

Accelerating High-Energy collisions calculations using analytic models to describe effective PDF's

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in collaboration with D. F. Rentería-Estrada,
R. J. Hernández-Pinto, G. F. R. Sborlini and Pia
Zurita.

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1. Parton Distribution Functions

1.1 Some history

1.2 How to compute them

2. Motivation

3. Machine Learning for PDFs

4. Results

5. Conclusions

Based on:

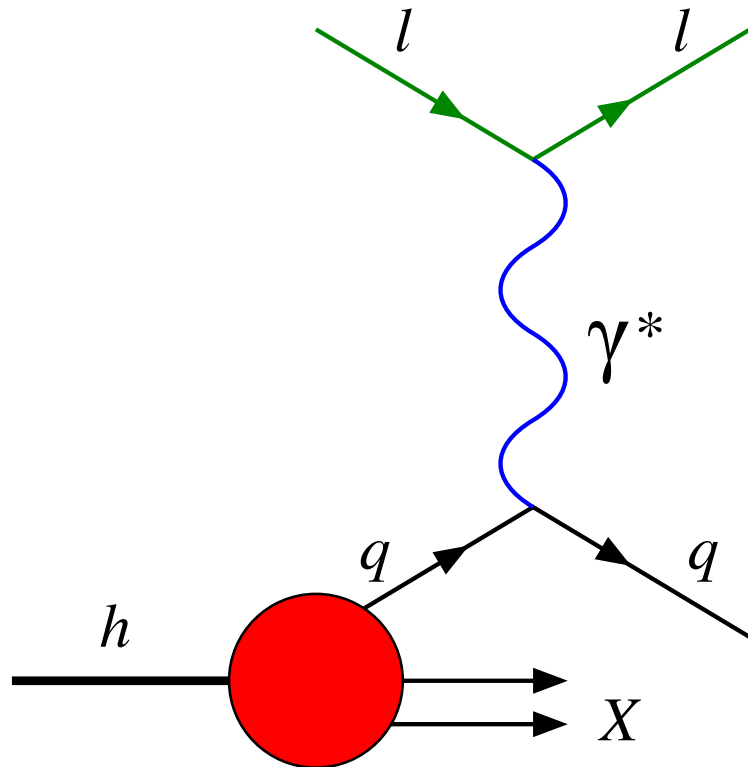
- S. A. Ochoa-Oregon, D. F. Rentería-Estrada, R. J. Hernández-Pinto, G. F.R. Sborlini and Pia Zurita, “**Using analytic models to describe effective PDFs**”, Phys. Rev. D 110, 036019



Parton Distribution Functions

Deep Inelastic Scattering

Parton distributions are present since 1960 when the determination of the cross section depends on the **structure functions** F_2 and F_L .



Kinematical variables

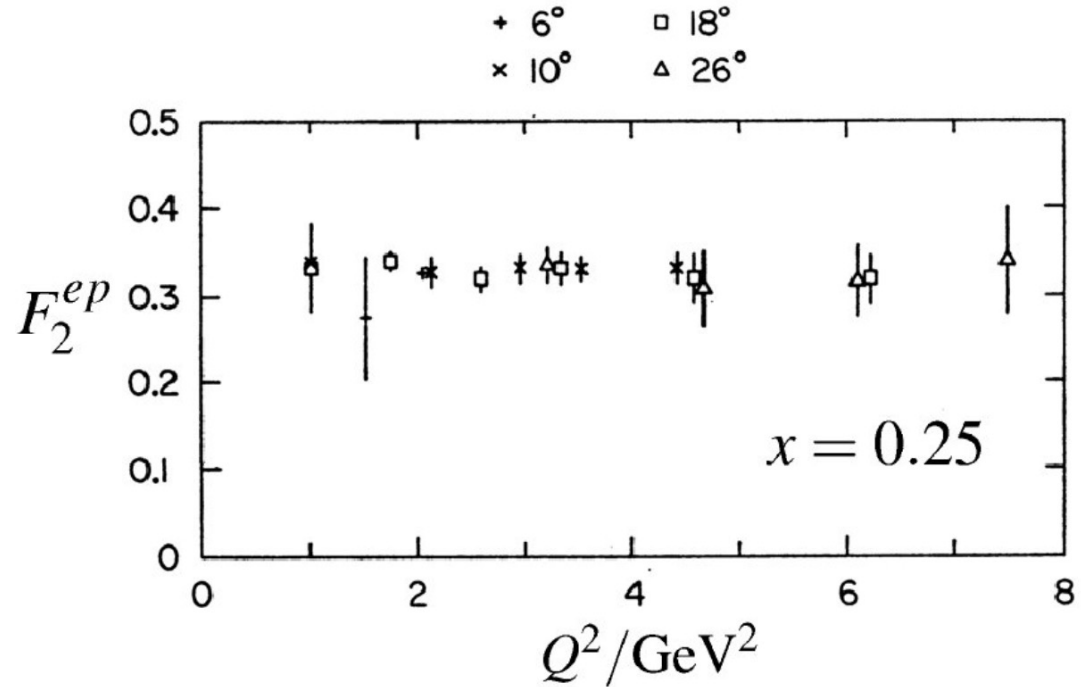
$$Q^2 = -(k - k')^2$$

$$x = \frac{Q^2}{2P \cdot Q} \quad y = \frac{P \cdot Q}{P \cdot k}$$

$$\frac{d^2\sigma}{dx dQ^2} \approx F_2(x, Q^2) - \frac{y^2}{1+(1-y)^2} F_L(x, Q^2)$$

Parton Distribution Functions

Experimental results of **structure functions** were



Then, a scaling was expected as

$$F_2^{L0}(x) = x \sum_{i=1}^{n_f} e_i^2 f_{i/h}(x)$$

Parton Distribution Functions

- Where $f_{i/h}$ is the probability density of **finding the parton i inside the hadron h** with a **fraction of momentum x** . They are called Parton Distribution Functions (PDFs).



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- At higher orders in the expansion the scaling breaks down and a **dependence on the renormalization scale μ** appears.
- The functional form of the PDFs is not known from first principles. Nevertheless, **DGLAP gives the evolution with the scale,**

$$\mu^2 \frac{d}{d\mu^2} f_{i/h}(x, \mu) = \int_{\mu}^1 \frac{d\xi}{\xi} \sum_b P_{a/b} \left(\frac{x}{\xi}, \alpha_s(\mu) \right) f_{b/h}(\xi, \mu)$$

with **$P_{a/b}$ the Altarelli-Parisi splitting functions.**

Parton Distribution Functions

One big assumption...

Universality holds for the PDFs, therefore, any process that is an inclusive hard scattering can be written as,

$$d\sigma^{\text{DIS}} = \sum_i d\sigma^{l+i \rightarrow l'} \otimes f_i \quad \text{and} \quad d\sigma^{\text{DY}} = \sum_{i,j} d\sigma^{i+j \rightarrow l+l'} \otimes f_i \otimes f_j$$

Factorization
scheme and fixed
order calculations

with the **same PDFs**. Also, the PDFs **contains the long distance structure of hadrons**.



We need global Fits

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We need global Fits

Without PDFs there are no theoretical predictions!

Parton Distribution Functions

Global Fits

- Steps in general. Choose: **i)** a factorization scheme, **ii)** an order in pQCD, **iii)** a starting scale Q_0 , **iv)** the data to be fitted, **v)** the heavy flavor scheme.



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- **Parametrize partonic distributions**, in general,

$$xf_i(x, Q_0^2) = A_i x^{\alpha_i} (1 - x)^{\beta_i} P(x, c_i)$$

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- **Solve the DGLAP equations** for the measured kinematics.
- Convolute PDFs and partonic Cross-sections.
- **Minimize** distance between theoretical predictions and experimental values.
- Use a method to estimate theoretical error bands.
- Create **grids in x and Q^2** , and provide an **interpolator for the grid**.

Process	NLO (CPU years)	NNLO (CPU years)	N3LO (CPU years)
pp → W/Z		0.6	160
pp → H		0.6	160
pp → $\gamma\gamma$		4.6	Process not available
pp → tt		20	Process not available
pp → $\gamma\gamma$ +2jets		2.4	Process not available
pp → 2 jets		10	Process not available
pp → H+jet		57	Process not available
pp → $\gamma\gamma\gamma$		31	Process not available
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pp → 3 jets		> 114	Process not available

Cieri, L. (2024, June 19). *Precise theoretical predictions at colliders*. LHCPHENO 2024, IFIC, Valencia, España.

Motivation

- All the running of MC codes **take a long time** to reach good precision.
- They carry a significant **environmental impact** (and to our pockets given the **cost of the CPU and then the electricity**)

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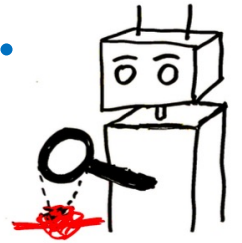
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- Most codes require **non perturbative** inputs (e.g. PDFs) and most of **them are provided as** grids and interpolate over them.
- A quick exploration shows that interpolation time could be **reduced 40-50%** if we had **analytical expressions for the PDFs**.

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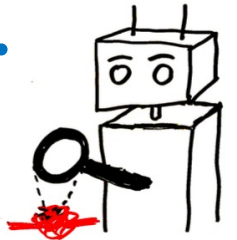
Machine Learning for PDFs

Goal: Find an analytical x and Q^2 form for a set of proton PDFs.



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- How? Inspired by **functional form of HERAPDF**, we propose a general functional form

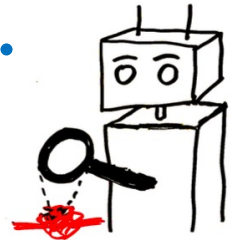


$$xf_i(x, Q^2) = A_i(Q^2)x^{\alpha_i(Q^2)}(1-x)^{\beta_i(Q^2)}P(x, c_i(Q^2)) \\ -\Theta(x_{c,i} - x)A'_i(Q^2)x^{\alpha'_i(Q^2)}(1-x)^{\beta'_i(Q^2)}P(x, c'_i(Q^2))$$



More details in: [Phys. Rev. D 110, 036019 \[hep-ph\]](#)

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- Our hypothesis is that the **Q^2 -dependence** of the PDFs is given by **the parameters**.
- The `heavyside` function is used to give more flexibility at low x . (Inspired by HERAPDF and gradient boosting algorithm)
- Fitted using Machine Learning tools and techniques.

