A semi-analytical x-space solution for parton evolution

Application to non-singlet and singlet DGLAP equation

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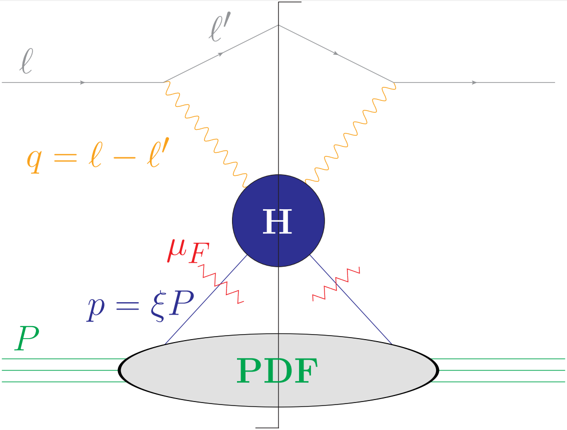
JH, Oliver Schüle, Fabian Wunder, arXiv:2404.18667 (to appear in JHEP)

Outline

1. Brief introduction to parton distributions and evolution
2. Semi-analytical x-space solution for parton evolution
3. Numerical analysis of our method applied to the DGLAP equation
4. Conclusion and Outlook

1. Brief introduction to parton distributions and evolution

Factorization in QCD



QCD factorization

$$\sigma_{eH \to eX}(P) = \sum_{i=q,\bar{q},g} \int_0^1 \mathrm{d}\xi \underbrace{f_{i/H}(\xi, \mu_F)}_{\text{non perturbative and collinear interaction}} \overbrace{\hat{\sigma}_{ei \to eX}(\xi P, \mu_F)}^{\text{only hard part H of the partonic scattering}} + \underbrace{\mathcal{O}\left(\Lambda_{\mathrm{QCD}}^2 / Q^2\right)}_{\text{e.g. multi-parton scat.}}$$

Scale dependence of parton distributions

Factorization theorem (schematic)

$$\sigma = f(\mu_\mathsf{F}) \otimes \hat{\sigma}(\mu_\mathsf{F})$$

Use factorization scale independence of full hadronic cross-section:

$$0 = \frac{\mathrm{d}}{\mathrm{d}\mu_\mathsf{F}} \sigma = \frac{\mathrm{d}}{\mathrm{d}\mu_\mathsf{F}} \left[f(\mu_\mathsf{F}) \otimes \hat{\sigma}(\mu_\mathsf{F}) \right]$$
$$= \left(\frac{\mathrm{d}f(\mu_\mathsf{F})}{\mathrm{d}\mu_\mathsf{F}} \right) \otimes \hat{\sigma}(\mu_\mathsf{F}) + f(\mu_\mathsf{F}) \otimes \left(\frac{\mathrm{d}\hat{\sigma}(\mu_\mathsf{F})}{\mathrm{d}\mu_\mathsf{F}} \right)$$

Solve for scale dependence of parton distribution:

Evolution equation (schematic)

$$\frac{\mathrm{d}f(\mu_\mathsf{F})}{\mathrm{d}\mu_\mathsf{F}} = \mathcal{P}(\mu_\mathsf{F}) \otimes f(\mu_\mathsf{F})$$

with perturbatively calculable evolution kernel $\mathcal{P}$.

⚠Proper derivation uses renormalization group (e.g. Collins 2011)⚠
⚠Less proper but simpler: based on col. subtr. (e.g. Ellis et al. 1996) ⚠

Example: DGLAP equation

- Evolution basis

$$q_{\mathrm{ns},\,ij} \equiv q_i - q_j \qquad \text{and} \qquad q_{\mathrm{s}} \equiv \sum_{i=1}^{n_{\mathrm{f}}} [q_i + \bar{q}_i]$$

- Non-singlet DGLAP equation

$$\frac{\mathrm{d}}{\mathrm{d}\ln\mu^2}\, q_{\mathrm{ns}}(\mu^2, x) = \frac{\alpha_s(\mu^2)}{2\pi} \int_x^1 \frac{\mathrm{d}\xi}{\xi}\, P_{qq}(\xi)\, q_{\mathrm{ns}}\left(\mu^2, \frac{x}{\xi}\right)$$

