}(\mu_{\rm r}^2)$ around $\mu_{\rm f}^2$, sort in $\alpha_{\rm s}(\mu_{\rm f}^2)$

$$
\begin{aligned}
P(x, \mu, \mu_r) \;&=\; a_{\rm s}(\mu_r^2)\, P^{(0)}(x) \\
&\quad + a_{\rm s}^2(\mu_r^2) \left(P^{(1)}(x) - \beta_0 P^{(0)}(x) L \right) \\
&\quad + a_{\rm s}^3(\mu_r^2) \left(P^{(2)}(x) - 2\beta_0 L\, P^{(1)}(x) - \left\{ \beta_1 L - \beta_0^2 L^2 \right\} P^{(0)}(x) \right)
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with $a_{\rm s} \equiv \frac{\alpha_{\rm s}}{4\pi}$, $L \equiv \ln(\mu^2/\mu_r^2)$. Assume fixed L: $\mu_{\rm r} \neq \mu$ no complication

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Note: no such restriction on μ/Q, e.g., $\mu^2 = Q^2 + 4m_c^2$ possible for $F_2^{c\bar{c}}$

Flavour decomposition of the evolution (I)

Quark-gluon and gluon-quark splitting functions: (anti-)flavour independent

$$P_{\mathrm{gq}} \equiv P_{\mathrm{gq}_i} = P_{\mathrm{g}\bar{\mathrm{q}}_i} \;, \qquad P_{\mathrm{qg}} \equiv 2n_f P_{\mathrm{q}_i\mathrm{g}} = 2n_f P_{\bar{\mathrm{q}}_i\mathrm{g}}$$

$\Rightarrow$ **quark-(anti-)quark differences** $q_i - q_k$ **and** $q_i - \bar{q}_k$ **decouple from** g

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General structure of the (anti-)quark (anti-)quark splitting functions

$$P_{\mathrm{q}_i\mathrm{q}_k} = P_{\bar{\mathrm{q}}_i\bar{\mathrm{q}}_k} = \delta_{ik} P^{\mathrm{v}}_{\mathrm{qq}} + P^{\mathrm{s}}_{\mathrm{qq}}$$
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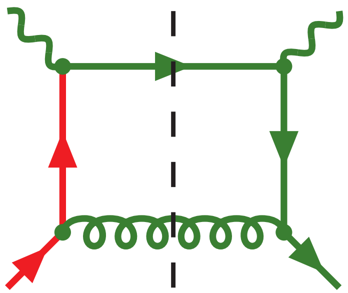
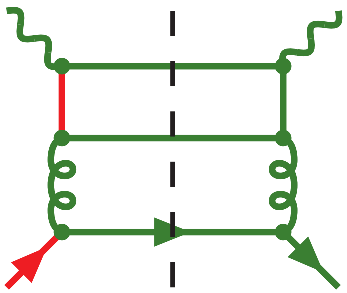


$P^{\mathrm{v}}_{\mathrm{qq}} = \mathcal{O}(\alpha_{\mathrm{s}})$



$P^{\mathrm{s}}_{\mathrm{qq}},\, P^{\mathrm{s}}_{\mathrm{q\bar{q}}} \;:\; \alpha_{\mathrm{s}}^2$

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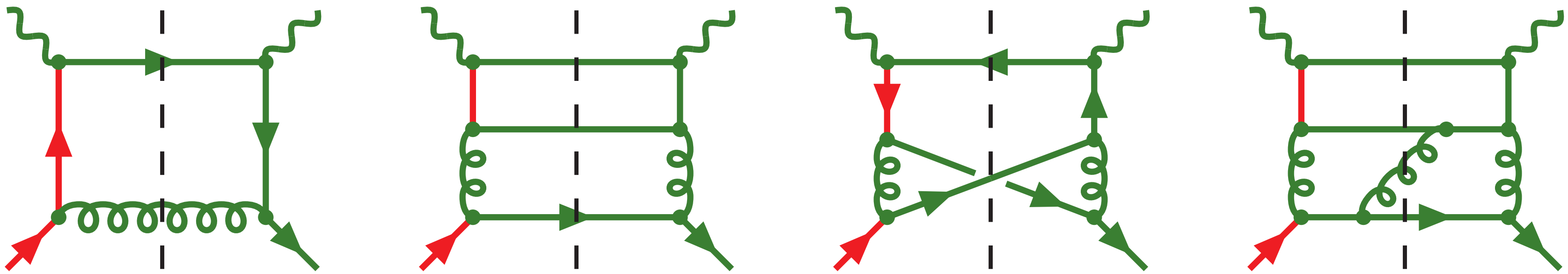

$P^{\rm v}_{\rm qq} = \mathcal{O}(\alpha_{\rm s})$ $\qquad$ $P^{\rm s}_{\rm qq},\, P^{\rm s}_{\rm q\bar{q}} \, : \, \alpha_{\rm s}^2$ $\qquad$ $P^{\rm v}_{\rm q\bar{q}} \, : \, \alpha_{\rm s}^2$ $\qquad$ $P^{\rm s}_{\rm q\bar{q}} \neq P^{\rm s}_{\rm qq} \, : \, \alpha_{\rm s}^3$

$\Rightarrow$ **three types of independent difference (non-singlet, ns) combinations:**

Flavour decomposition of the evolution (II)

$2(n_f - 1)$ **flavour asymmetries of** $q_i \pm \bar{q}_i$ **+ one total valence distribution**

$$q^{\pm}_{\mathrm{ns},ik} = q_i \pm \bar{q}_i - (q_k \pm \bar{q}_k) \ , \quad q^{\mathrm{v}}_{\mathrm{ns}} = \sum_{r=1}^{n_f} (q_r - \bar{q}_r)$$

with

$$P^{\pm}_{\mathrm{ns}} = P^{\mathrm{v}}_{\mathrm{qq}} \pm P^{\mathrm{v}}_{\mathrm{q\bar{q}}}$$

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Flavour-singlet quark distribution q_{s} **[or** Σ **(older)]: maximal coupling to** g

$$q_{\mathrm{s}} = \sum_{r=1}^{n_f} (q_r + \bar{q}_r) \ , \quad \frac{d}{d \ln \mu^2} \begin{pmatrix} q_{\mathrm{s}} \\ g \end{pmatrix} = \begin{pmatrix} P_{\mathrm{qq}} & P_{\mathrm{qg}} \\ P_{\mathrm{gq}} & P_{\mathrm{gg}} \end{pmatrix} \otimes \begin{pmatrix} q_{\mathrm{s}} \\ g \end{pmatrix}$$

with (ps = 'pure singlet')

$$P_{\mathrm{qq}} = P^{+}_{\mathrm{ns}} + n_f (P^{\mathrm{s}}_{\mathrm{qq}} + P^{\mathrm{s}}_{\mathrm{\bar{q}q}}) \equiv P^{+}_{\mathrm{ns}} + P_{\mathrm{ps}}$$

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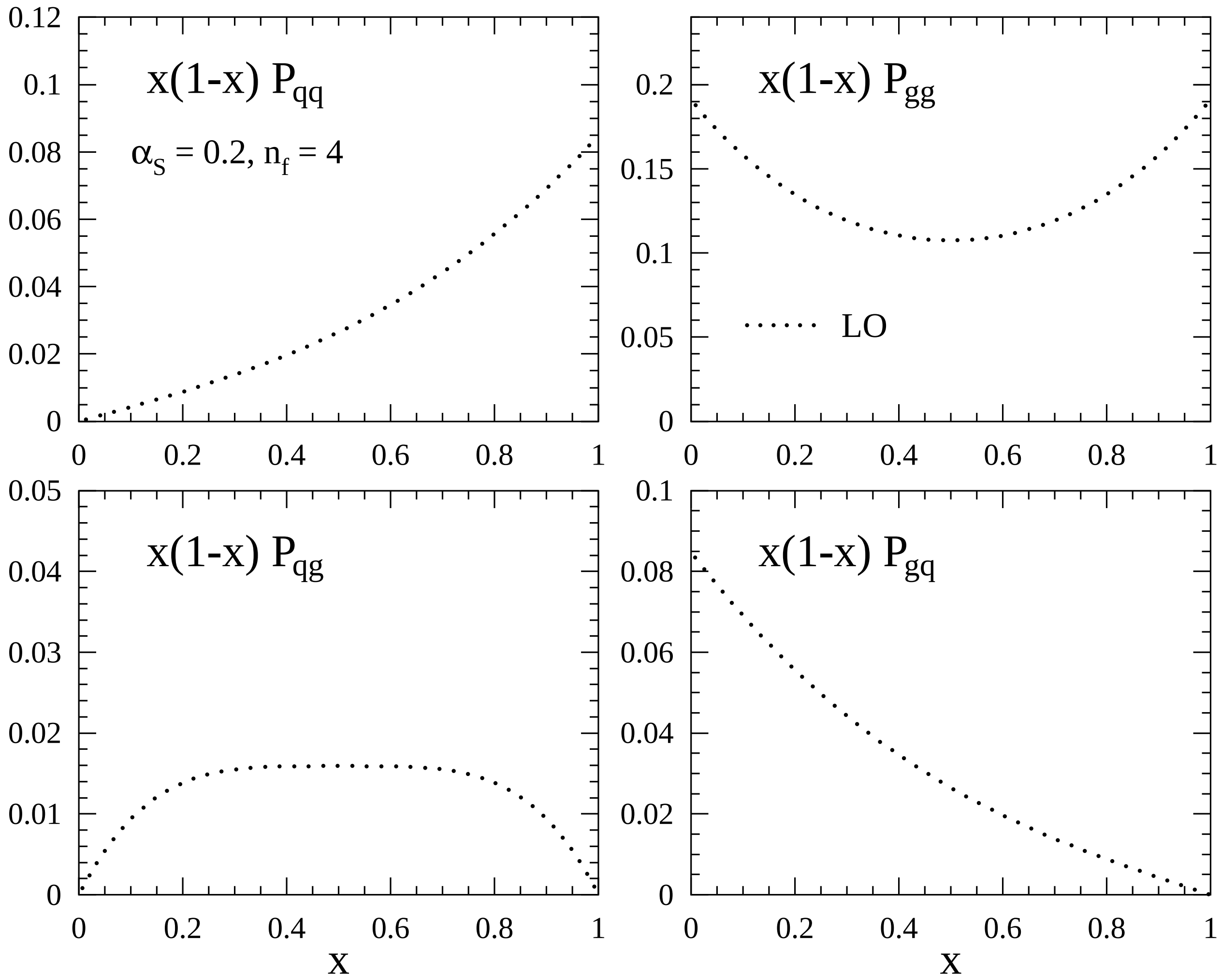
$$P_{\mathrm{qq}} \;=\; P^{+}_{\mathrm{ns}} + n_f (P^{\mathrm{s}}_{\mathrm{qq}} + P^{\mathrm{s}}_{\mathrm{\bar{q}q}}) \;\equiv\; P^{+}_{\mathrm{ns}} + P_{\mathrm{ps}}$$