More details in: Phys. Rev. D 110, 036019 [hep-ph]

Fitting procedure

- We generate a grid of 5,000-10,000 random points in $\{x, Q^2\}$ using HERAPDF20_NLO_EIG (HERAPDF 2.0)
- The range was chosen in accordance to HERAPDF
- Furthermore, we use for light quarks and gluons $Q_{\text{Min}} = Q_0 \approx 1.37$ GeV, whilst $Q_0 = 1.5$ GeV and $Q_0 = 4.5$ GeV for the charm and bottom quarks, respectively

Note: We are fitting the results of an existing fit.

More details in: Phys. Rev. D 110, 036019 [hep-ph]

Finding the best fit: cost function

- Since HEP phenomenology is **not only interested in the central value** of the PDF, we rather define the best fitting parameters through the **cost function**,

$$\Delta_i(Q^2) = \frac{I[f_i^{\text{ML}}(x, Q^2), Q^2] - I[f_i^{\text{HERA}}(x, Q^2), Q^2]}{I[f_i^{\text{HERA}}(x, Q^2), Q^2]},$$



Inspired by
Factorization
Theorem

- which takes care of the integral error of the determination of the PDFs, through the integration operator,

$$I[f, Q^2] = \int_{10^{-4}}^1 dx f(x, Q^2).$$

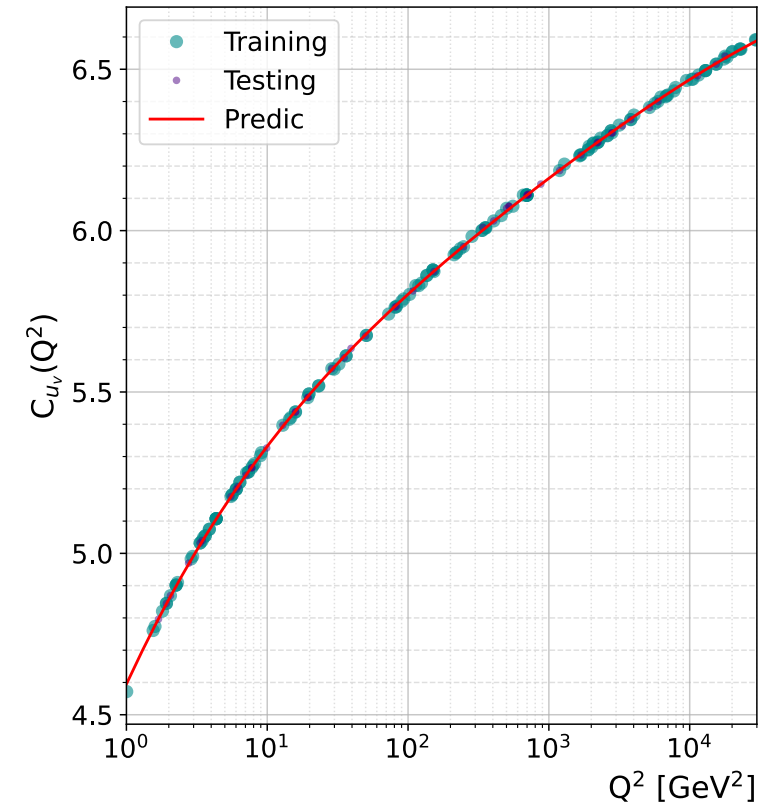
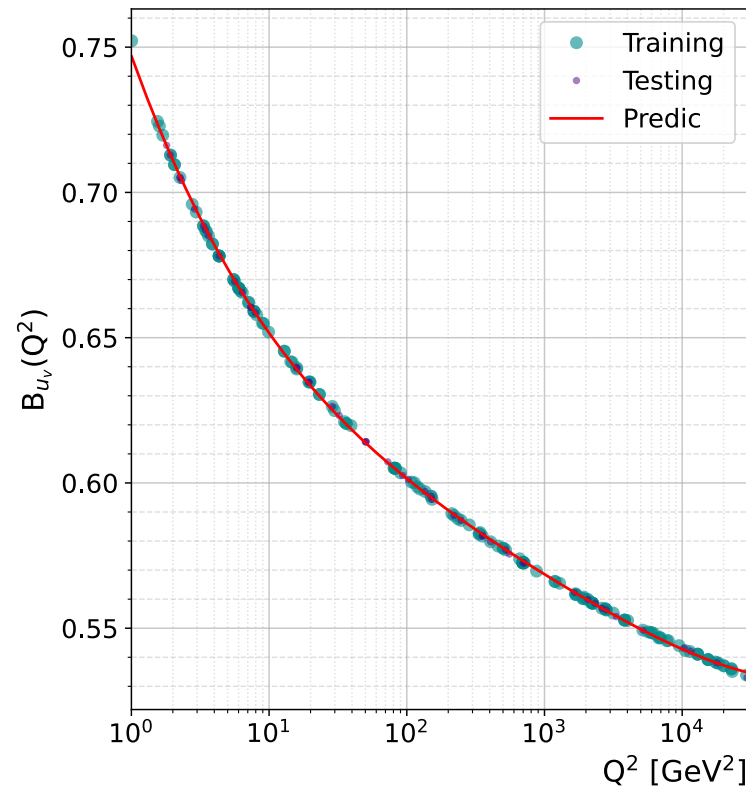
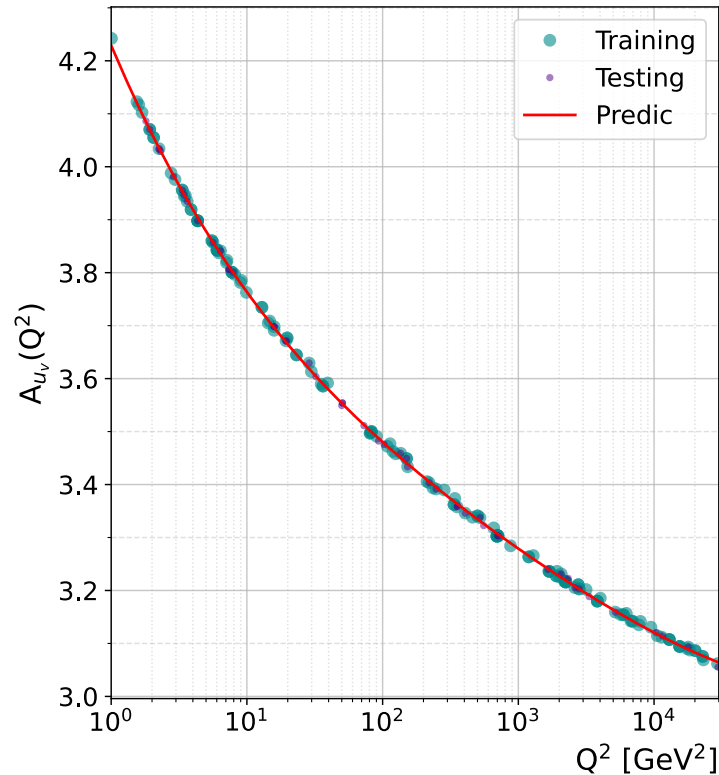
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Machine Learning for PDFs

xu_ν distribution coefficients

- We use ML to find all coefficients.

More details in: [Phys. Rev. D 110, 036019 \[hep-ph\]](#)