- Singlet DGLAP equation

$$\frac{\mathrm{d}}{\mathrm{d}\ln\mu^2} \begin{pmatrix} q_{\mathrm{s}}(\mu^2, x) \\ g(\mu^2, x) \end{pmatrix} = \frac{\alpha_s(\mu^2)}{2\pi} \int_x^1 \frac{\mathrm{d}\xi}{\xi} \begin{pmatrix} P_{qq}(\xi) & 2n_{\mathrm{f}} P_{qg}(\xi) \\ P_{gq}(\xi) & P_{gg}(\xi) \end{pmatrix} \begin{pmatrix} q_{\mathrm{s}}\left(\mu^2, \frac{x}{\xi}\right) \\ g\left(\mu^2, \frac{x}{\xi}\right) \end{pmatrix}$$

- Momentum and flavor sum rules

$$(i):\ \int_0^1 \mathrm{d}x\, \left(q_i(\mu^2, x) - \overline{q}_i(\mu^2, x)\right) = \text{number of valence quarks } i\,,$$

$$(ii):\ \int_0^1 \mathrm{d}x\, x \left(q_{\mathrm{s}}(\mu^2, x) + g(\mu^2, x)\right) = 1$$

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Existing methods

Key question

How to solve integro-differential equation?

Two main strategies

A) Mellin-space methods:

- Convolution becomes multiplication in Mellin space → analytic solution in Mellin-space → numerical transformation to x-space
  `partonevolution`, `QCD-PEGASUS`, `EKO`

B) x-space methods:

- Discretization in x with interpolation ansatz to transform evolution equation into ordinary differential equation (ODE)
  `QCDnum`, `APFEL`, `HOPPET`, `ChiliPDF`

2. Semi-analytical x-space solution for parton evolution

General idea of our method

- General integro-differential equation with integral operator $\mathbf{P}\otimes$ in $\vec{x}$-space

$$\frac{\mathrm{d}}{\mathrm{d}\mu}\mathbf{f}(\mu,\vec{x}) = (\mathbf{P}\otimes\mathbf{f})(\mu,\vec{x}) \tag{1}$$

- Ansatz with suitable set of spanning functions $\mathbf{f}_m$

$$\mathbf{f}(\mu,\vec{x}) = \sum_m a_m(\mu)\,\mathbf{f}_m(\vec{x})$$

- Transform (1) into ODE for coefficients

$$\frac{\mathrm{d}}{\mathrm{d}\mu}a_m(\mu) = \mathcal{P}_{mn}(\mu)\,a_n(\mu)\,.$$

- Truncate to finite system and solve numerically via matrix exponential
- Evolution matrix $\mathcal{P}$ can be applied to any initial condition

Our idea applied to DGLAP

- x-space ansatz for parton distributions
- Overcomplete family of spanning functions closed under evolution equation $\left(\frac{\ln^m(x)x^n}{m!} \text{ for DGLAP}\right)$
- Grasp analytic behaviour in x generated by evolution equation
- Transforms evolution equation into ODE for scale-dependent coefficients, solved via matrix exponential
- Truncate ODE to finite subsystem, solve numerically

Simplest example: Test idea on LO DGLAP equation

Very explicit, very small example

- Take non-singlet LO DGLAP equation

$$\frac{\mathrm{d}}{\mathrm{d}\ln\mu^2}\, q\left(\mu^2, x\right) = \frac{\alpha_s\left(\mu^2\right)}{2\pi} \int_x^1 \frac{\mathrm{d}\xi}{\xi}\, P_{qq}^{(0)}(\xi)\, q\left(\mu^2, \frac{x}{\xi}\right) \qquad (2)$$

where $\frac{\mathrm{d}}{\mathrm{d}\ln\mu^2} = \mu^2 \frac{\mathrm{d}}{\mathrm{d}\mu^2}$ and

$$P_{qq}^{(0)}(\xi) = C_F \left(\frac{1+\xi^2}{(1-\xi)_+} + \frac{3}{2}\delta(1-\xi) \right)$$

- Plug in ansatz

$$q\left(\mu^2, x\right) = a_{00}\left(\mu^2\right) + a_{01}\left(\mu^2\right) x + a_{10}\left(\mu^2\right) \ln x + \dots$$

- DGLAP eq. (2) becomes

$$\frac{\mathrm{d}a_{00}}{\mathrm{d}\ln\mu^2} + \frac{\mathrm{d}a_{01}}{\mathrm{d}\ln\mu^2} x + \frac{\mathrm{d}a_{10}}{\mathrm{d}\ln\mu^2} \ln x + \dots$$

$$= \frac{\alpha_s}{2\pi}\left[a_{00} \int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi) + a_{01} \int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi) \frac{x}{\xi} + a_{10} \int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi) \log\frac{x}{\xi} + \dots \right]$$