Evolution: transform quark input to ‘evolution basis’ of q_{s}, $q^{\mathrm{v}}_{\mathrm{ns}}$ and, e.g.,

$$v^{\pm}_l \;=\; \sum_{i=1}^{k} (q_i \pm \bar{q}_i) - k(q_k \pm \bar{q}_k)\,, \quad k = 2, \ldots, n_f\;, \; l \equiv k^2 - 1\;,$$

evolve non-singlet / singlet, and transform back to, say, $u \pm \bar{u}$, $d \pm \bar{d}$ etc

Singlet splitting functions $P(x < 1)$ to NNLO



Note: Plotted information incomplete for (math.) distributions P_{qq} and P_{gg}

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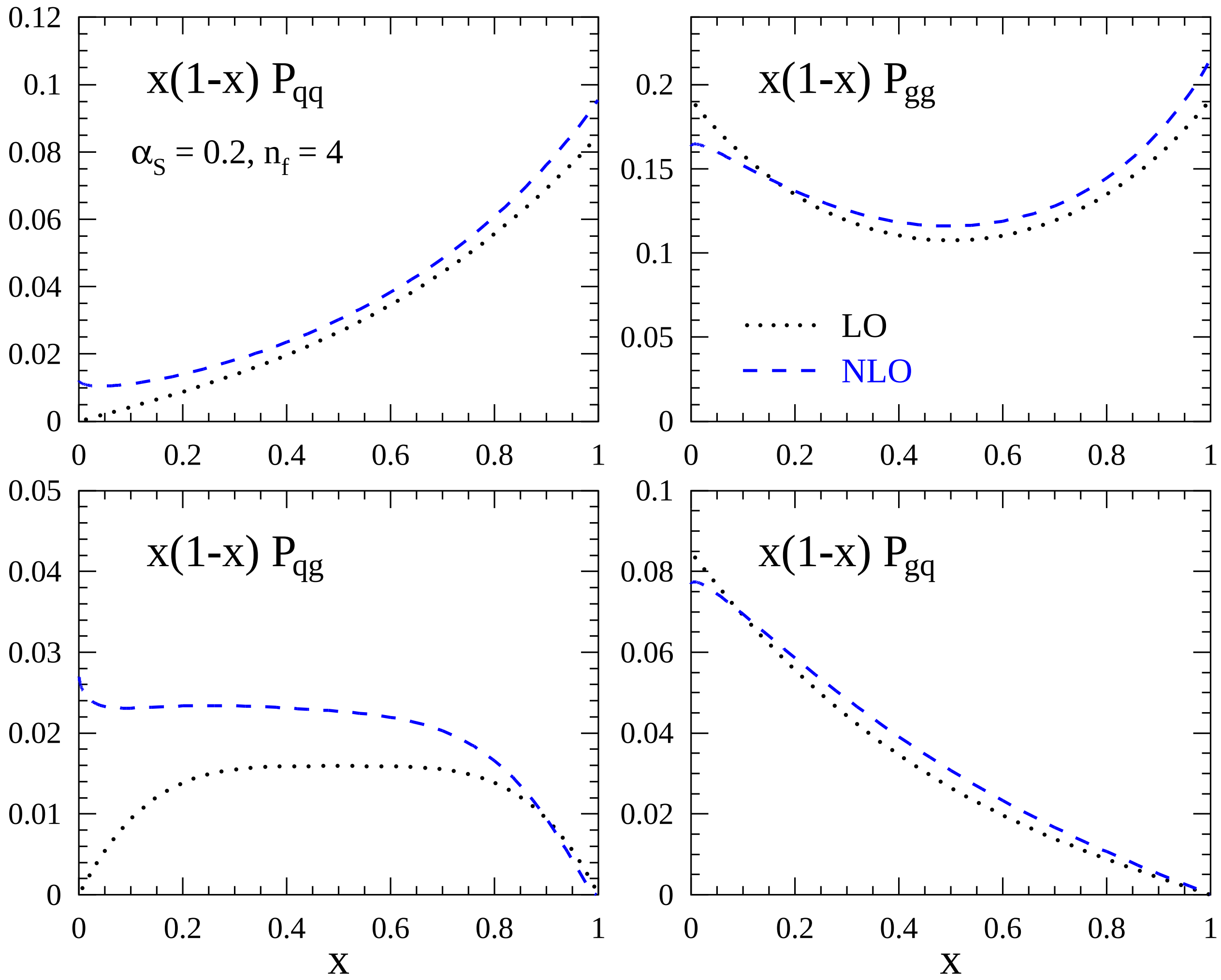

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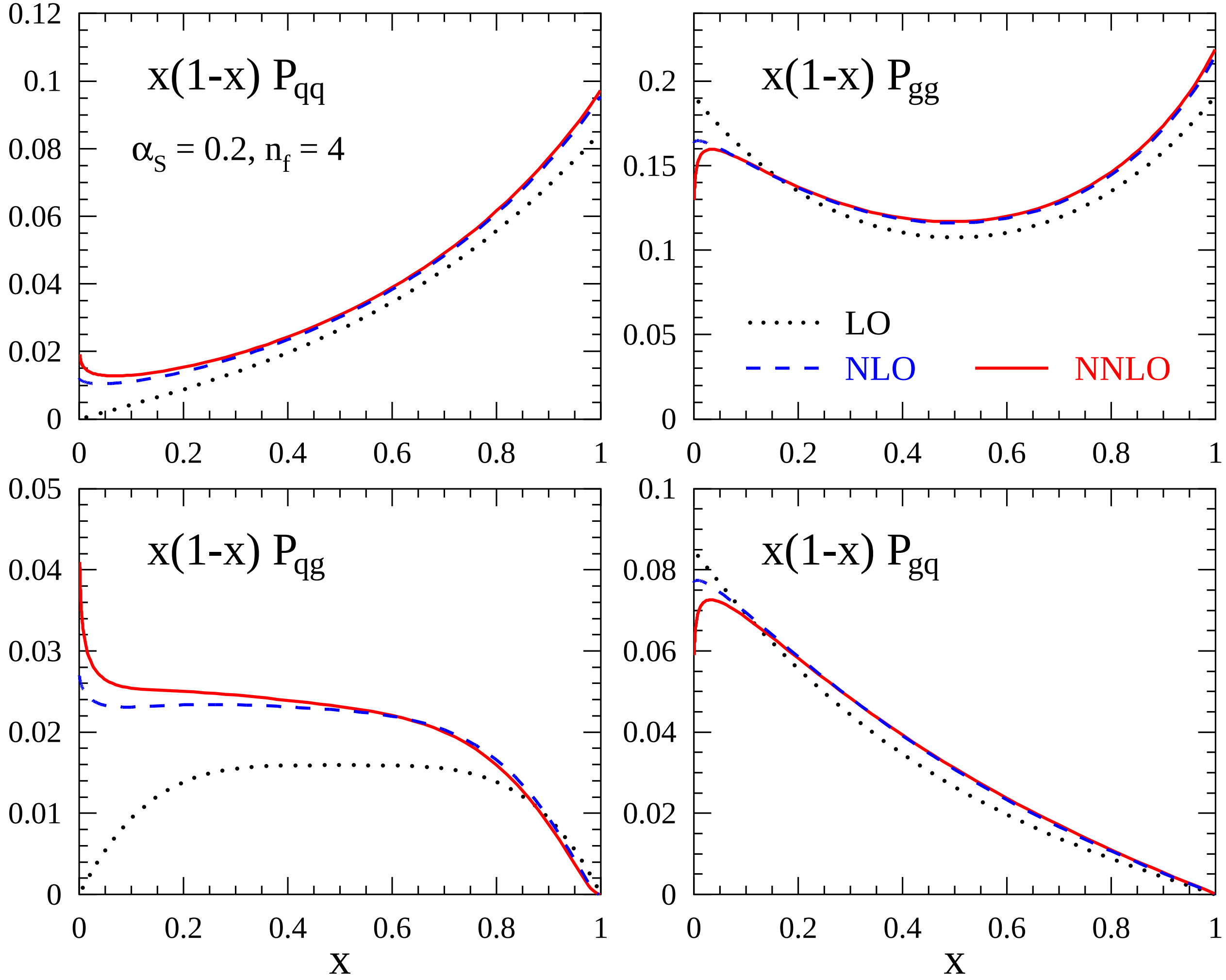

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Stability of the perturbative expansion an issue only at small values of x

Large-x behaviour of the splitting functions

Diagonal entries: form stable in $\overline{\text{MS}}$ to (at least) three loops

$$P^{(n)}_{\mathrm{aa},\,x\to 1}(x) \;=\; \frac{A_n^{\mathrm{a}}}{(1-x)_+} \;+\; \widetilde{B}_n^{\mathrm{a}}\,\delta(1-x) \;+\; C_n^{\mathrm{a}}\;\ln(1-x) \;+\; \mathcal{O}(1)$$

All orders: Korchemsky (89) for +-distribution and $\delta(1-x)$, with $qq/gg = C_F/C_A$

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Leading coefficients A_n^{a} $\Leftrightarrow$ universal 'cusp anomalous dimension'

$$A_3^{\mathrm{q}} \;=\; 16\,C_F C_A^2 \left[\frac{245}{24} - \frac{67}{9}\,\zeta_2 + \frac{11}{6}\,\zeta_3 + \frac{11}{5}\,\zeta_2^2\right] \;-\; 16\,C_F n_f^2 \left[\frac{1}{27}\right]$$
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Gracey (94) [n_f^2]; C.Berger (02), MVV (02) [n_f]; MVV (04); Bern, Dixon, Smirnov (05) [ζ_2^2]

Large-x behaviour of the splitting functions

Diagonal entries: form stable in $\overline{\text{MS}}$ to (at least) three loops

$$P^{(n)}_{\mathrm{aa},x\to 1}(x) \;=\; \frac{A_n^{\mathrm{a}}}{(1-x)_+} \;+\; \widetilde{B}_n^{\mathrm{a}}\,\delta(1-x) \;+\; C_n^{\mathrm{a}}\;\ln(1-x) \;+\; \mathcal{O}(1)$$