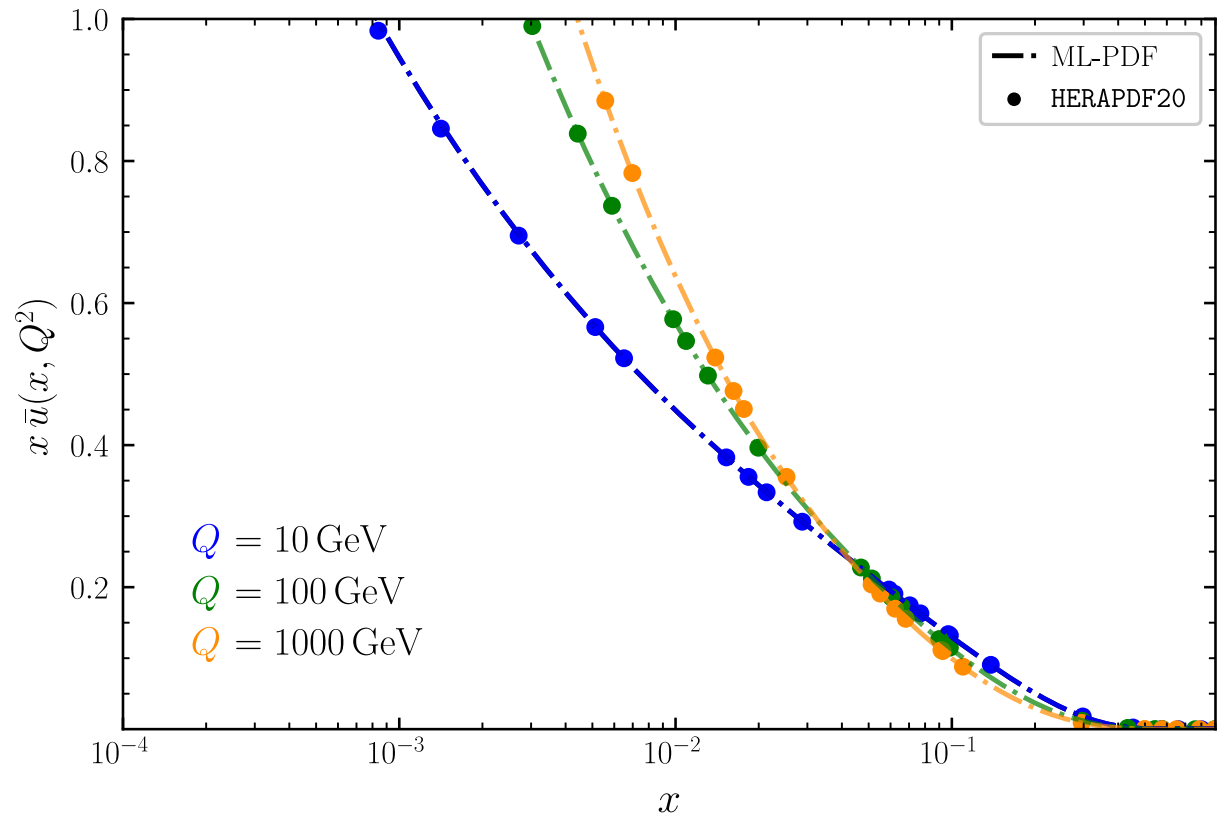
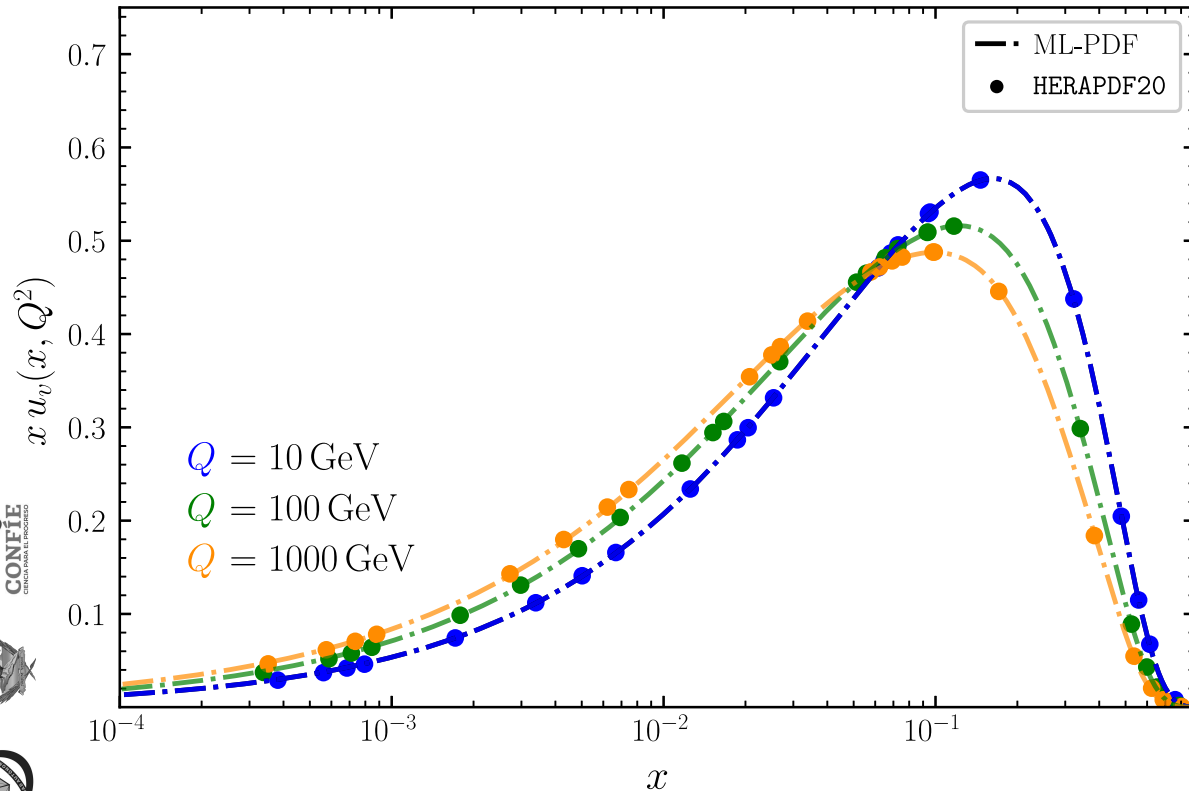


- For this particular case, a **polynomial function** was sufficient. In many cases it was necessary to propose a **more complicated basis**.



Machine Learning for PDFs

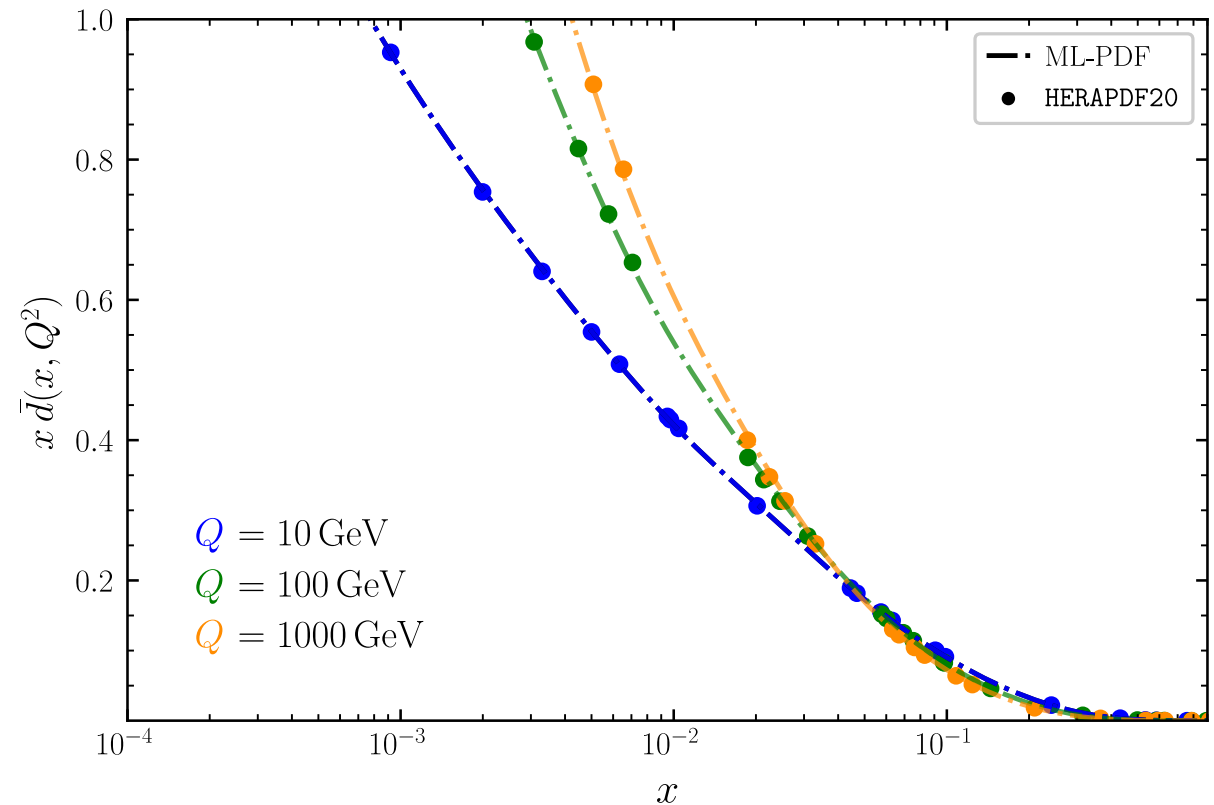
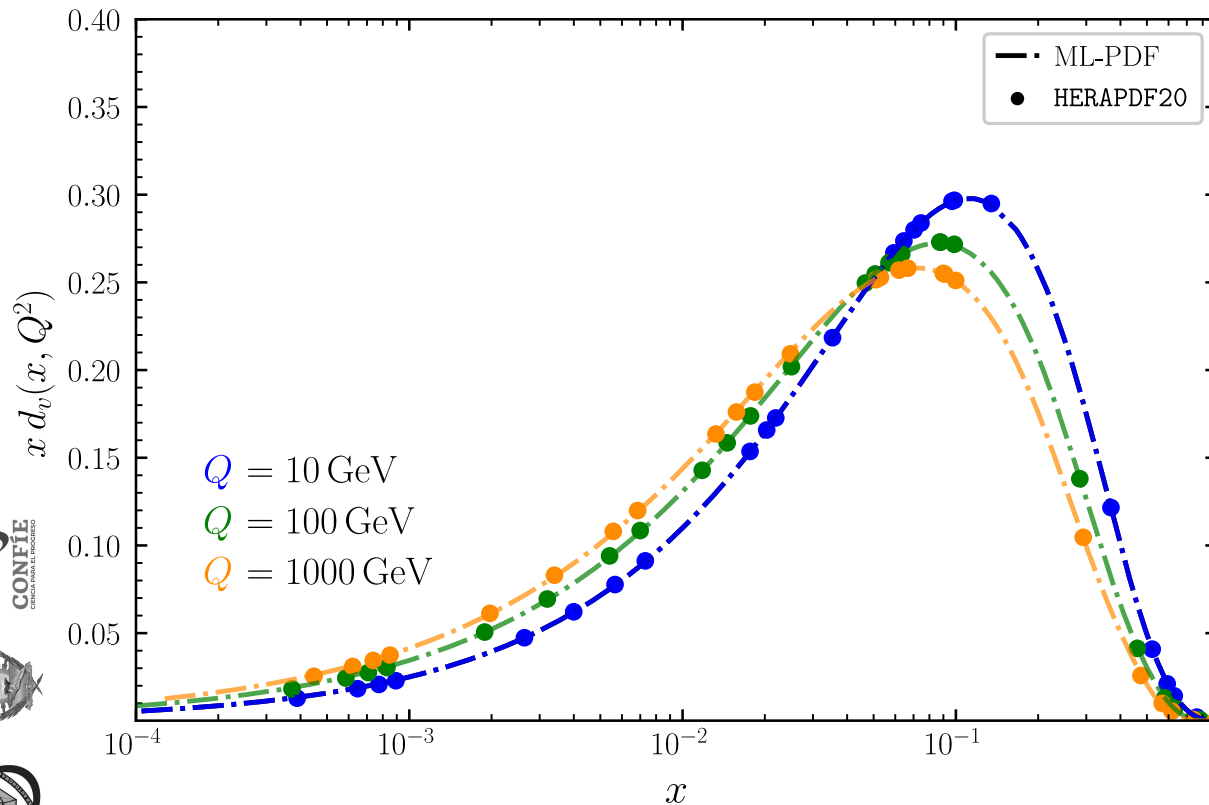
Up quark distributions