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- Calculate remaining integrals analytically:

$$\frac{1}{C_\mathrm{F}}\int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi) = \frac{1}{2} + x - \ln x + 2\underbrace{\ln(1-x)}_{-x+\dots} = \frac{1}{2} - x - \ln x + \dots$$

$$\frac{1}{C_\mathrm{F}}\int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi)\,\frac{x}{\xi} = 1 + \frac{x}{2} + \dots$$

$$\frac{1}{C_\mathrm{F}}\int_x^1 \frac{\mathrm{d}\xi}{\xi} P_{qq}^{(0)}(\xi)\log\frac{x}{\xi} = \frac{\pi^2}{3} - 1 - x + \frac{1}{2}\ln x + \dots$$

- Write DGLAP eq. in matrix form w.r.t. basis $(1, x, \ln x, \dots)$

Very explicit, very small example

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- Solve (numerically) with your preferred method for ODEs $\rightarrow$ diagonalize (impractical for large matrices) or use **(numerical) matrix exponential** or use Runge-Kutta or ...
- Solution in our example:

$$\begin{pmatrix} a_{00}(\mu^2) \\ a_{01}(\mu^2) \\ a_{10}(\mu^2) \end{pmatrix} = \exp\left[\frac{C_\mathrm{F}}{2\pi} \overbrace{\int_{\ln\mu_0^2}^{\ln\mu^2} \mathrm{d}\ln\mu_1^2\, \alpha_s(\mu_1^2)}^{\text{integral over running coupling}} \begin{pmatrix} \frac{1}{2} & 1 & \frac{\pi^2}{3} - 1 \\ -1 & \frac{1}{2} & -1 \\ -1 & 0 & \frac{1}{2} \end{pmatrix}\right] \begin{pmatrix} a_{00}(\mu_0^2) \\ a_{01}(\mu_0^2) \\ a_{10}(\mu_0^2) \end{pmatrix}$$

- Running coupling at LO (known to N^{4}LO): $\alpha_s(\mu^2) = \frac{4\pi}{\beta_0 \ln\left(\frac{\mu^2}{\Lambda_{\mathrm{QCD}}^2}\right)}$ with $\beta_0 = 11 - \frac{2}{3} n_\mathrm{f}$ and QCD mass scale Λ_{QCD}.

Very explicit, very small example

- Write DGLAP eq. in matrix form w.r.t. basis $(1, x, \ln x)$:

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with $\beta_0 = 11 - \frac{2}{3} n_f$ and QCD mass scale Λ_{QCD}.

Solving the LO DGLAP equation with more basis functions

- Ansatz: $$q_{\text{ns}}(\mu^2, x) = \sum_{m,n=0}^{\infty} a_{mn}(\mu^2) \frac{\ln^m(x)\, x^n}{m!}$$

- Plug into LO DGLAP equation
$$\sum_{m,n=0}^{\infty} \frac{\mathrm{d}a_{mn}(\mu^2)}{\mathrm{d}\ln\mu^2} \frac{\ln^m(x)\, x^n}{m!} = \frac{\alpha_s(\mu^2)}{2\pi} C_F \sum_{m,n=0}^{\infty} a_{mn}(\mu^2)$$
$$\times \left[\frac{1}{x} I_1^{m,n+1} + x\, I_1^{m,n-1} + 2\, I_2^{m,n} + 2\, \ln(1-x) \frac{\ln^m(x)\, x^n}{m!} + \frac{3}{2} \frac{\ln^m(x)\, x^n}{m!}\right]$$

- Collect w.r.t. spanning functions
$$\frac{\mathrm{d}a_{MN}(\mu^2)}{\mathrm{d}\ln\mu^2} = \frac{\alpha_s(\mu^2)}{2\pi} \mathcal{P}_{MN}^{(0),ij} a_{ij}(\mu^2)$$

- Truncate infinite system of equations
$$q(\mu^2, x) = \sum_{m=0}^{M_{\max}} \sum_{n=0,-1}^{N_{\max}(m)} a_{mn}(\mu^2) \frac{\ln^m(x)\, x^n}{m!}$$

Solving the LO DGLAP equation with more basis functions

- Differential equation for the coefficients

$$\frac{\mathrm{d}a_{MN}(\mu^2)}{\mathrm{d}\ln\mu^2} = \frac{\alpha_s(\mu^2)}{2\pi}\,\mathcal{P}^{(0),ij}_{MN}\,a_{ij}(\mu^2)$$

- Solved numerically by matrix exponential

$$a_{MN}(\mu^2) = \exp\left[\Omega(\mu^2,\mu_0^2)\right] a_{MN}(\mu_0^2)$$

- With

$$\Omega(\mu^2,\mu_0^2) = \int_{\ln\mu_0^2}^{\ln\mu^2} \mathrm{d}\ln\mu_1^2\,\alpha_s(\mu_1^2)\,\mathcal{P}^{(0)}$$

Key questions

- How large is the error induced by the truncation to a finite number of basis functions?
- How many do we need for good accuracy?
- Which basis functions should we choose?