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$$A_{\mathrm{q}}(\alpha_{\mathrm{s}}, n_f = 4) \;\cong\; 0.424\,\alpha_{\mathrm{s}}\left(1 + 0.638\,\alpha_{\mathrm{s}} + 0.510\,\alpha_{\mathrm{s}}^2 + \{\,0.4_{\,\mathrm{Pade}}\;\alpha_{\mathrm{s}}^3 + \}\;\ldots\right)$$

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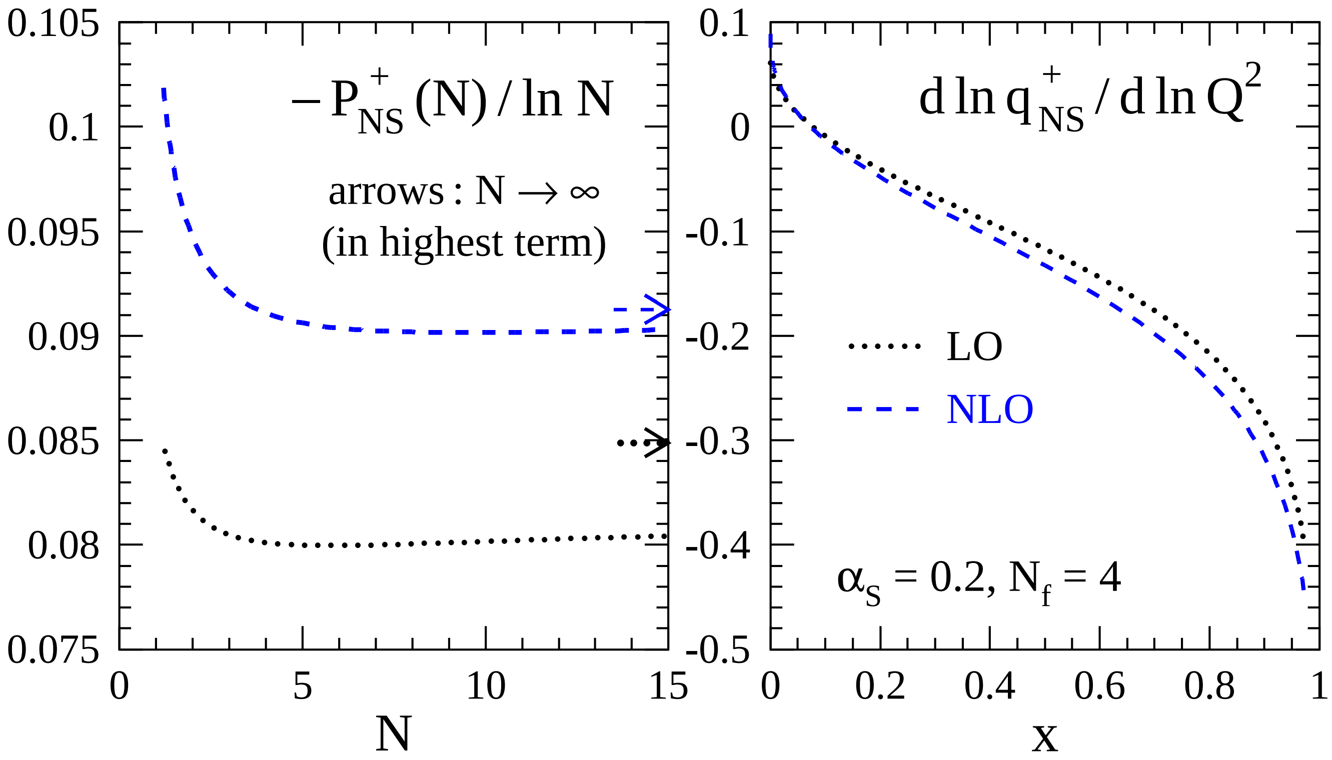
Subleading C_3^{a} : surprising relation, suggesting a general structure

$$C_1^{\mathrm{a}} = 0\,, \quad C_2^{\mathrm{a}} = (A_1^{\mathrm{a}})^2\,, \quad C_3^{\mathrm{a}} = 2\,A_1^{\mathrm{a}}\,A_2^{\mathrm{a}}$$

Taken up, extended: Dokshitzer, Marchesini, Salam (05); Basso, Korchemsky (06); . . .

$\overline{\text{MS}}$ non-singlet evolution at large N / large x

Moments: $A^N = \int_0^1 dx\, x^{N-1} A(x)\,, \quad (1-x)_+^{-1} \leftrightarrow \ln N + \gamma_e + \mathcal{O}(1/N)$



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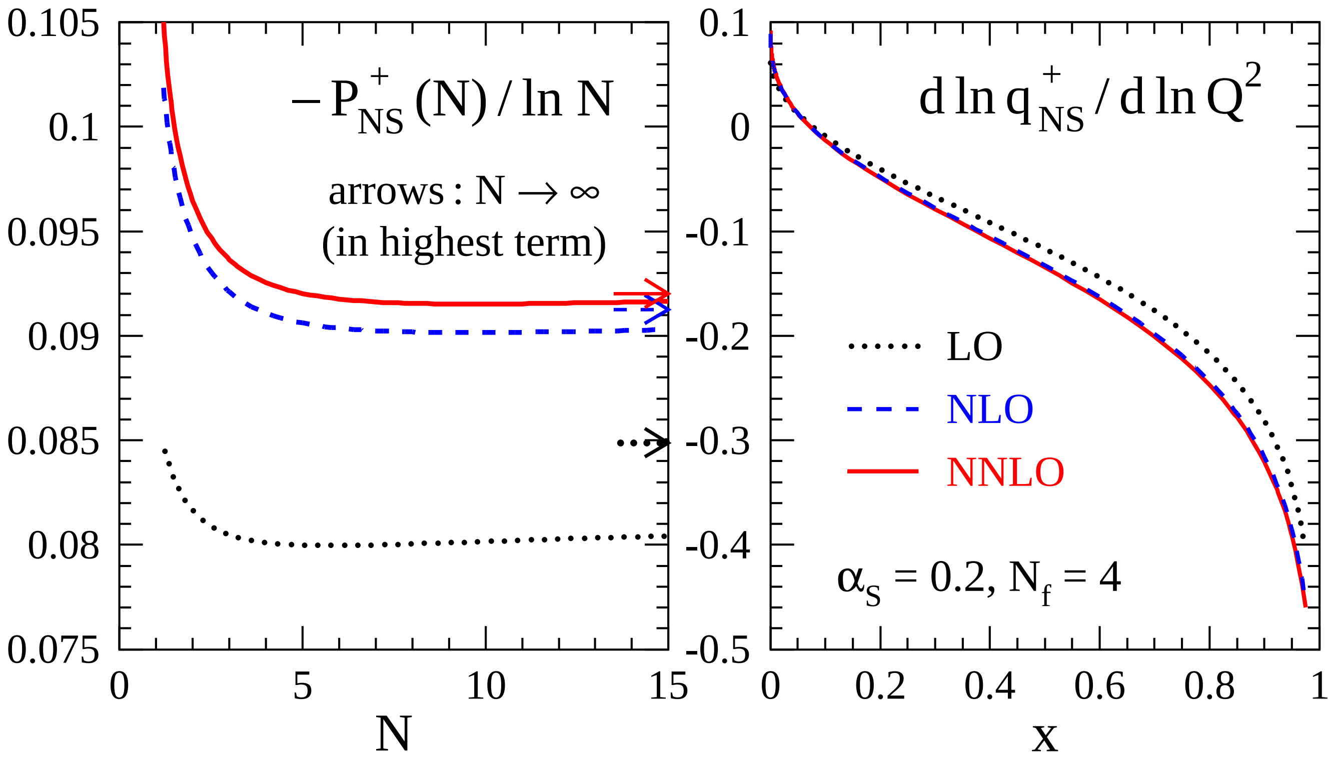

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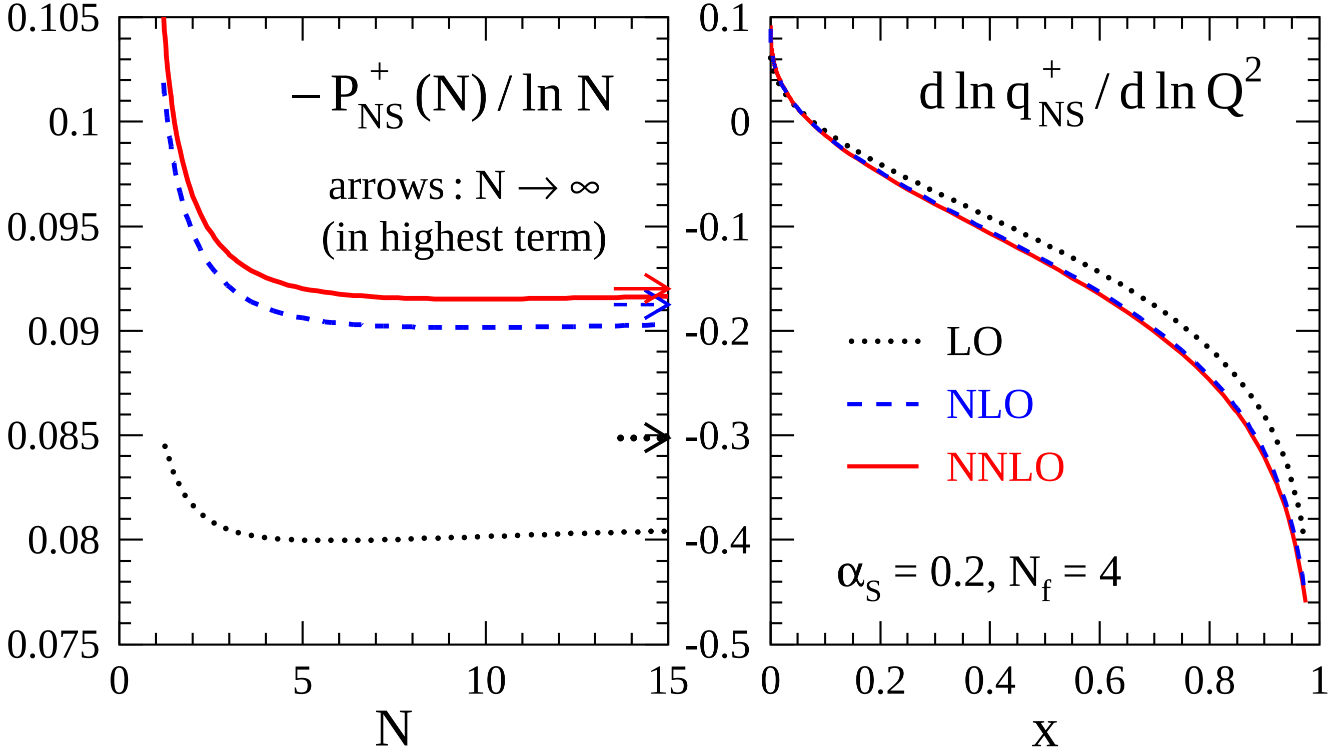