- We found a **good agreement** and only use **one region to $x\bar{u}$** and **two regions to xu_v** .
- We can obtain u -quark distribution by: $xu = x\bar{u} + xu_v$

Machine Learning for PDFs

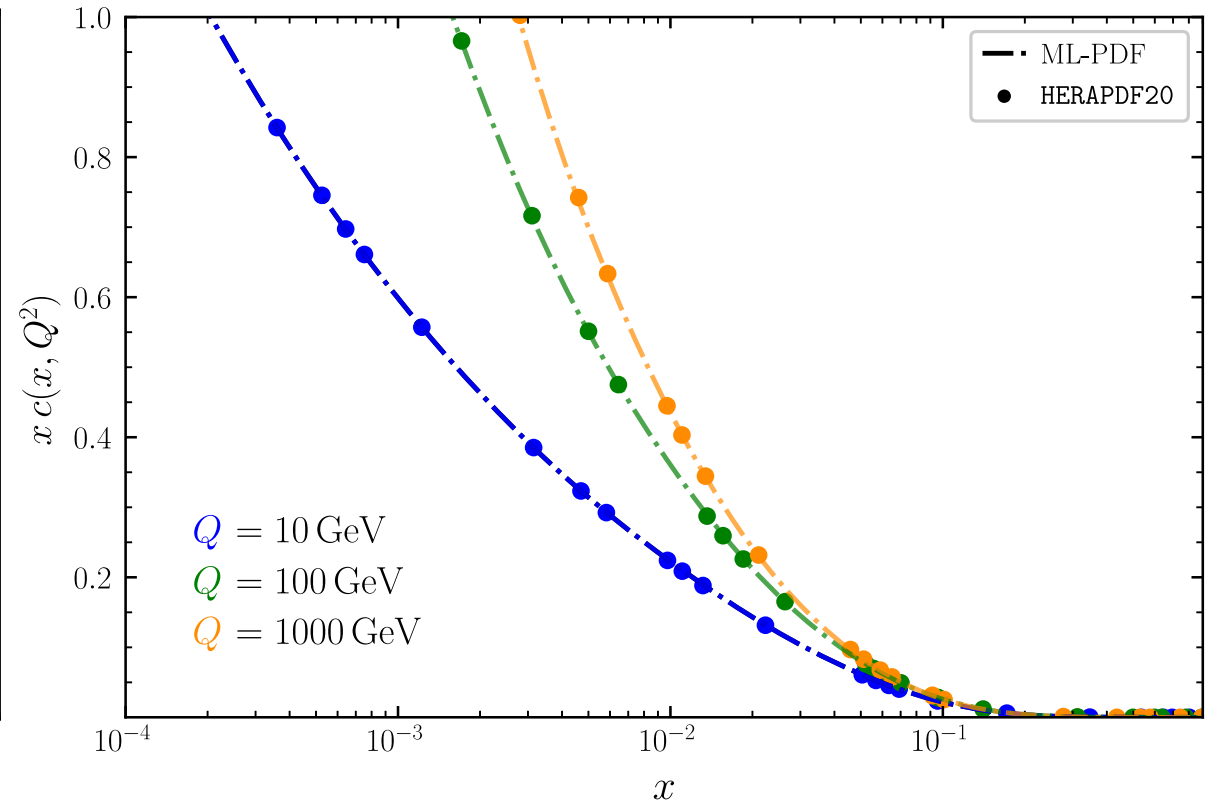
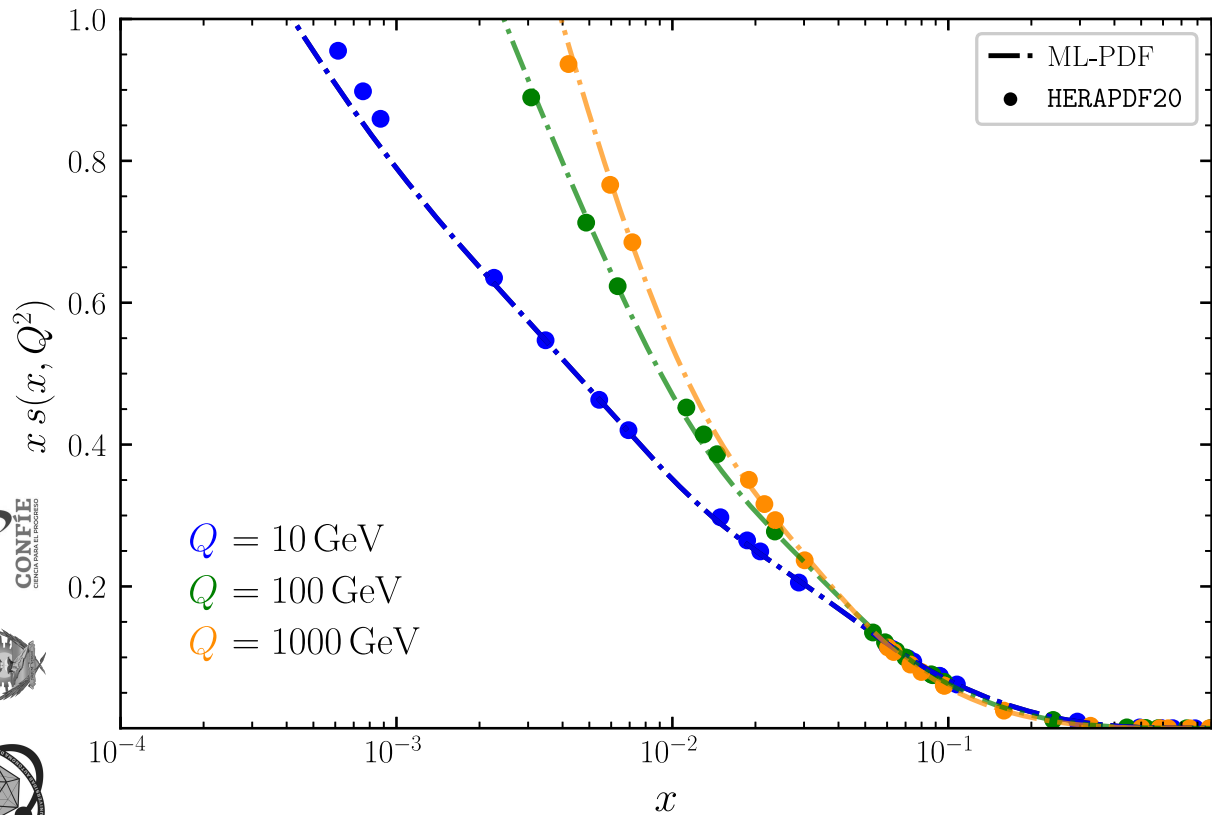
Down quark distributions



- Similar to the u -quark, we found a **good agreement** and in this case we only use **one region** to both distributions.
- Similarly, d -quark distribution by: $xd = x\bar{d} + xd_v$