$\Longrightarrow$ Check numerical performance for sufficiently realistic example

Solving the LO DGLAP equation with more basis functions

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Key questions

- How large is the error induced by the truncation to a finite number of basis functions?
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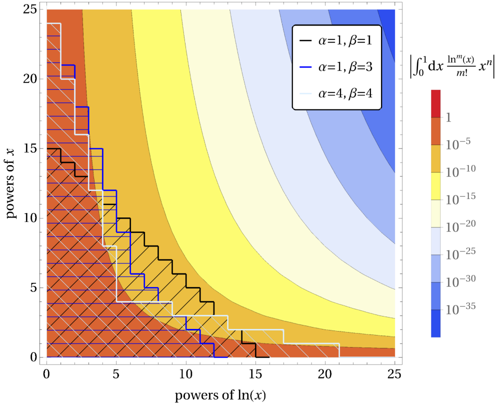
$\Longrightarrow$ Check numerical performance for sufficiently realistic example

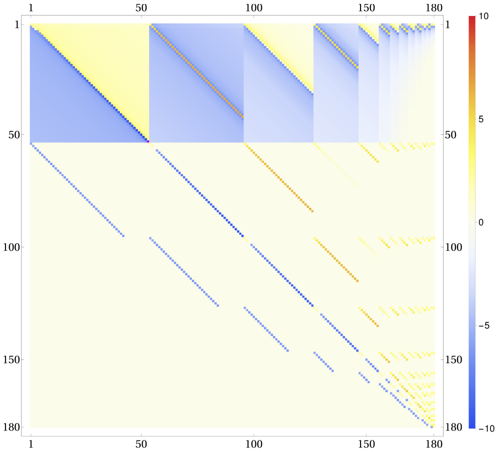
3. Numerical analysis of our method applied to the DGLAP equation

Contribution of different basis functions



$$N_{\max}^{\alpha,\beta}(m) = \begin{cases} \left\lfloor \frac{M_{\max} - m}{\alpha} \right\rfloor & \text{if } (\alpha+1)\, m > M_{\max} \\ \left\lfloor -\beta\, m + \frac{1+\beta}{1+\alpha} M_{\max} \right\rfloor & \text{else} \end{cases}$$

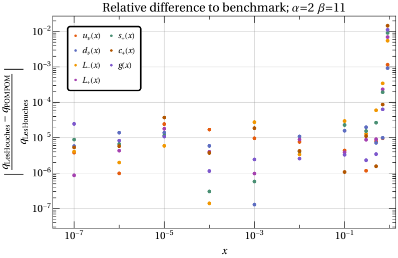
Magnitude of entries in the non-singlet evolution matrix

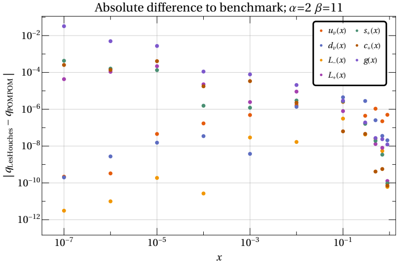


- Ordered by (m, n), i.e. $(1, x, x^2, \ldots, \ln(x), x\ \ln(x), \cdots)$
- Cut-off parameters $(\alpha, \beta) = (2, 11)$

Comparison to Les Houches benchmark tables

- Benchmark values for checking PDF evolution codes [hep-ph/02043160]
- Parametrize input distributions in terms of spanning functions
- Evolve from $\mu_0^2 = 2\,\mathrm{GeV}^2$ to $\mu^2 = 10^4\,\mathrm{GeV}^2$ using `POMPOM` Mathematica code for LO DGLAP evolution





Check sum rule violation

Recap:

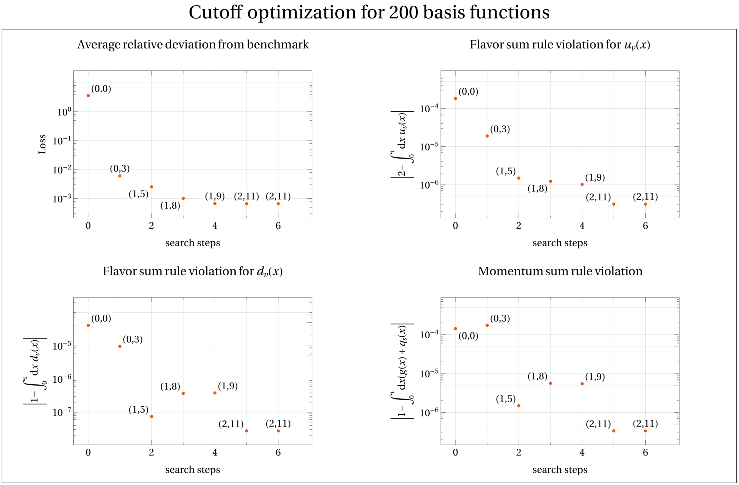
- **Momentum sum rule**

$$\int_0^1 \mathrm{d}x\, x\,(q_s(x) + g(x)) = 1$$

- **Flavor sum rule**

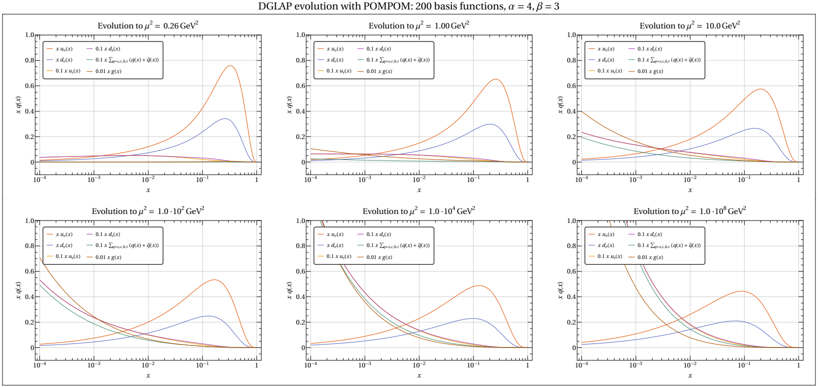
$$\int_0^1 \mathrm{d}x\, q_{v,i}(x) = \int_0^1 \mathrm{d}x\, (q_i(x) - \overline{q}_i(x)) = \text{number of valence quarks } i$$

Comparison to Les Houches benchmark tables



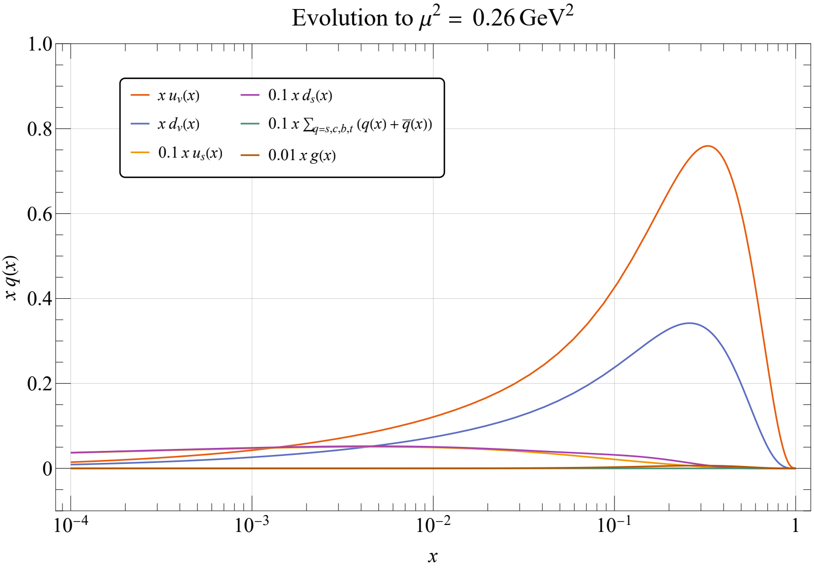
- Use gradient descent on cutoff parameters (α, β)
- Tested for 50, 100, 150, 200 basis functions