N^{3}LO: P_{ns}^+ **computed for** $N = 2\,,\ n_f = 3$ **Baikov, Chetyrkin (06)**

$$P_{ns}^+ \;=\; -\,0.283\,\alpha_s\,[\,1 \;+\; 0.869\,\alpha_s \;+\; 0.798\,\alpha_s^2 \;+\; 0.926\,\alpha_s^3 \;+\; \ldots\,]$$

$N > 2\,,\ n_f > 3:$ **similar / smaller** $\ln N$ **coeff's.** $\simeq$ **1% accuracy at** $\alpha_s \lesssim 0.25$

Small-x behaviour of the splitting functions

NNLO non-singlet : $P^{(2)i}_{x\to 0}(x) \; = \; D^i_0 \ln^4 x \; + \; \ldots \; + \; D^i_3 \ln x \; + \; \mathcal{O}(1)$

Generally terms up to $\ln^{2k} x$ at order α_s^{k+1}

D^i_0 **: Blümlein, A.V. (95)**

Coefficients for 'plus' case, like $u+\bar{u}-(d+\bar{d})$ for $n_f = 4$

$$D^+_0 \cong 1.580\,, \quad D^+_1 \cong 20.18\,, \quad D^+_2 \cong 175.3\,, \quad D^+_3 \cong 720.3$$

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NNLO singlet : $P^{(2)}_{\mathrm{ab},x\to 0}(x) \;=\; E^{\mathrm{ab}}_1 \frac{\ln x}{x} \;+\; E^{\mathrm{ab}}_2 \frac{1}{x} \;+\; \mathcal{O}(\ln^4 x)$

Generally terms up to $x^{-1}\ln^k x$ (gb) and $x^{-1}\ln^{k-1} x$ (qb) at order α_s^{k+1}

E^{qb}_1 : Catani, Hautmann (94), E^{gg}_1 : Fadin, Lipatov (98)

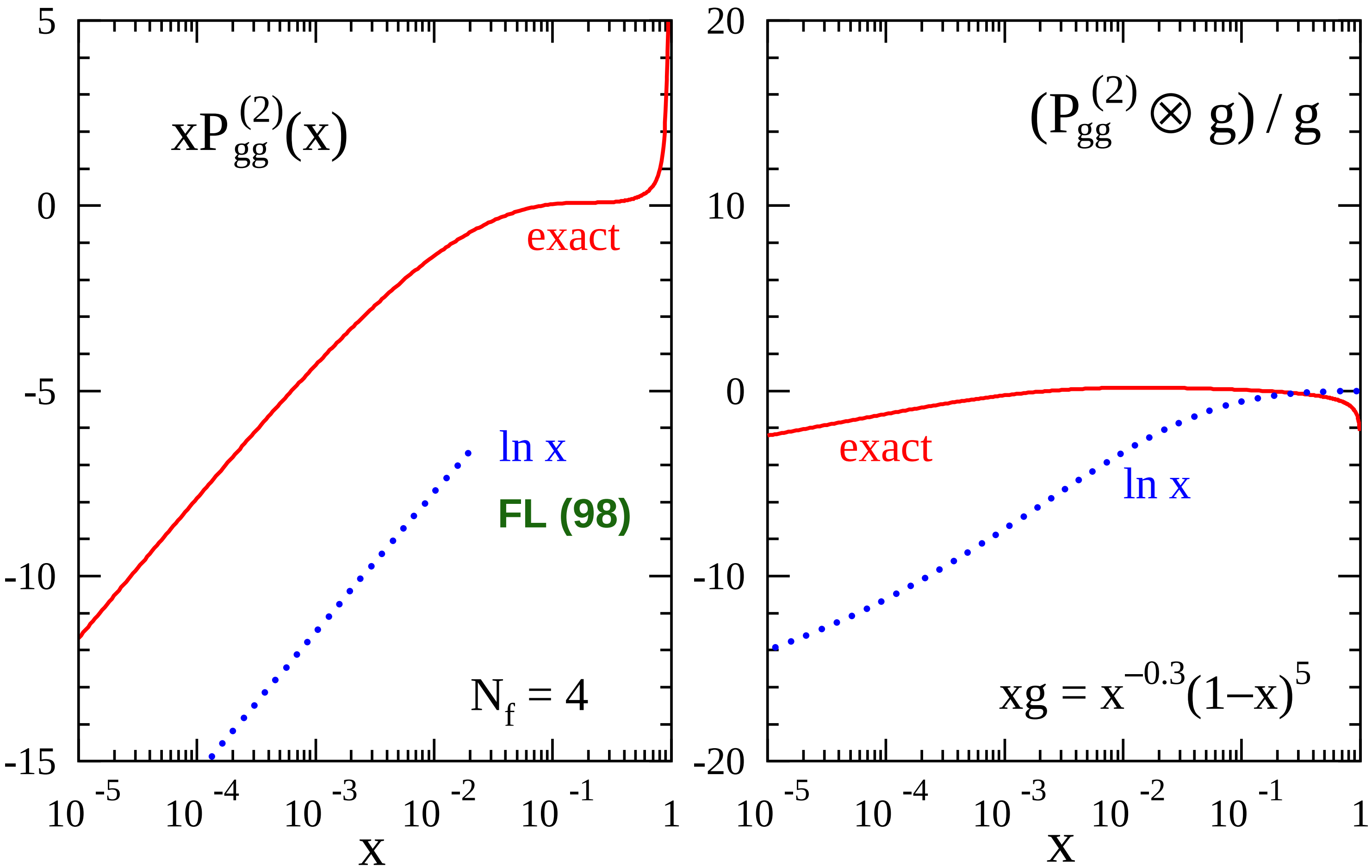
$n_f = 4$:

$$E^{\mathrm{qg}}_1 \cong -1194.7 \;, \quad E^{\mathrm{qg}}_2 = -4999.9$$
$$E^{\mathrm{gg}}_1 \cong +3304.9 \;, \quad E^{\mathrm{gg}}_2 = +14901$$

More often than not, **Large** logarithms have small coefficients

Singlet splitting and evolution at small x

Splitting functions $\longrightarrow$ observables: **Mellin convolutions** $\int_x^1 \frac{dy}{y} P(y)\, f\left(\frac{x}{y}\right)$



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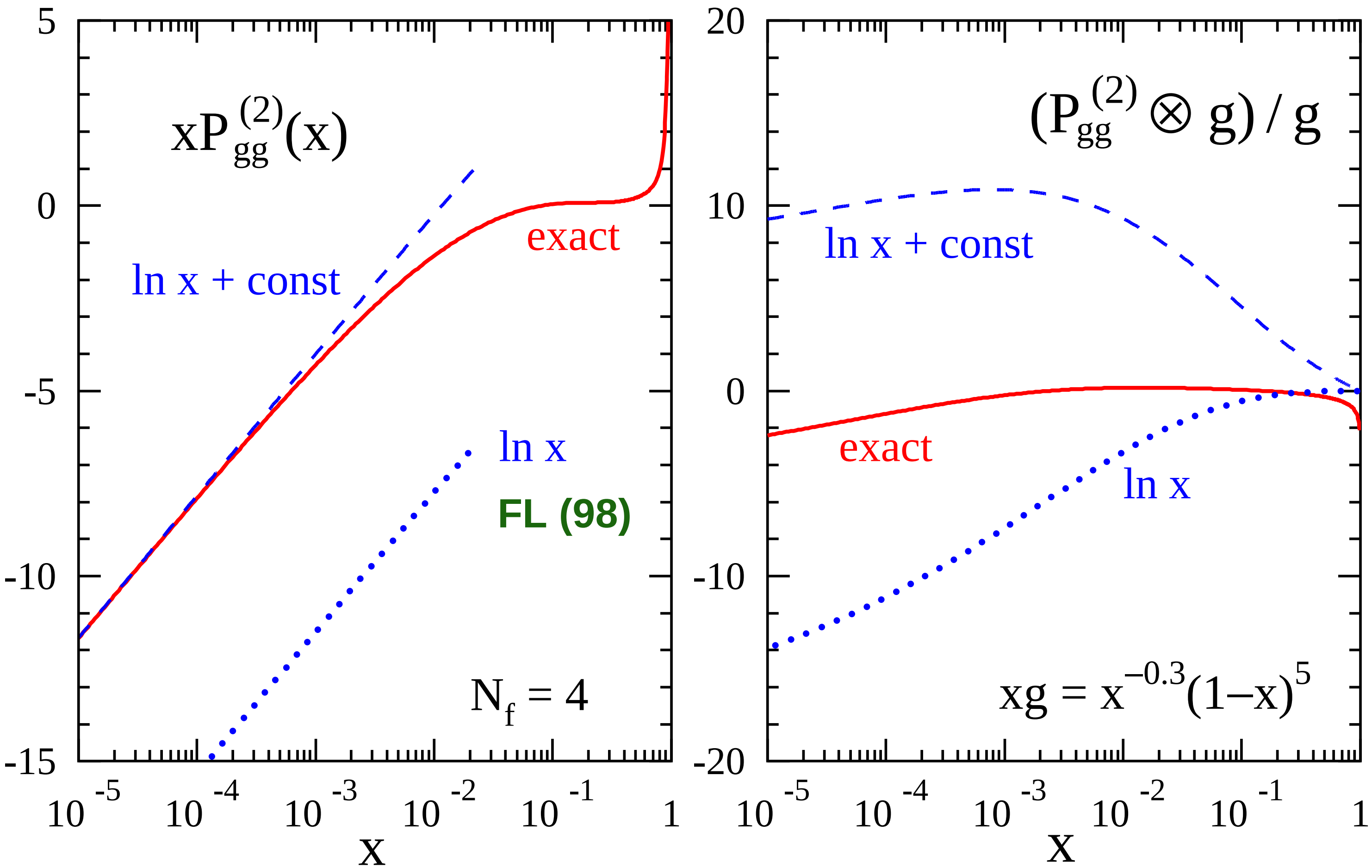
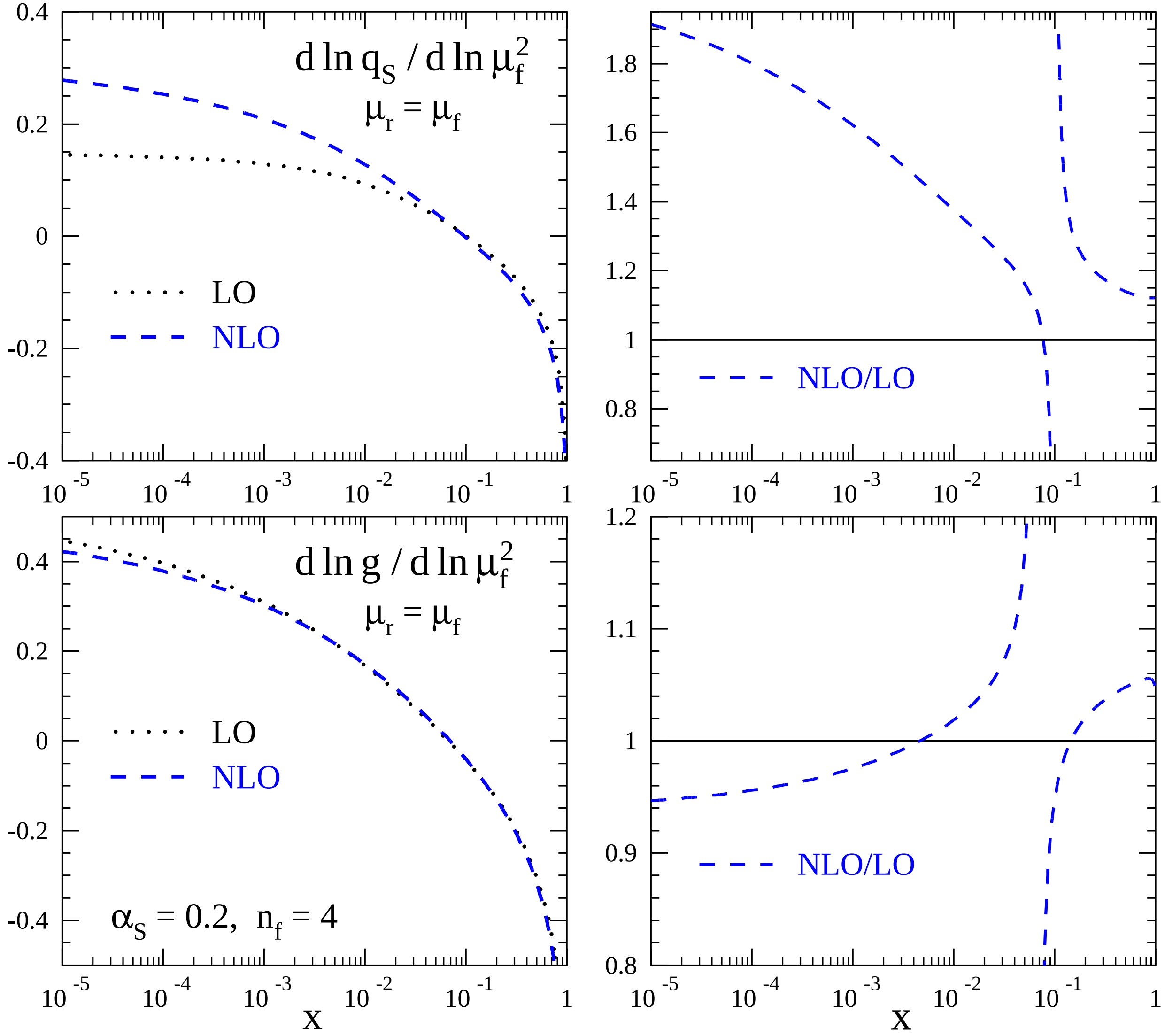