Machine Learning for PDFs

Strange and Charm quark distributions

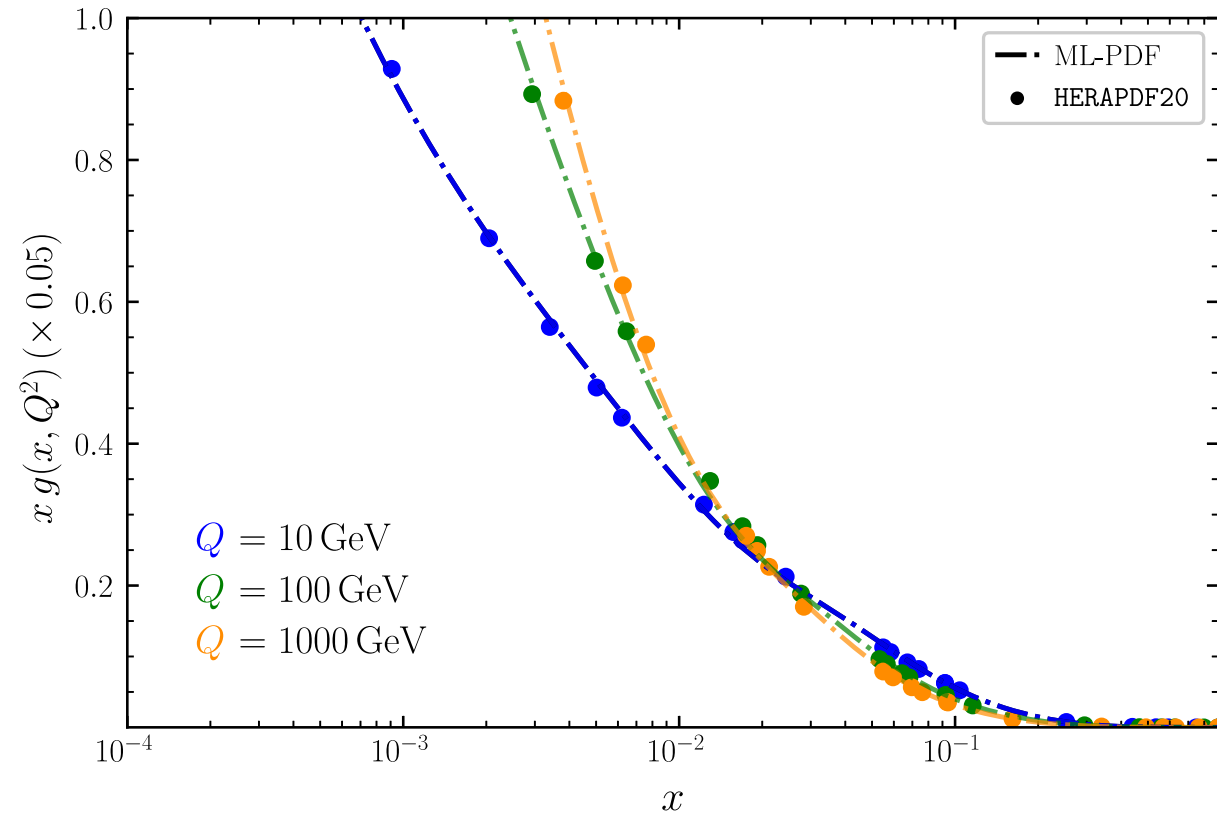
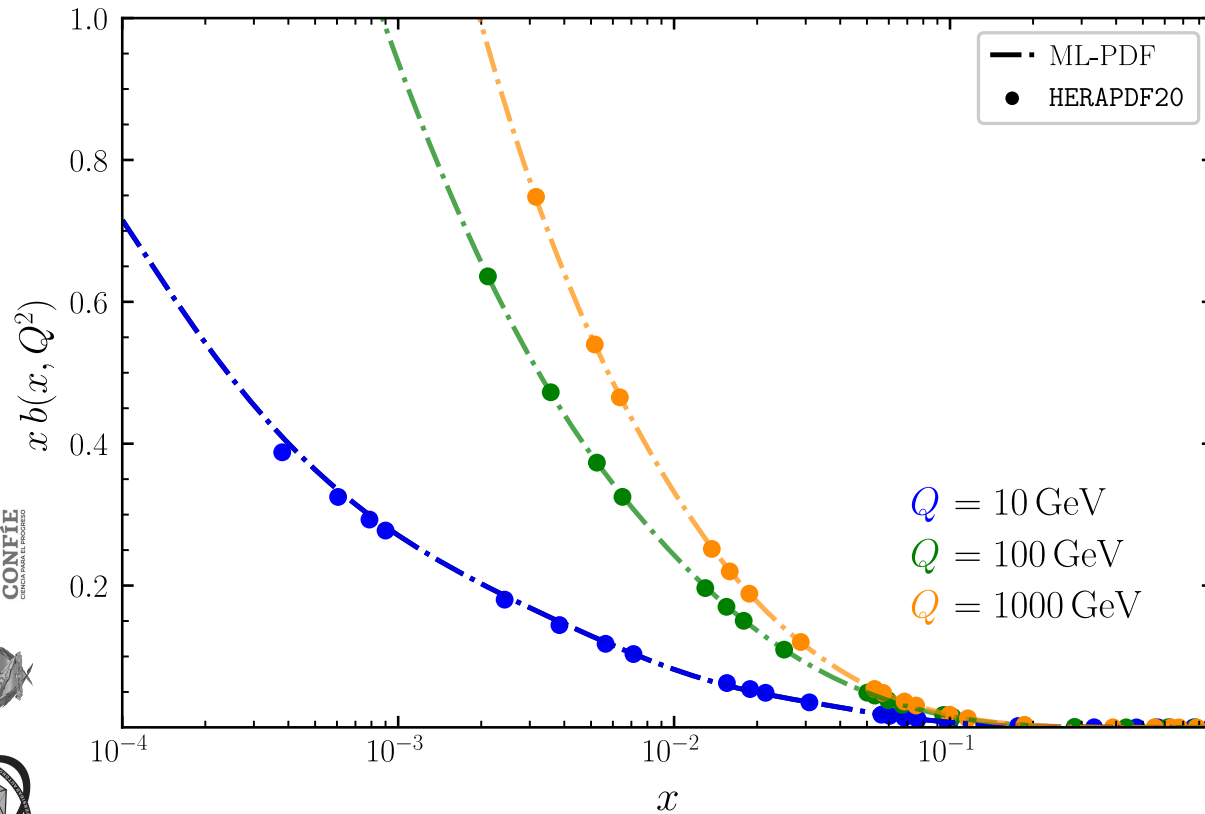


- For s -quark and c -quark we used **two regions**.
- Only **small discrepancies** for $x < 10^{-3}$ at $Q = 10$ GeV in s -quark distribution are present.



Machine Learning for PDFs

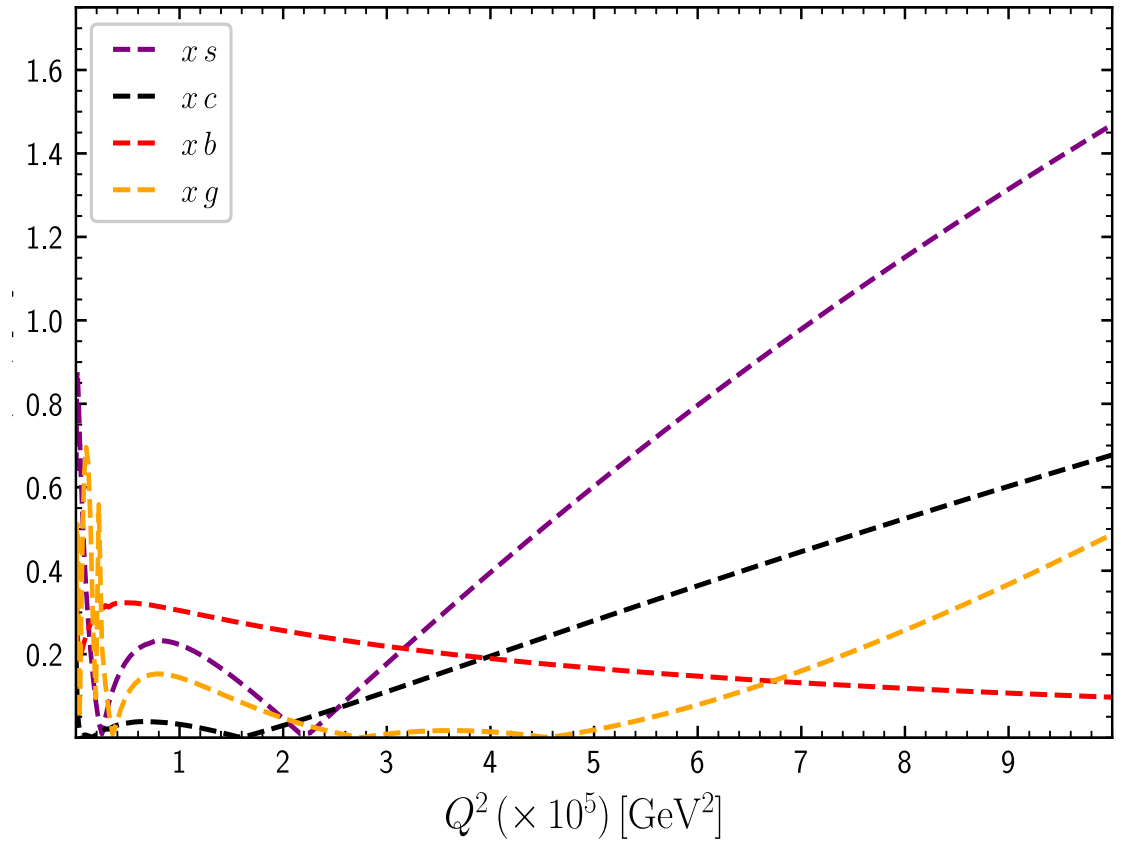
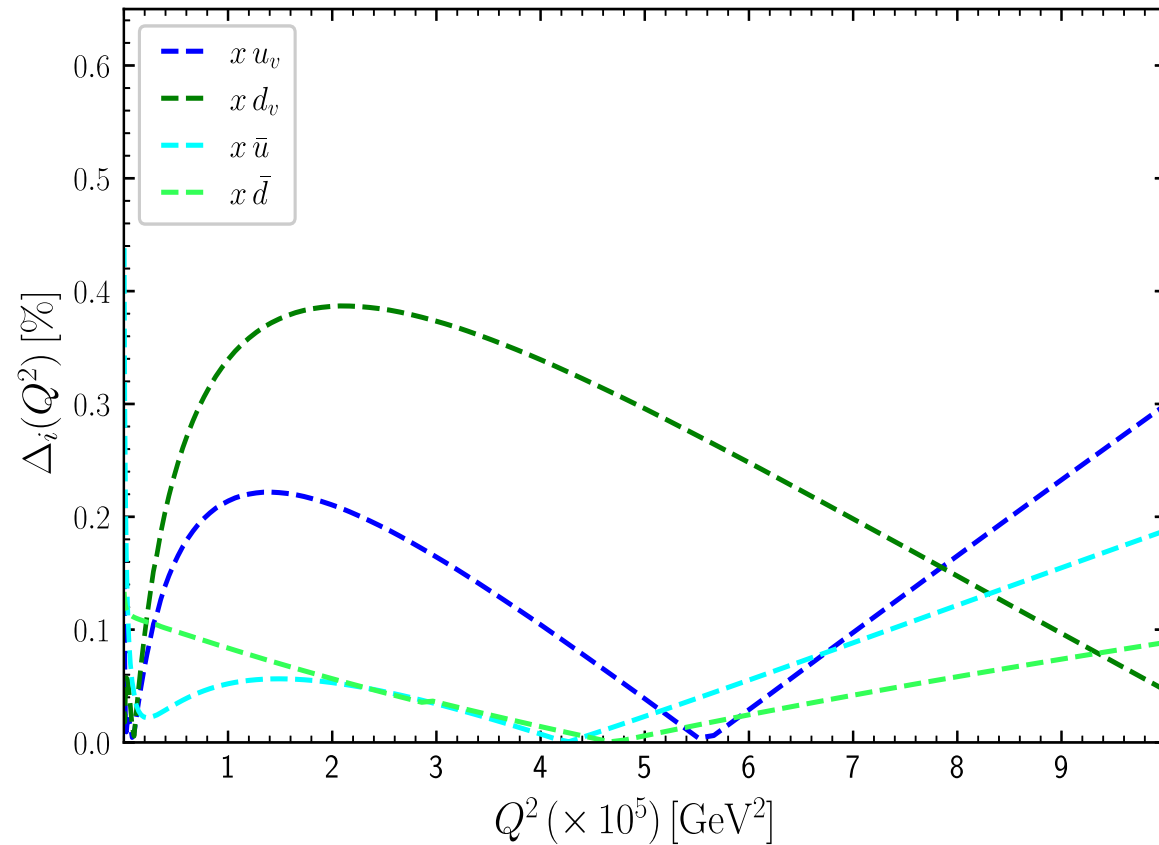
Bottom quark and Gluon distributions



- For the b -quark we split into **two regions** and for the gluon we split into **four regions**.
- **Small deviations** of the central value for $x < 10^{-3}$ in b -quark were found.