Evolution of a full set of PDFs

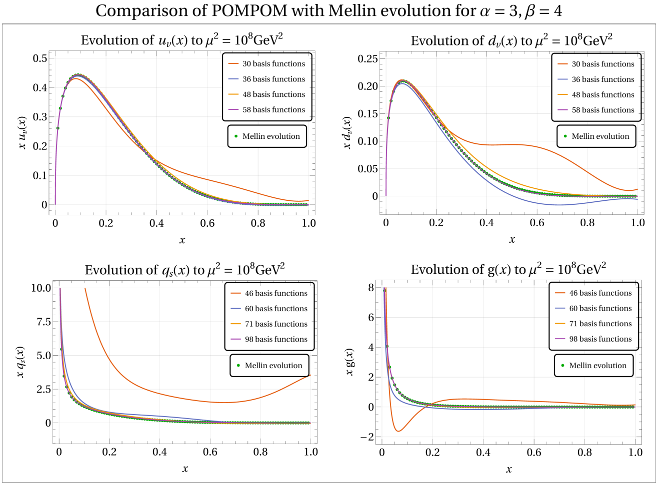


- GRV98 input distributions at $\mu_0^2 = 0.26\,\mathrm{GeV}^2$ [hep-ph/9806404]
- Sum-rule violation as metric to optimize cutoff
- Variable flavor number scheme

Evolution of a full set of PDFs



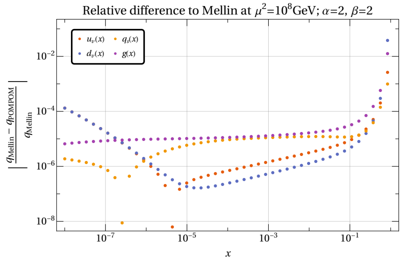
Comparison to Mellin-space evolution: Convergence

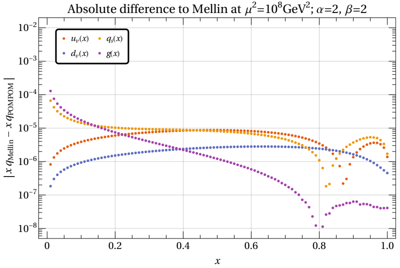


- $\sim$ 50 basis functions valence-like distributions and $\sim$ 100 for sea (additional $1/x$ terms for sea)

Comparison to Mellin-space evolution: Larger basis

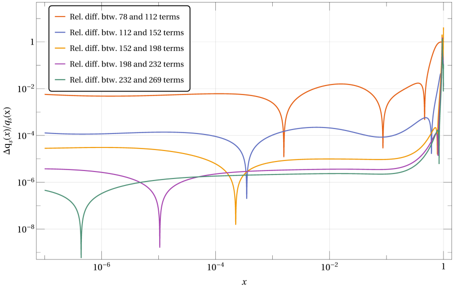
- 200 basis functions



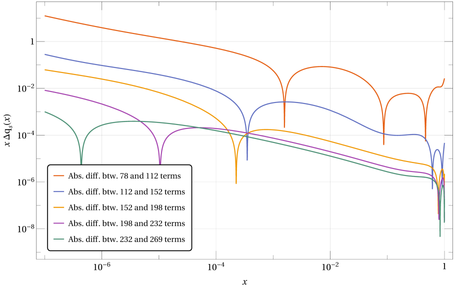


Difference between singlet PDFs $x\,q_s(x)$ for increasing number of basis functions

- Evolve from scale $\mu_0^2 = 0.26\,\mathrm{GeV}^2$ to $\mu^2 = 10^8\,\mathrm{GeV}^2$
- Cut-off parameters $\alpha = \beta = 2$



Relative difference



Absolute difference

4. Conclusion and Outlook

Conclusion and Outlook

Conclusion:

- Good agreement with Les Houches benchmarks and Mellin evolution
- Sum rule violations $< 10^{-6}$ for $\mathcal{O}(200)$ basis functions
- Truncation effects under control, can be systematically improved
- `POMPOM`: `Mathematica` and `Python` implementation of LO DGLAP

Outlook:

- Higher order DGLAP evolution
- Apply POMPOM-method to similar evolution equations
- Improve cut-off optimization

Outlook: Generalization to higher order DGLAP equation

- Differential equation for the coefficients

$$\frac{\mathrm{d}a_{MN}(\mu^2)}{\mathrm{d}\ln\mu^2} = \frac{\alpha_s(\mu^2)}{2\pi}\,\mathcal{P}^{ij}_{MN}\,a_{ij}(\mu^2)$$

- Solved numerically by matrix exponential

$$a_{MN}(\mu^2) = \prod_{k=1}^{K}\exp\left[\Omega\left(\mu_k^2,\mu_{k-1}^2\right)\right]a_{MN}(\mu_0^2)\,,\ \text{with } \mu_K^2 = \mu^2$$