General: small-x limits of pQCD functions insufficient due to convolutions

Scale derivatives of singlet parton densities



scale ≈ 30 GeV^2

quark distrib'n

gluon distrib'n

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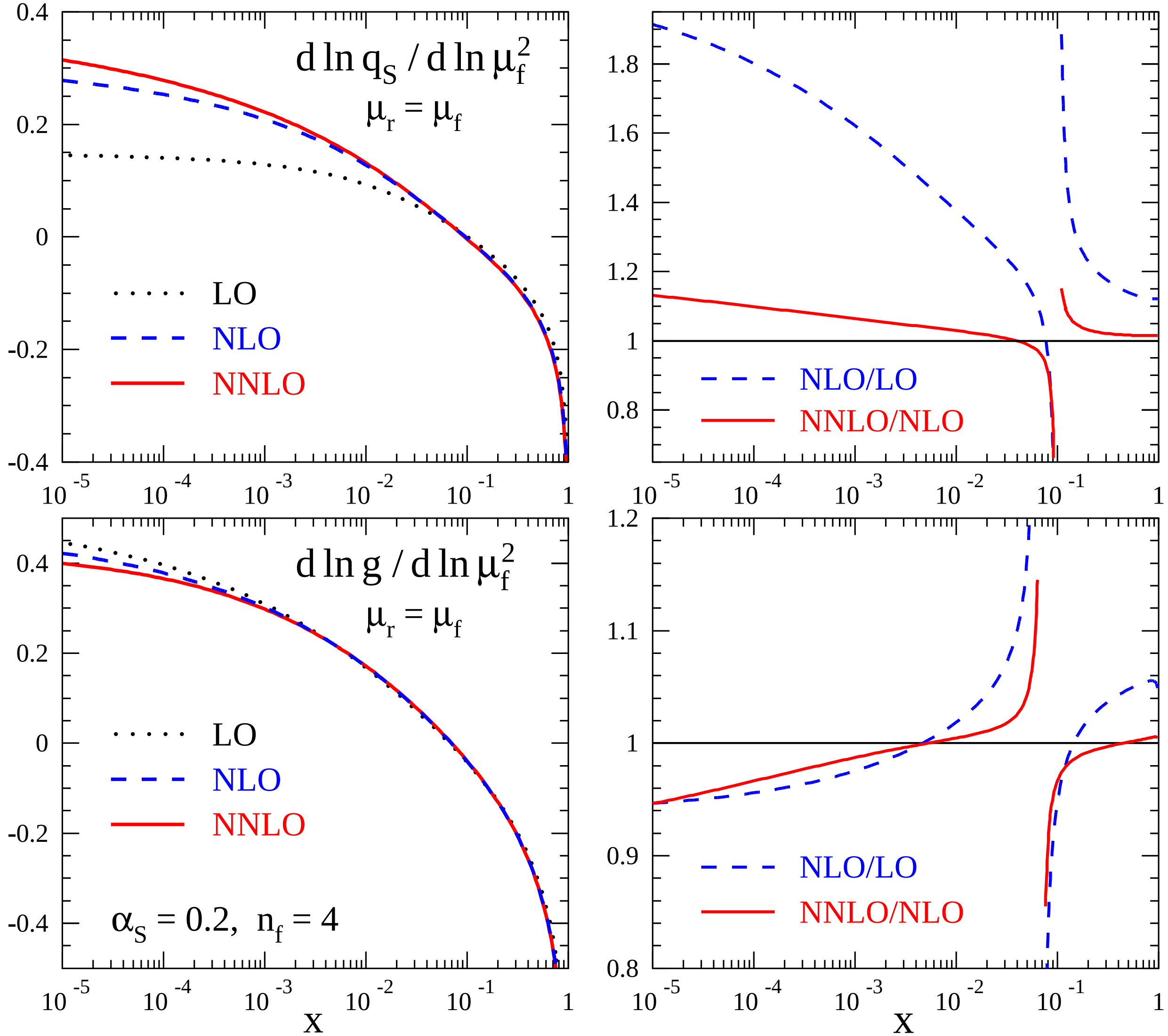

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Good convergence at collider-x – but NNLO is 10% for q_s at $x = 10^{-4}$

The evolution equations in Mellin-N space

Moments of all x-dependent quantities: convolutions turn into products

$$\boldsymbol{a(N) \;=\; \int_0^1 dx\, x^{N-1}\, a(x) \quad \Rightarrow \quad [a \otimes b](N) \;=\; a(N)\, b(N)}$$

$\Rightarrow$ **Evolution equations in N $=$ system of ordinary differential equations**

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Transformation of independent variable to $a_{\rm s} = \frac{\alpha_{\rm s}(\mu_r^2)}{4\pi}$ (for fixed μ_r/μ)

$$\frac{\partial q(N,\alpha_{\rm s})}{\partial \alpha_{\rm s}} \;=\; \{\beta(\alpha_{\rm s})\}^{-1}\, P_{\rm N^mLO}(N,\alpha_{\rm s})\; q(N,\alpha_{\rm s})$$

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&=\; -\frac{1}{\beta_0 \alpha_s}\Big[P^{(0)}(N) + \alpha_s\Big(P^{(1)}(N) - b_1 P^{(0)}(N)\Big) \\
&\qquad + \alpha_s^2\Big(P^{(2)}(N) - b_1 P^{(1)}(N) + (b_1^2 - b_2) P^{(0)}(N)\Big) + \ldots\Big]\; q(N,\alpha_s)
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&=\; -\alpha_s^{-1}\Big[R_0(N) + \textstyle\sum_{k=1}^{\infty} \alpha_s^k R_k(N)\Big] q(N,\alpha_s)
\end{aligned}$$

with

$$R_0 \;\equiv\; \frac{1}{\beta_0} P^{(0)} \;, \quad R_k \;\equiv\; \frac{1}{\beta_0} P^{(k)} - \textstyle\sum_{i=1}^{k} b_i\, R_{k-i} \;, \quad b_i = \frac{\beta_i}{\beta_0}$$

N$^{\mathrm{m}}$LO approximation: retain expansion coefficients $b_{l\le m}$ and $P^{(l\le m)}(N)$

The symbolic U-matrix solutions

Singlet part: splitting function matrices of different orders do not commute,

$$[R_i, R_k] \neq 0 \quad \text{for} \quad i \neq k$$

$\Rightarrow$ **no solution in closed exponential form beyond leading order ($m = 0$)**

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Cf. Schrödinger equation with $[H(t_1), H(t_2)] \neq 0$ – here $t = \ln \frac{\alpha_s(\mu_{r,0}^2)}{\alpha_s(\mu_r^2)}$:

interaction picture, time-ordered exponential solution for $|\psi(t)\rangle$

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Leading order

$$q_{\rm LO}(N, \alpha_s) \;=\; \left(\frac{a_0}{a_s}\right)^{R_0(N)} q(N, a_0) \;\equiv\; L(N, a_s, a_0)\, q(N, a_0)$$