Results

How good is good ?



- The estimator $\Delta_i(Q^2)$ shows **small integral error** (maximum of 1.5% for all partons)

Results

How fast is fast?

$$\text{Gain}(\%) = 100 \times \frac{\text{time}_{\text{LHAPDF}} - \text{time}_{\text{ML-PDF}}}{\text{time}_{\text{LHAPDF}}}$$

N_{points}	LHAPDF (s)	ML-PDFs (s)	Gain(%)
10^3	$3.76 \cdot 10^{-2}$	$2.92 \cdot 10^{-4}$	99.22
10^4	$4.20 \cdot 10^{-2}$	$2.50 \cdot 10^{-3}$	94.05
10^5	$8.94 \cdot 10^{-2}$	$2.50 \cdot 10^{-2}$	72.10
10^6	0.56	0.25	55.46
10^7	5.25	2.50	52.49
10^8	52.04	24.92	52.11

- Comparison of the time (in seconds) required to compute N_{points} evaluations of HERAPDF2.0 within LHAPDF framework, and our ML-PDF analytic approximation.
- The gains seems to approach a **plateau around 50%**.

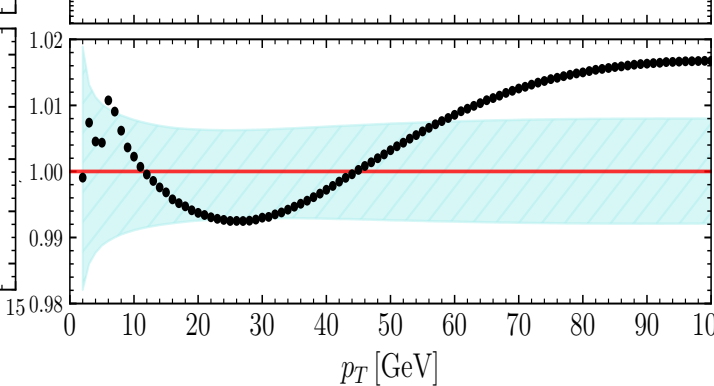
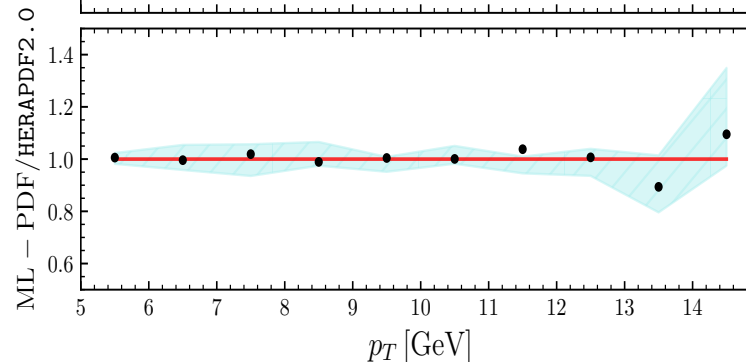
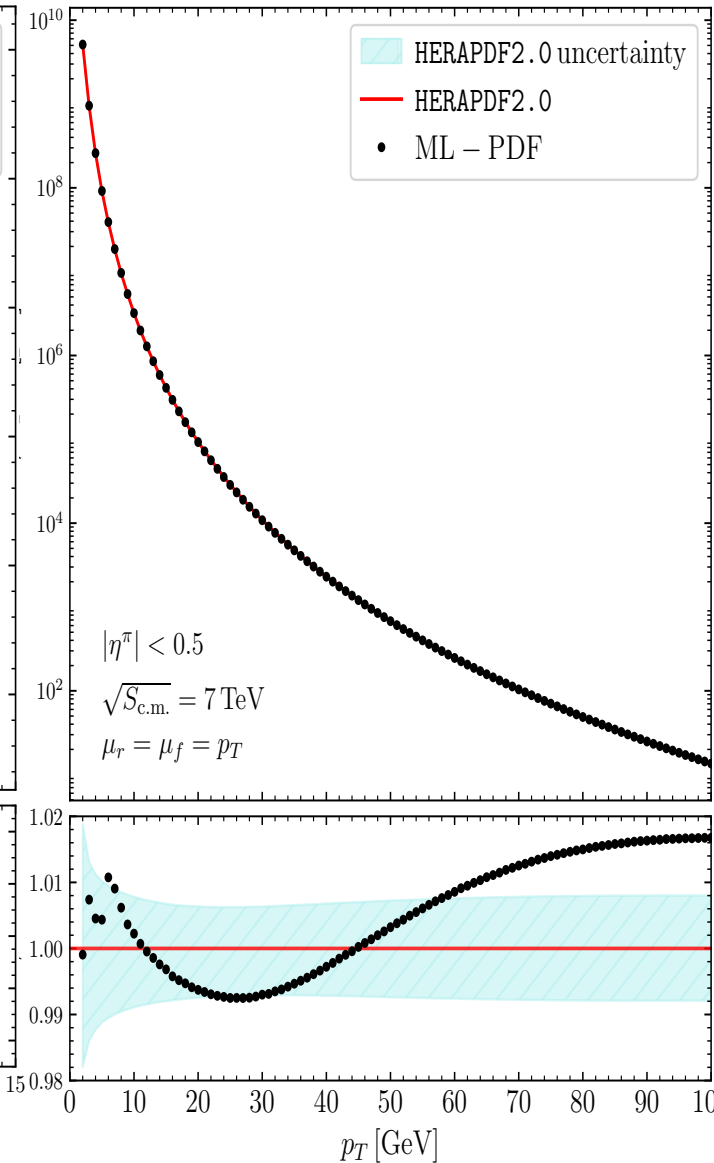
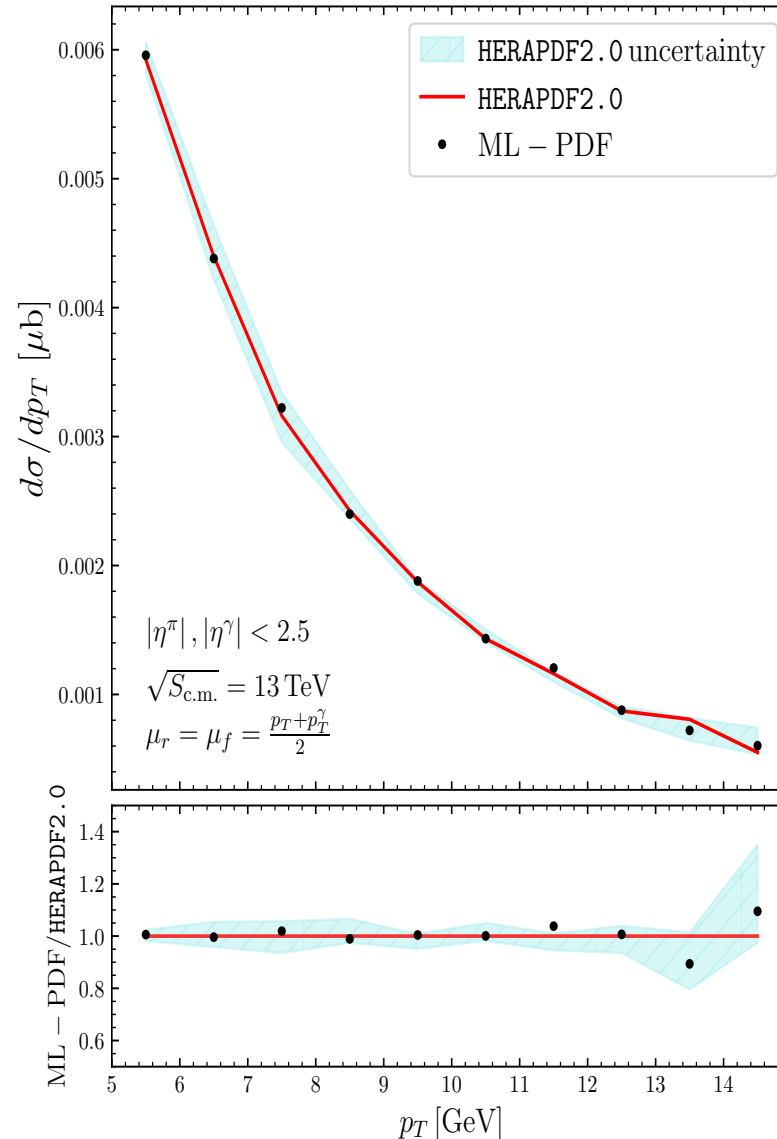


Results

The final test ...

- We test our results with two observables:
 - $p + p \rightarrow \pi$ and
 - $p + p \rightarrow \pi + \gamma$ at NLO.
- We find an almost perfect agreement ($\approx 1\%$ difference)
- Time consumption is also improved!