- With Magnus expansion, $\Omega = \Omega_1 + \Omega_2 + \ldots$,

$$\Omega_1(\mu^2,\mu_0^2) = \int_{\ln\mu_0^2}^{\ln\mu^2}\mathrm{d}\ln\mu_1^2\left(\alpha_s(\mu_1^2)\,\mathcal{P}^{(0)} + \alpha_s^2(\mu_1^2)\,\mathcal{P}^{(1)} + \alpha_s^3(\mu_1^2)\,\mathcal{P}^{(2)} + \mathcal{O}(\alpha_s^4)\right)$$

$$\Omega_2(\mu^2,\mu_0^2) = \frac{1}{2}\int_{\ln\mu_0^2}^{\ln\mu^2}\mathrm{d}\ln\mu_1^2\int_{\ln\mu_0^2}^{\ln\mu_1^2}\mathrm{d}\ln\mu_2^2\,\alpha_s(\mu_1^2)\,\alpha_s^2(\mu_2^2)\left[\mathcal{P}^{(0)},\,\mathcal{P}^{(1)}\right] + \mathcal{O}(\alpha_s^4)$$

  LO, NLO, NNLO contribution
- Sufficiently large number of slices K to ensure convergence of expansion

Outlook: Generalization to twist-3 evolution

Singlet ETQS equation:

$$\frac{\mathrm{d}}{\mathrm{d}\ln\mu^2}\begin{pmatrix}\mathfrak{S}^\pm\\ \mathfrak{F}^\pm\end{pmatrix} = -\frac{\alpha_s(\mu^2)}{2\pi}\begin{pmatrix}\mathbb{H}^\pm_{QQ} & \mathbb{H}^\pm_{QF}\\ \mathbb{H}^\pm_{FQ} & \mathbb{H}^\pm_{FF}\end{pmatrix}\begin{pmatrix}\mathfrak{S}^\pm\\ \mathfrak{F}^\pm\end{pmatrix},$$

where $\mathfrak{S}^\pm$ and $\mathfrak{F}^\pm$ are functions of two momentum fractions.

- Existing codes use discretization (`Honeycomb`/`Snowflake` 2024)
- First step for applying the presented method: Come up with suitable two-variable basis functions
- Higher dimensionality requires more basis functions, therefore more important to select "important" ones to be computationally feasible

Outlook: Improve choice of basis cut-off

Numerical performance may be spoiled by

(1) omitting "large" basis functions

(2) omitting matrix elements strongly coupling to initial condition

(3) large coefficients / very large number of non-negligible coefficients in initial conditions

- Choose suitable basis functions to avoid (3)
- (1) and (2) determine sensible cut-off
- Finite cut-off always leads to (1), precise evolution possible if omitted basis functions do not couple strongly to initial conditions
- Rescaling basis functions shuffles overall factors between (1) - (3)

Idea

Use machine learning techniques for parametrization-independent optimization

5. Backup slides

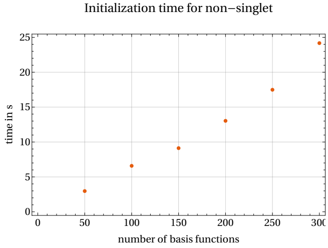
Relation to Mellin-space

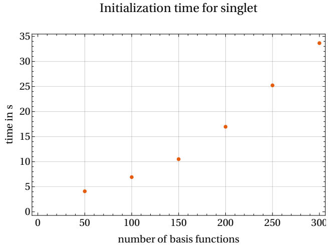
- Mellin transform $\mathcal{M}$ of the non-singlet pdf

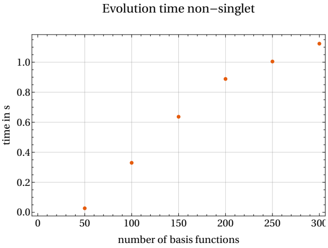
$$\mathcal{M}[q_{\mathrm{ns}}](\mu^2, s) = \int_0^1 \mathrm{d}x\, x^{s-1}\, q_{\mathrm{ns}}(\mu^2, x) = \sum_{m,n=0}^{\infty} a_{mn}(\mu^2)\, \frac{(-1)^m}{(n+s)^{m+1}}$$