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Higher orders

$$\begin{aligned} q(N, \alpha_s) \;&=\; U(N, a_s) L(N, a_s, a_0) U^{-1}(N, a_0)\; q(N, a_0) \\ &=\; \Big[1 + \sum_{k=1} a_s^k U_k(N)\Big] L(a_s, a_0, N) \Big[1 + \sum_{k=1} a_0^k U_k(N)\Big]^{-1} q(N, a_0) \end{aligned}$$

U^{-1} term with $a_0 = a_s(\mu_{r,0}^2)$: normalization at μ_0^2 – important, see below

Construction of the U-matrices (I)

LO splitting function matrix in terms of eigenvalues $r_\pm$ and projectors $e_\pm$

$$\boldsymbol{R_0 = r_- e_- + r_+ e_+}$$

with

$$\begin{aligned} \boldsymbol{r_\pm} &= \frac{1}{2\beta_0}\left[P^{(0)}_{\rm qq} + P^{(0)}_{\rm gg} \pm \sqrt{\left(P^{(0)}_{\rm qq} - P^{(0)}_{\rm gg}\right)^2 + 4P^{(0)}_{\rm qg}P^{(0)}_{\rm gq}}\right] \\ \boldsymbol{e_\pm} &= \frac{1}{r_\pm - r_\mp}\left[R_0 - r_\mp \mathbf{1}\right] \end{aligned}$$

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$\Rightarrow$ **representation of LO evolution operator** **(cf. two-level system in QM)**

$$L(a_s, a_0, N) = e_-(N)\left(\frac{a_s}{a_0}\right)^{-r_-(N)} + e_+(N)\left(\frac{a_s}{a_0}\right)^{-r_+(N)}$$

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U-ansatz + evolution eqs. $\Rightarrow$ recursive commutation relations for $U_k(N)$

$$\begin{aligned} [U_1, R_0] &= R_1 + U_1 \\ [U_2, R_0] &= R_2 + R_1 U_1 + 2U_2 \\ &\vdots \\ [U_k, R_0] &= R_k + \sum_{i=1}^{k-1} R_{k-i} U_i + k U_k \equiv \widetilde{R}_k + k U_k \end{aligned}$$

Construction of the U-matrices (II)

$e_{\pm}$ **projectors** ($e_{\pm}^2 = e_{\pm}\,,\ e_{\pm}e_{\mp} = 0\,,\ e_{-} + e_{+} = 1$) $\Rightarrow$ **identity**

$$U_k \ = \ e_{-}U_k e_{-} + e_{-}U_k e_{+} + e_{+}U_k e_{-} + e_{+}U_k e_{+}$$

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Insertion into commutation relations: iterative solutions for matrices U_k

$$U_k \;=\; -\frac{1}{k}\left[e_- \widetilde{R}_k e_- + e_+ \widetilde{R}_k e_+\right] + \frac{e_+ \widetilde{R}_k e_-}{r_- - r_+ - k} + \frac{e_- \widetilde{R}_k e_+}{r_+ - r_- - k}$$

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What about the poles at N-values with $r_- - r_+ \pm k = 0$?

[Not harmless, recall $a(N) \;=\; (N - N_0)^{-1} \;\Leftrightarrow\; a(x) = x^{-N_0}$]

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[Not harmless, recall $a(N) \;=\; (N - N_0)^{-1} \;\Leftrightarrow\; a(x) = x^{-N_0}$ **]**

Insert into $q(N, a_{\rm s})$**, expand** U^{-1} **factor [here to first order], re-sort terms**

$$q(a_{\rm s}) \;=\; \left\{ \left(\frac{a_{\rm s}}{a_0}\right)^{-r_-} \left[e_- + (a_0 - a_{\rm s})\, e_- R_1 e_- \right.\right.$$
$$\left.\left. - \left(a_0 - a_{\rm s} \left(\frac{a_{\rm s}}{a_0}\right)^{r_- - r_+} \right) \frac{e_- R_k e_+}{r_+ - r_- - 1} \right] + \{+ \leftrightarrow -\} \right\} q(a_0)$$

$\Rightarrow U^{-1}(a_0)$ **cancels the poles, e.g., round bracket = 0 for** $r_- - r_+ = 1$

Approximation options beyond leading order

Various ways to define the N^{m}LO solution, difference: terms of order $n > m$

- Exact ('iterated') sol'n of equation in $d/d\ln\mu^2$: keep $P_{n\leq m}$ and 'all' U_n

  Equivalent to widely used numerical x-space solutions; group property

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- **Truncated solution of equation in $d/d\alpha_s$: keep $R_{n\le m}$ and $U_{n\le m}$ only**

$$
\begin{aligned}
q_{\mathrm{N^3LO}}(a_s) \;=\; \Big[& L + a_s U_1 L - a_0 L U_1 \\
& + a_s^2 U_2 L - a_s a_0 U_1 L U_1 + a_0^2 L \left(U_1^2 - U_2\right) \\
& + a_s^3 U_3 L - a_s^2 a_0 U_2 L U_1 + a_s a_0^2 U_1 L \left(U_1^2 - U_2\right) \\
& \quad - a_0^3 L \left(U_1^3 - U_1 U_2 - U_1 U_2 + U_3\right) \Big]\, q(a_0)
\end{aligned}
$$

  Close to scheme-indep. expressions for observables; no group property

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q_{\mathrm{N^3LO}}(a_s) \;=\; & \Big[L + a_s U_1 L - a_0 L U_1 \\
& + a_s^2 U_2 L - a_s a_0 U_1 L U_1 + a_0^2 L \left(U_1^2 - U_2\right) \\
& + a_s^3 U_3 L - a_s^2 a_0 U_2 L U_1 + a_s a_0^2 U_1 L \left(U_1^2 - U_2\right) \\
& - a_0^3 L \left(U_1^3 - U_1 U_2 - U_1 U_2 + U_3\right) \Big]\, q(a_0)
\end{aligned}
$$

Close to scheme-indep. expressions for observables; no group property

Differences $\approx$ lower limits for the uncertainties due to missing higher orders

All above options available in QCD-Pegasus via parameter IMODEV = 1, 2, 0

Flavour symmetry breaking by evolution

Input $u = u_{\rm v} + \bar{u}$, $d = d_{\rm v} + \bar{d}$ **with SU(2) - symm. sea,** $\bar{u}(\mu_0^2) = \bar{d}(\mu_0^2)$

$\Rightarrow \; v_3^+ \; = \; u_{\rm v} + 2\bar{u} - d_{\rm v} - 2\bar{d} \; = \; u_{\rm v} - d_{\rm v} \; = \; v_3^-$ **at input scale** μ_0^2

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(Truncated) NLO evolution

$$v_3^-(a_s) = \left\{1 + (a_s - a_0)\, R_1^-\right\} \left(\frac{a_s}{a_0}\right)^{-R_0^{\mathrm{ns}}} (u_{\mathrm{v}} - d_{\mathrm{v}})(a_0)$$

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SU(2) sea symmetry not preserved by NLO evolution for $u_v \neq d_v$ **(p)**

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Analogous situation: $s \neq \bar{s}$ at NNLO even for $(s - \bar{s})(\mu_0^2) = 0$:

small effects, ‘dynamical’ $s - \bar{s}$ looked at for $\sin^2\theta_{\rm weak}$ from $\nu/\bar{\nu}$ DIS

Heavy quarks in hard proton processes

$$m_u\,,\, m_d \ll \Lambda_{\rm QCD}\;,\;\; m_s \lesssim \Lambda_{\rm QCD}$$

Can neglect 'light quark' masses in description of hard proton processes

$\Rightarrow$ **mass singularities, scale-dependent** u, d, s, g **parton distributions**

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$Q \gg m_c$ **: terms $m_c/Q \neq 0$, but quasi-collinear logs $\ln(Q/m_c)$ large,**

$n_f = 4$ pdf's, 'interpolating' coeff. functions ($\Leftarrow$ prescriptions)

(General-mass) variable flavour-number scheme, (GM-)VFNS

Heavy quarks in the evolution of PDFs and α_s

Here: disregard 'intrinsic charm/bottom' – might be relevant at large x

cf. Pumplin, Lai, Tung (2007)

$\overline{\text{MS}}$ evolution of parton densities and α_s with variable number n_f of flavours: matching of effective theories.

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$$
\begin{aligned}
l_i^{(n_f+1)} &= l_i^{(n_f)} + \theta_{m2}\, a_s^2\, A_{qq,h}^{ns,(2)} \otimes l_i^{(n_f)} + \dots \\
g^{(n_f+1)} &= g^{(n_f)} + \theta_{m2}\, a_s^2 \left[A_{gq,h}^{s,(2)} \otimes q_s^{(n_f)} + A_{gg,h}^{s,(2)} \otimes g^{(n_f)} \right] + \dots \\
(h+\bar{h})^{(n_f+1)} &= \theta_{m2}\, a_s^2 \left[A_{hq}^{s,(2)} \otimes q_s^{(n_f)} + A_{hg}^{s,(2)} \otimes g^{(n_f)} \right] + \dots
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Advantage of this choice: partons continuous at thresholds at LO and NLO

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Corresponding N^{m}LO relation for the coupling constant at $\mu_r^2 = \kappa\mu^2$

$$a_s^{(n_f+1)}(\kappa m_h^2) = a_s^{(n_f)}(\kappa m_h^2) + \sum_{n=1}^{m} \left(a_s^{(n_f)}(\kappa m_h^2) \right)^{n+1} \sum_{l=0}^{n} c_{n,l} \ln^l \kappa$$

$c_{1,0} = 0\,,\; c_{1,1} \neq 0,\; c_{2,0} \neq 0 \;\;\Rightarrow\;\; \alpha_s$ continuous only at NLO with $\kappa = 1$

Available evolution codes including NNLO

x-space: discretization in x, $\mu_{\mathbf{f}}$ of coupled integro-differential equations

QCDNUM (M. Botje, now v.17β), http://www.nikhef.nl/~h24/qcdnum/

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N-space: ordinary diff. eqs., symbolic U-matrix solution, $N \rightarrow x$ numerical