Obs.	LHAPDF (s)	ML-PDFs (s)	Gain(%)
$p + p \rightarrow \pi$	628.320	558.854	11.06
$p + p \rightarrow \gamma + \pi$	12452.273	8671.827	30.36



Results

The final test


Published July 15, 2024 | Version v2

Computational notebook

Open

Ancillary files for "Using analytic models to describe effective PDFs"

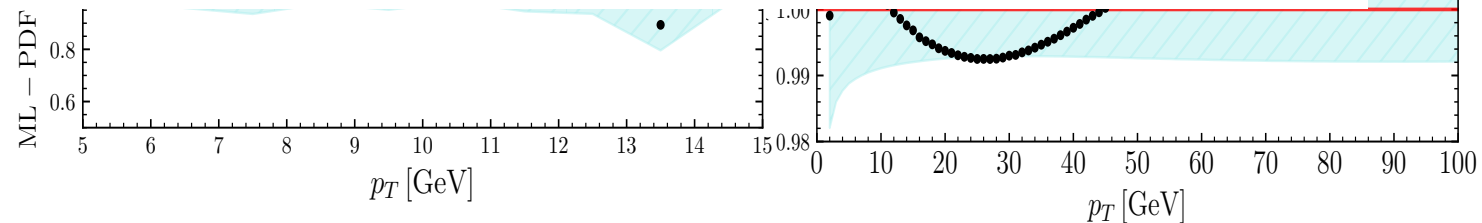
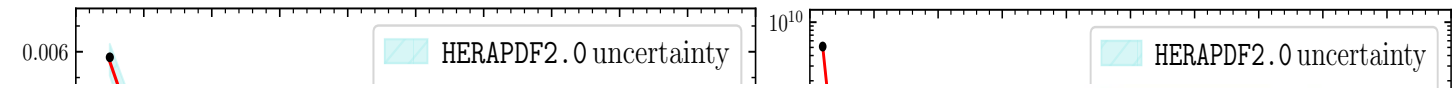
Ochoa-Oregon, Salvador (Researcher)¹ 

Rentería-Estrada, David (Researcher)² 

Hernández-Pinto, Roger (Researcher)¹ ; Sborlini, German (Researcher)³ 

Zurita, Pía (Researcher)⁴ 

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S. A. Ochoa-Oregon et al arXiv:2404.15175 [hep-ph].

FF: DEHSS2014



Conclusions

- **PDFs** are **key ingredients** for any phenomenological theoretical predictions.
- Since MC simulations are taking the CPU cost to the extreme, we exploited ML to extract **analytical PDFs** to avoid running interpolations techniques.
- We compared our results w.r.t. LHAPDF within **two benchmarks** finding an **improvement in the CPU time** of around **11%** for $p + p \rightarrow \pi$ and more than **30%** for $p + p \rightarrow \pi + \gamma$, both at NLO.
- The code (FORTRAN) with the PDFs can be found at **<https://zenodo.org/records/12745978>**.



THANKS!



BACKUP SLIDES



Regions

xu_ν distribution

$$R_1 = \{Q_0 \leq Q \leq 10 \text{ GeV}\}$$

$$R_2 = \{10 \text{ GeV} \leq Q \leq 1000 \text{ GeV}\}$$

xs distribution

$$R_1 = \{Q_0 \leq Q \leq 4.5 \text{ GeV}\}$$

$$R_2 = \{4.5 \text{ GeV} \leq Q \leq 1000 \text{ GeV}\}$$

xb distribution

$$R_1 = \{4.5 \leq Q \leq 15 \text{ GeV}\}$$

$$R_2 = \{15 \text{ GeV} \leq Q \leq 1000 \text{ GeV}\}$$

xc distribution

$$R_1 = \{1.47 \leq Q \leq 3 \text{ GeV}\}$$

$$R_2 = \{3 \text{ GeV} \leq Q \leq 1000 \text{ GeV}\}$$

xg distribution

$$R_1 = \{Q_0 \leq Q \leq 2.5 \text{ GeV}\}$$

$$R_2 = \{2.5 \text{ GeV} \leq Q \leq 5 \text{ GeV}\}$$

$$R_3 = \{5 \text{ GeV} \leq Q \leq 5 \text{ GeV}\}$$

$$R_4 = \{150 \text{ GeV} \leq Q \leq 1000 \text{ GeV}\}$$



Functional Forms

Up distributions

$$xu_v(x, Q^2) = A_{u_v}(Q^2)x^{B_{u_v}(Q^2)}(1-x)^{C_{u_v}(Q^2)} \\ \times [1 + D_{u_v}(Q^2)x + E_{u_v}(Q^2)x^2 \\ + F_{u_v}(Q^2)x^3 + G_{u_v}(Q^2)x^4 + H_{u_v}(Q^2)x^5]$$

For R_1 :

$$x\bar{u}(x, Q^2) = A_{\bar{u}}(Q^2)x^{B_{\bar{u}}(Q^2)}(1-x)^{C_{\bar{u}}(Q^2)} \\ \times [1 + D_{\bar{u}}(Q^2)x + E_{\bar{u}}(Q^2)x^2 \\ + F_{\bar{u}}(Q^2)x^3 + G_{\bar{u}}(Q^2)x^4 + H_{\bar{u}}(Q^2)x^5]$$

For R_2 :

$$x\bar{u}(x, Q^2) = A_{\bar{u}}(Q^2)x^{B_{\bar{u}}(Q^2)}(1-x)^{C_{\bar{u}}(Q^2)} \\ \times [1 + D_{\bar{u}}(Q^2)x + E_{\bar{u}}(Q^2)x^2 \\ + F_{\bar{u}}(Q^2)x^3 + G_{\bar{u}}(Q^2)x^4 + H_{\bar{u}}(Q^2)x^5]$$

Down distributions

$$xd_v(x, Q^2) = A_{d_v}(Q^2)x^{B_{d_v}(Q^2)}(1-x)^{C_{d_v}(Q^2)} \\ \times [1 + D_{d_v}(Q^2)x^2 + E_{d_v}(Q^2)x^4 \\ + F_{d_v}(Q^2)x^6],$$

$$x\bar{d}(x, Q^2) = A_{\bar{d}}(Q^2)x^{B_{\bar{d}}(Q^2)}(1-x)^{C_{\bar{d}}(Q^2)} \\ - \Theta(x_{C,\bar{d}} - x)A'_{\bar{d}}(Q^2)x^{B'_{\bar{d}}(Q^2)}(1-x)^{C'_{\bar{d}}(Q^2)} \\ \times [1 + D'_{\bar{d}}(Q^2)x^2 + E'_{\bar{d}}(Q^2)x^4],$$



Strange distribution

For R_1 :

$$x s(x, Q^2) = A_s(Q^2) x^{B_s(Q^2)} (1-x)^{C_s(Q^2)} \\ - \Theta(x_{C,s}(R_1) - x) A'_s(Q^2) x^{B'_s(Q^2)} \\ \times (1-x)^{C'_s(Q^2)}$$

For R_2 :

$$x s(x, Q^2) = A_s(Q^2) x^{B_s(Q^2)} (1-x)^{C_s(Q^2)} \\ - \Theta(x_{C,s}(R_2) - x) A'_s(Q^2) x^{B'_s(Q^2)} \\ \times (1-x)^{C'_s(Q^2)} [1 + D'_s(Q^2) x^2]$$

Charm distribution

For R_1 :

$$x c(x, Q^2) = A_c(Q^2) x^{B_c(Q^2)} (1-x)^{C_c(Q^2)} [1 + D_c(Q^2) x^2] \\ - \Theta(x_{C,c}(R_1) - x) A'_c(Q^2) x^{B'_c(Q^2)} \\ \times (1-x)^{C'_c(Q^2)} [1 + D'_c(Q^2) x^2]$$

For R_1, R_2 :

$$x c(x, Q^2) = A_c(Q^2) x^{B_c(Q^2)} (1-x)^{C_c(Q^2)} \\ \times (1 + D_c(Q^2) x + E_c(Q^2) x^2) \\ - \Theta(x_{C,c}(R_2) - x) A'_c(Q^2) x^{B'_c(Q^2)} \\ \times (1-x)^{C'_c(Q^2)} (1 + D'_c(Q^2) x^2)$$



Bottom distribution

For R_1 :

$$\begin{aligned}
 xb(x, Q^2) &= A_b(Q^2)x^{B_b(Q^2)}(1-x)^{C_b(Q^2)}[1 + D_b(Q^2)x^2] \\
 &\quad - \Theta(x_{C,b}(R_1) - x)A'_b(Q^2)x^{B'_b(Q^2)} \\
 &\quad \times (1-x)^{C'_b(Q^2)}[1 + D'_b(Q^2)x^2]
 \end{aligned}$$

For R_2 :

$$\begin{aligned}
 xb(x, Q^2) &= A_b(Q^2)x^{B_b(Q^2)}(1-x)^{C_b(Q^2)} \\
 &\quad \times [1 + D_b(Q^2)x + E_b(Q^2)x^2] \\
 &\quad - \Theta(x_{C,b}(R_2) - x)A'_b(Q^2)x^{B'_b(Q^2)} \\
 &\quad \times (1-x)^{C'_b(Q^2)}[1 + D'_b(Q^2)x^2],
 \end{aligned}$$

Gluon distribution

For R_1 :

$$\begin{aligned}
 xg(x, Q^2) &= A_g(Q^2)x^{B_g(Q^2)}(1-x)^{C_g(Q^2)} \\
 &\quad - \Theta(x_{C,g} - x)A'_g(Q^2)x^{B'_g(Q^2)} \\
 &\quad \times (1-x)^{C'_g(Q^2)}
 \end{aligned}$$