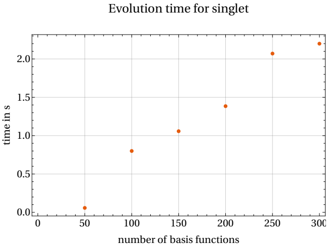
- Coefficients a_{mn} in Mellin-space identical to coefficients in x-space
- Scale evolution decouples from switch x-space $\leftrightarrow$ Mellin-space
- Spanning functions $\frac{(-1)^m}{(n+s)^{m+1}}$ are meromorphic functions of s on $\mathbb{C}$, poles on real axis for $s = n$
- Exploit to obtain simple analytic form of Mellin transform of PDF

Timing

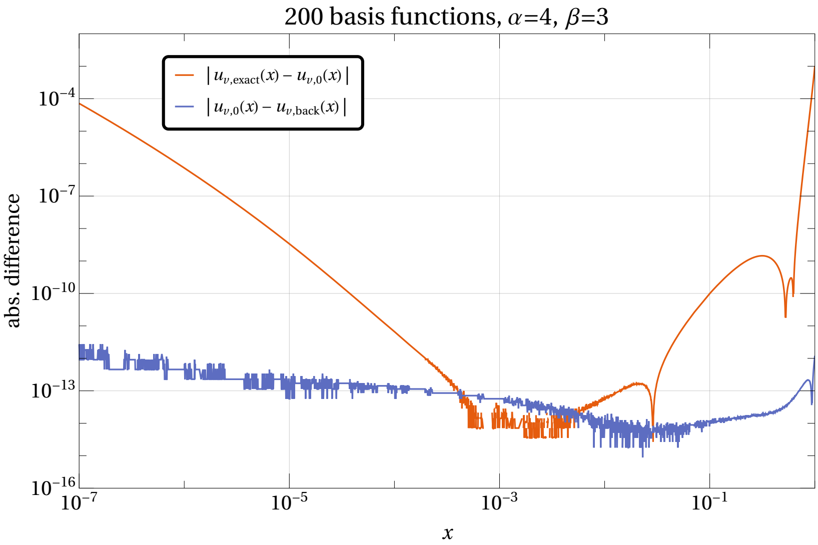

Initialization time for non−singlet
time in s
0
5
10
15
20
25
0
50
100
150
200
250
300
number of basis functions


Initialization time for singlet
time in s
0
5
10
15
20
25
30
35
0
50
100
150
200
250
300
number of basis functions


Evolution time non−singlet
time in s
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200
250
300
number of basis functions


Evolution time for singlet
time in s
0.0
0.5
1.0
1.5
2.0
0
50
100
150
200
250
300
number of basis functions

Back Evolution



GRV98 input distributions and parameters

- LO input distributions at $\mu_0^2 = 0.26\,\mathrm{GeV}^2$ $(\Delta \equiv \bar{d} - \bar{u})$

$$
\begin{aligned}
x\,u_v\left(x, \mu_0^2\right) &= 1.239\,x^{0.48}\,(1-x)^{2.72}\left(1 - 1.8\sqrt{x} + 9.5x\right)\\
x\,d_v\left(x, \mu_0^2\right) &= 0.614\,(1-x)^{0.9}\,x\,u_v\left(x, \mu_0^2\right)\\
x\,\Delta\left(x, \mu_0^2\right) &= 0.23\,x^{0.48}\,(1-x)^{11.3}\left(1 - 12.0\sqrt{x} + 50.9x\right)\\
x\,(\bar{u} + \bar{d})\left(x, \mu_0^2\right) &= 1.52\,x^{0.15}\,(1-x)^{9.1}\left(1 - 3.6\sqrt{x} + 7.8x\right)\\
x\,g\left(x, \mu_0^2\right) &= 17.47\,x^{1.6}\,(1-x)^{3.8}\\
x\,s\left(x, \mu_0^2\right) &= x\,\bar{s}\left(x, \mu_0^2\right) = 0
\end{aligned}
$$

- Running coupling $\alpha_s\left(\mu^2\right) = \frac{4\pi}{\beta_0 \ln\left(\frac{\mu^2}{\Lambda_{\mathrm{QCD}}^2}\right)}$ with $\beta_0 \equiv 11 - \frac{2}{3} n_{\mathrm{f}}$

- QCD mass scale $\Lambda_{\mathrm{QCD}}^{(n_{\mathrm{f}}=3,4,5,6)} = 204, 175, 132, 66.5\,\mathrm{MeV}$

- Thresholds for $n_{\mathrm{f}} = 4, 5, 6$ at $\mu^2 = 1.96, 20.25, 30625\,\mathrm{GeV}^2$