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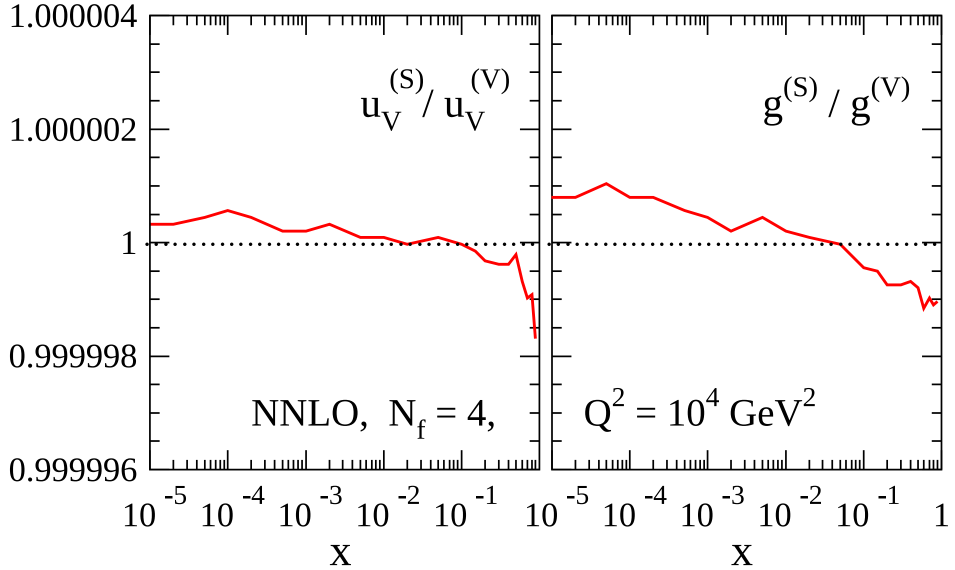
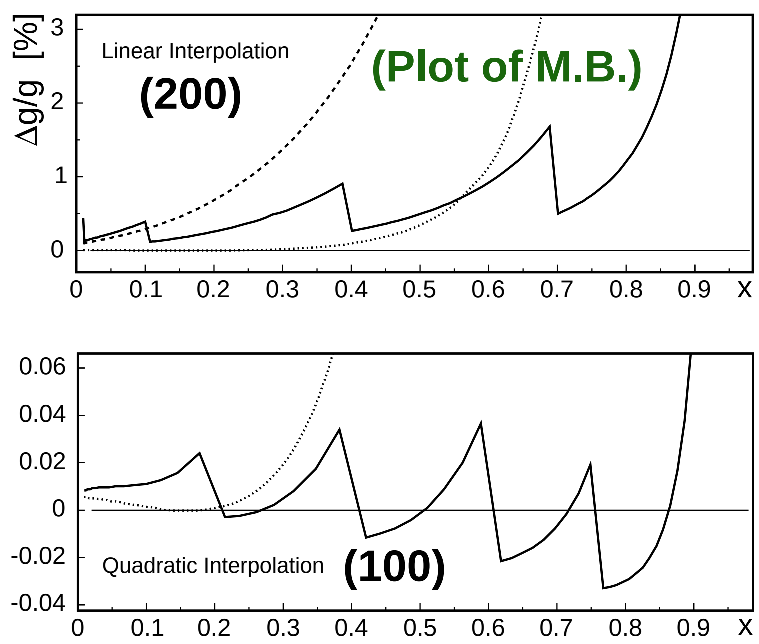
Sample comparisons





Benchmark tables for the parton evolution

Evolution of Les Houches (2001) reference input at scale $\mu_{\rm f,0}^2 = 2$ GeV^2

$$\begin{aligned} xu_v(x,\mu_{\rm f,0}^2) &= 5.1072\ x^{0.8}\ (1-x)^3 \quad , \quad \ldots \\ xg\ (x,\mu_{\rm f,0}^2) &= 1.7000\, x^{-0.1}\, (1-x)^5 \end{aligned}$$

with

$$\alpha_{\rm s}(\mu_{\rm r}^2 = 2\ \text{GeV}^2) \;=\; 0.35$$

at LO, NLO and NNLO, for $\mu_{\rm r} = \{0.5,\ 1,\ 2\}\, \mu_{\rm f}$, with fixed and variable n_f

Use of two completely different codes. G. Salam, A.V. (2002, 05)

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Five-digit agreement over wide range in x, μ_f^2 $\Rightarrow$ reference tables

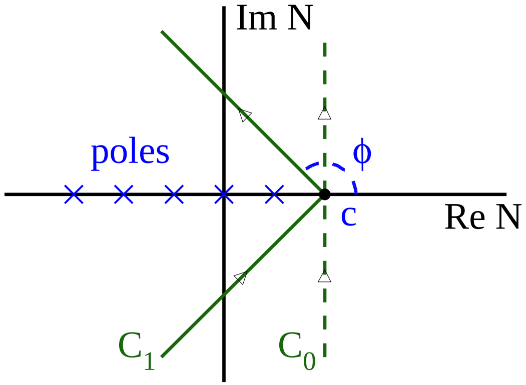
Example: (iterated) NNLO results, $\mu_r = 2\mu_f$, $n_f = 4$ at $\mu_f^2 = 10^4$ GeV^2

$$x = 10^{-5}\ ,\quad xu_v = 2.9032 \cdot 10^{-3}\ ,\quad \ldots\ ,\quad xg = 2.2307 \cdot 10^{2}$$
$$\ldots x = 0.9\ ,\quad xu_v = 3.6527 \cdot 10^{-4}\ ,\quad \ldots\ ,\quad xg = 1.2489 \cdot 10^{-6}$$

Full tables in hep-ph/0204316 (Les Houches), hep-ph/0511119 (HERA-LHC)

Mellin inversion in QCD-Pegasus (I)

Inverse transformation of Mellin-moment solution, using $a^*(N) = a(N^*)$



$$a(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} dN \, x^{-N} \, a(N)$$

$$= \frac{1}{\pi} \int_0^\infty dz \, \mathrm{Im} \left[e^{i\phi} x^{-c-ze^{i\phi}} a(N = c + ze^{i\phi}) \right]$$

$\mathcal{C}_1$ **: exponential damping** $\sim \; \exp\left(z \ln(1/x) \cos\phi\right)$

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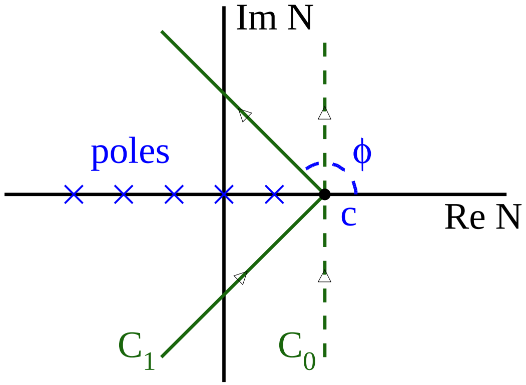

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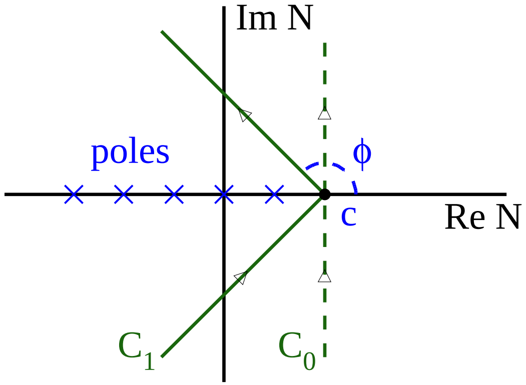

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Practical choice (speed – accuracy compromise for cases in QCD evolution)

$c = 1.9$, $\phi = \frac{3}{4}\pi$, **18 fixed subintervals in** z **up to** $z_{\max} = 80$

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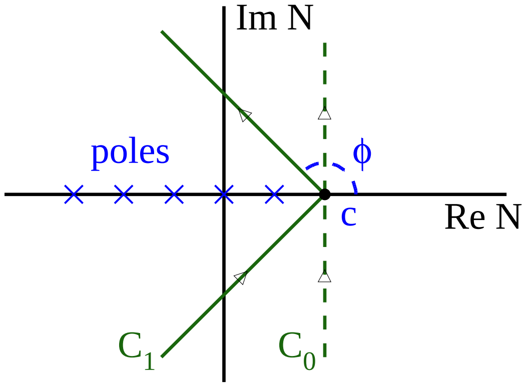

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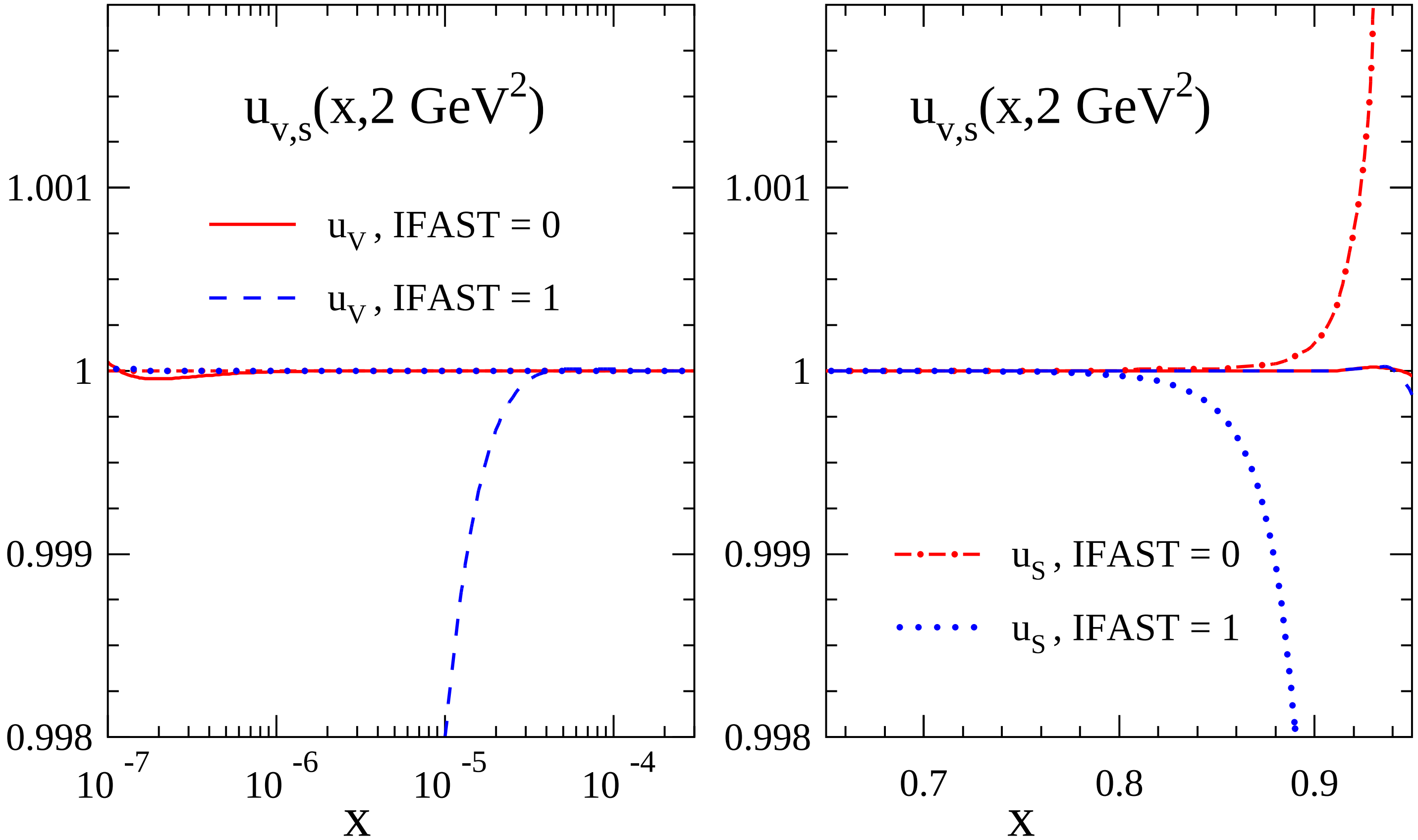
Faster (less accurate) option available: 18 $\longrightarrow$ 10 intervals, 144 $\longrightarrow$ 80 points