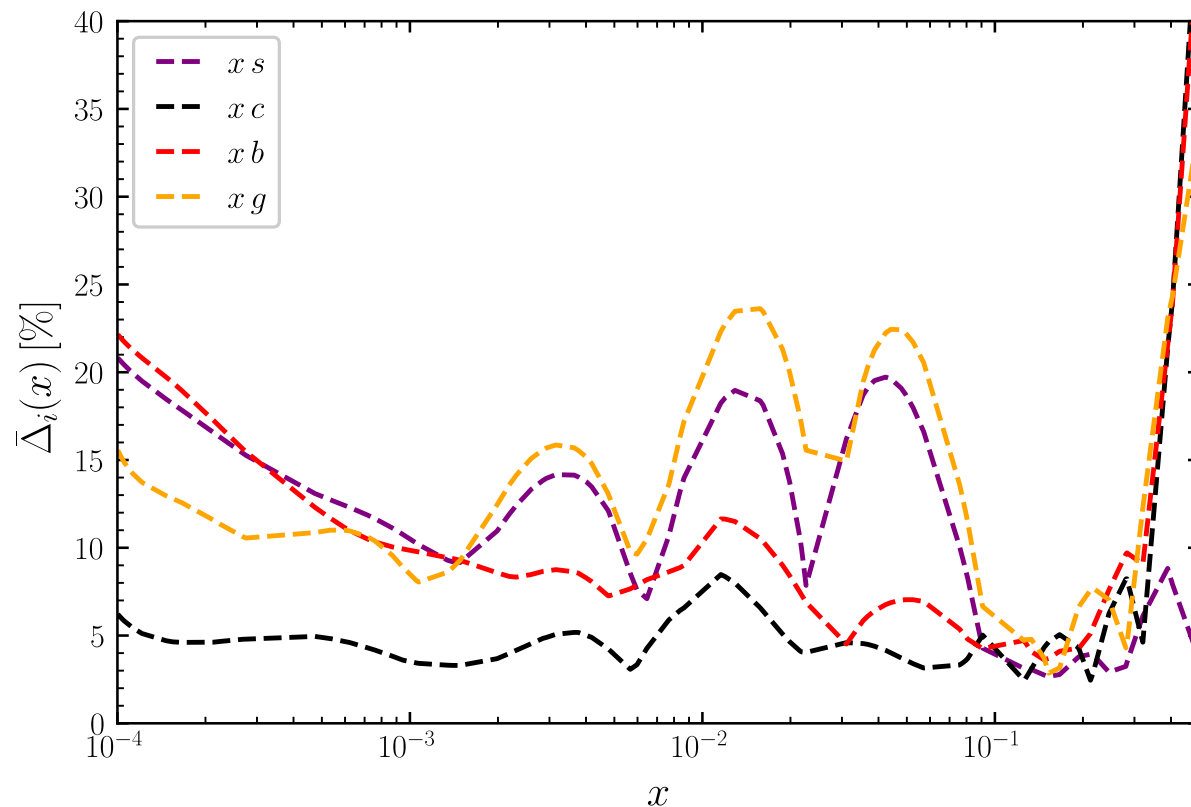
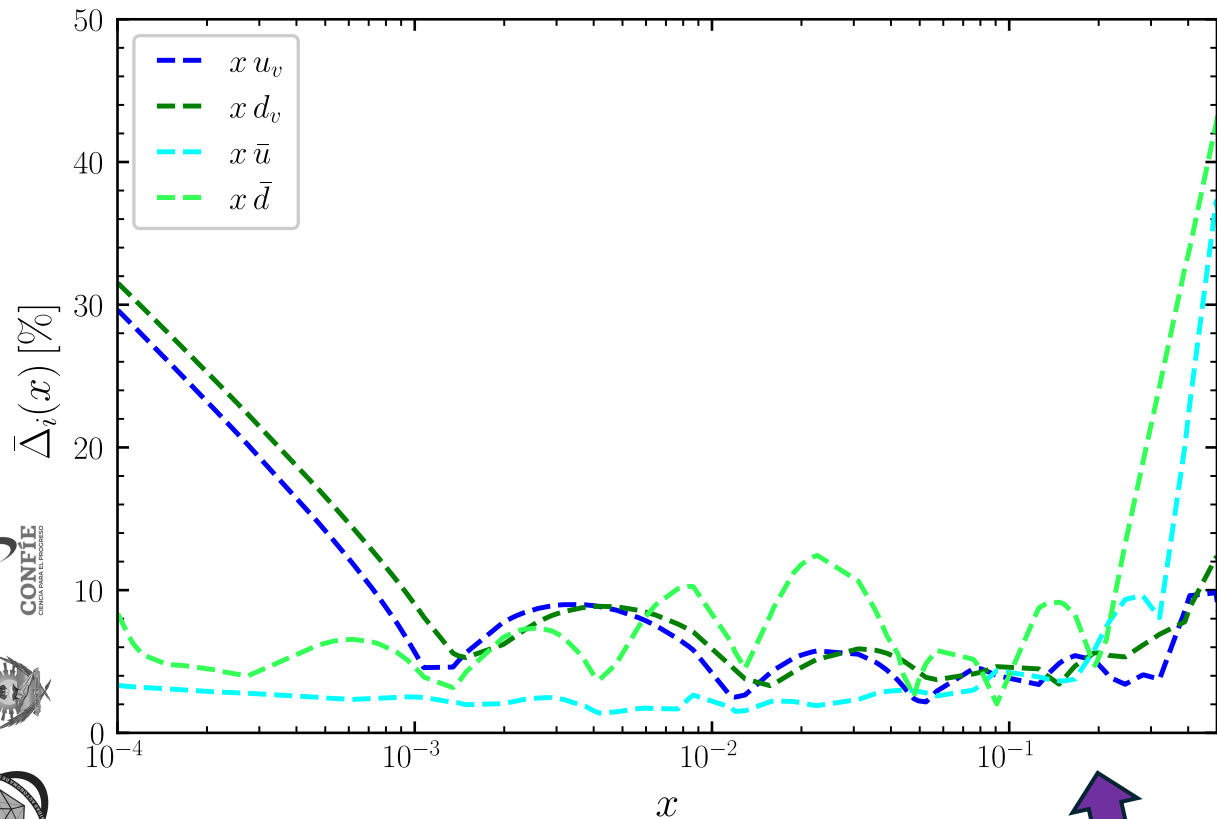
For R_1, R_2 and R_3 :

$$\begin{aligned}
 xg(x, Q^2) &= A_g(Q^2)x^{B_g(Q^2)}(1-x)^{C_g(Q^2)} \\
 &\quad - \Theta(x_{C,g} - x)A'_g(Q^2)x^{B'_g(Q^2)} \\
 &\quad \times (1-x)^{C'_g(Q^2)}
 \end{aligned}$$



Another Cost-Function

Error Shape



$N = 50,000$ and $Q \in \{10 \text{ GeV}, 1000 \text{ GeV}\}$

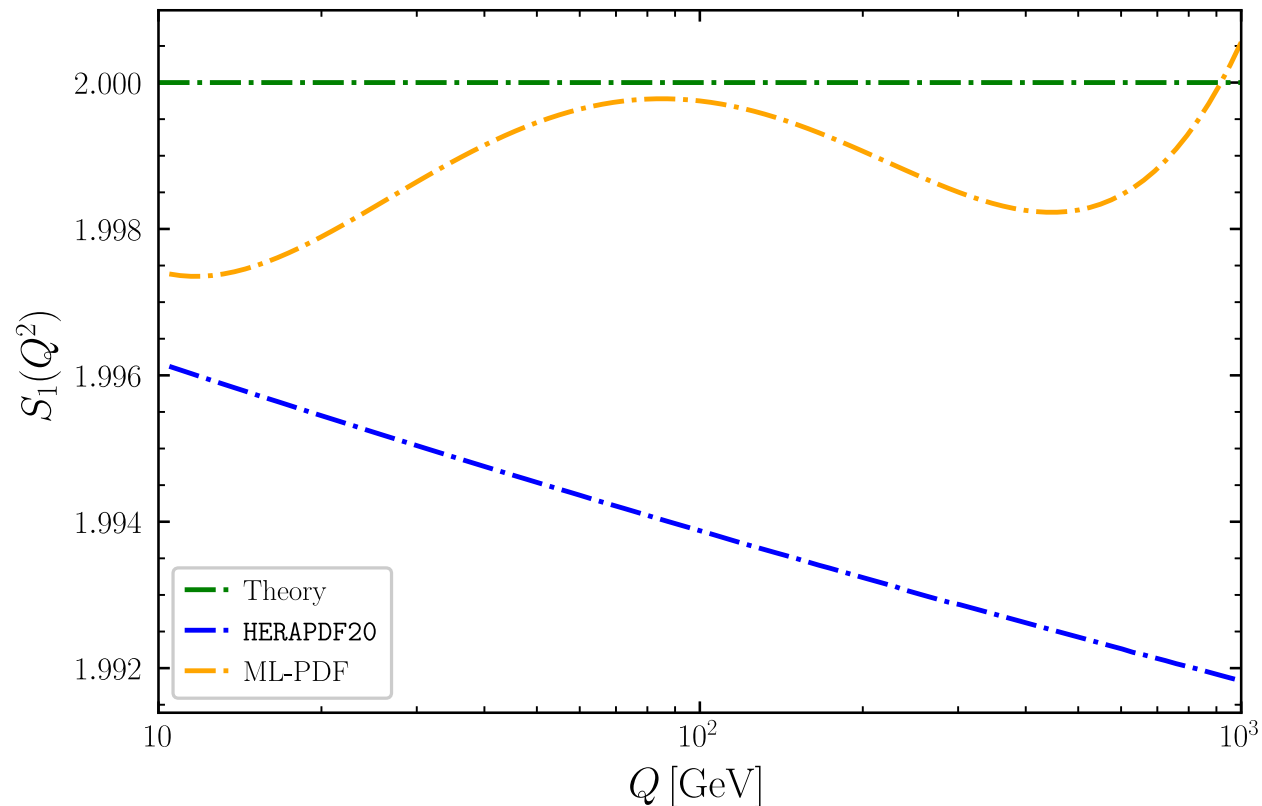
$$\bar{\Delta}_i(x) = \frac{1}{N} \sum_{j=1}^N \left| 1 - \frac{f_i^{\text{ML}}(x, Q_j^2)}{f_i^{\text{HERA}}(x, Q_j^2)} \right|$$



Validity of the sum rules

Sum rules for any energy scale Q

$$S_1(Q^2) = \int_0^1 dx u_v(x, Q^2) = 2 \quad S_2(Q^2) = \int_0^1 dx d_v(x, Q^2) = 1 \quad S_3(Q^2) = \int_0^1 dx x \left[g(x, Q^2) + \sum_{i \in \{q, \bar{q}\}} f_i(x, Q^2) \right] = 1$$



Validity of the sum rules

Sum rules for any energy scale Q