Mellin inversion in QCD-Pegasus (II)

Inversion accuracy: use initial scale μ_0^2, divide by x-space reference inputs



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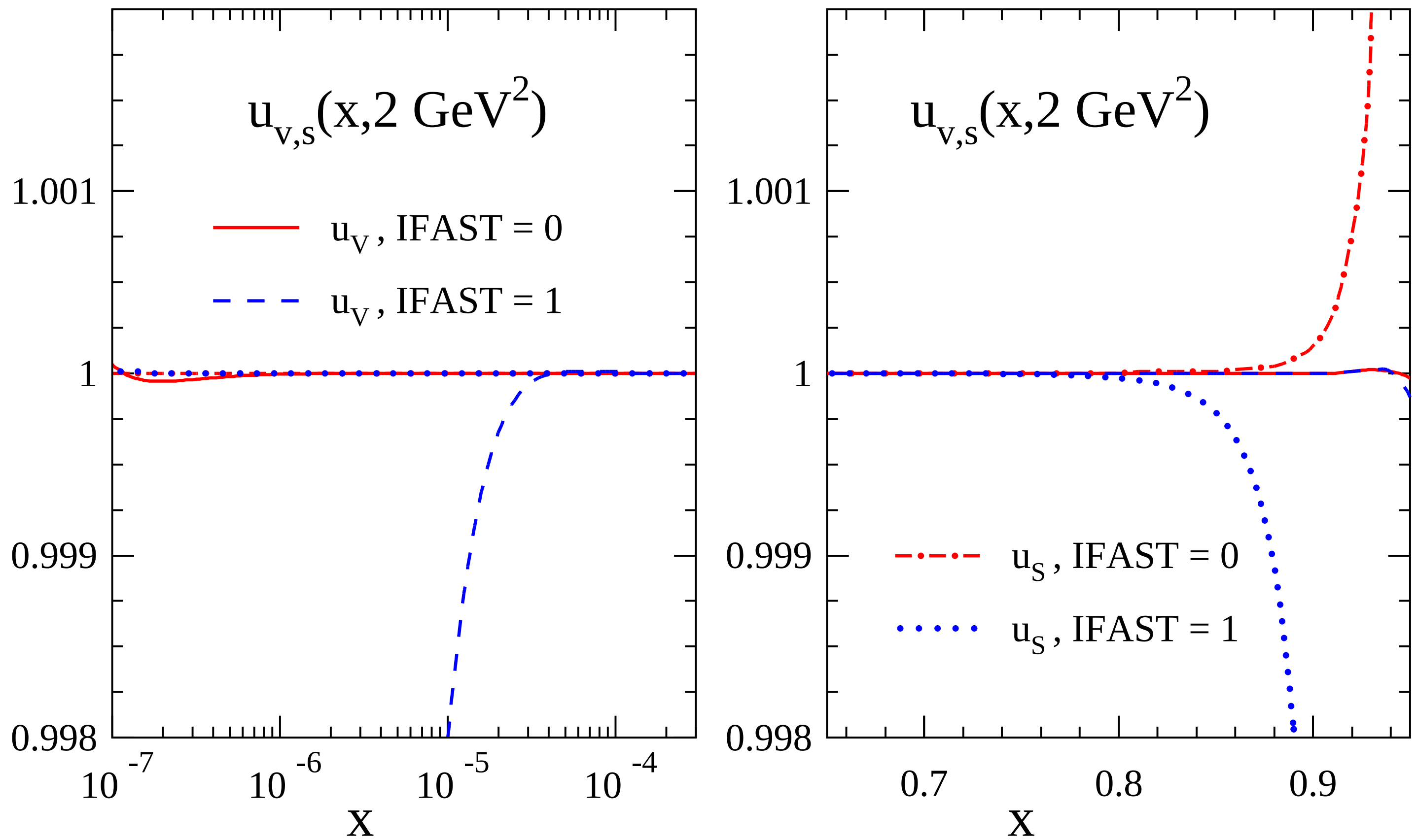

Fast option safe at least at $10^{-4} \lesssim x \lesssim 0.7$, but often over full range shown

Large-x limitation: suppressed $xu_s \sim (1-x)^7$. Small-x: $xu_v \sim x^{0.8}$

Splitting functions and initial distributions

Mellin inversion (in particular) on contour $\mathcal{C}_1$: 'proper' analytic continuations

$\Rightarrow$ **work from accurate parametrizations of (parts of) splitting functions etc**

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Practically sufficient, recall 10^{-6} agreement with x-space code HOPPET

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Initial distributions: choose functional forms with 'easy' moments such as

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(use via NFORM = 1, 2 in Pegasus). Many more flexible forms no problem

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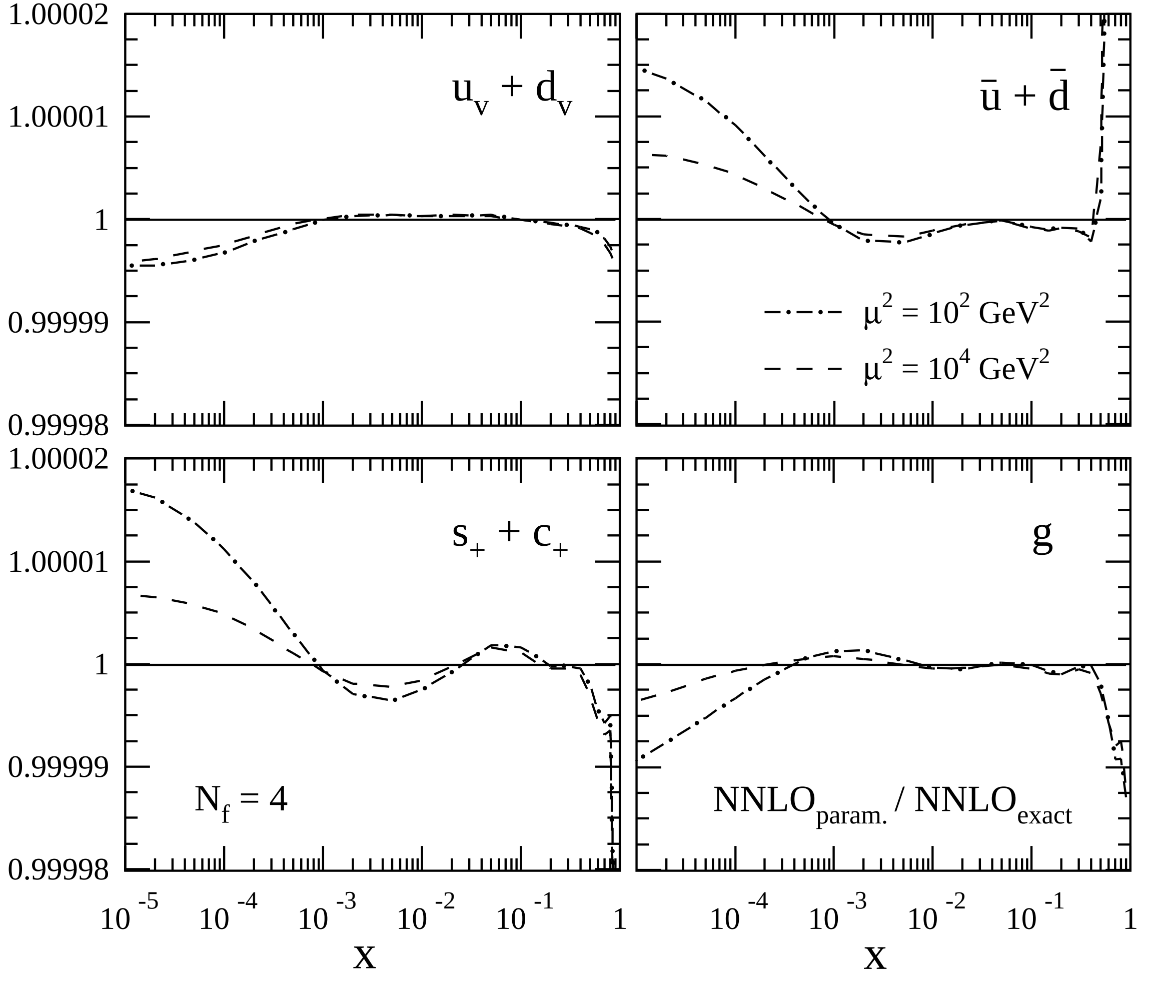
Disclaimer: moments not trivial for, e.g., input form of CTEQ6 analysis

$$xf_i(x,\mu_0^2) \;=\; N_i\, x^{a_i} (1-x)^{b_i}\, (1 + A_i\, x)^{c_i}\, e^{d_i x}$$

Parametrizations of NNLO splitting functions

Complete NNLO splitting functions parametrized with inaccuracies $< 0.1\%$

MVV (04)



Relative deviations from evolution with exact functions well below 10^{-4}

Performing the evolution with QCD-Pegasus

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Make sure that any modified version, or any other evolution program you write or use, agrees with the Les Houches and HERA-LHC benchmark tables – and say so in papers

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Performing the evolution with QCD-Pegasus

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Make sure that any modified version, or any other evolution program you write or use, agrees with the Les Houches and HERA-LHC benchmark tables – and say so in papers

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- **In case of questions/problems: contact me via Andreas.Vogt@liv.ac.uk**
  but carefully study the manual before becoming too aggressive

And now let's see it in practice . . .