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A NEW GENERATION OF SIMULTANEOUS FITS TO LHC DATA USING DEEP LEARNING

DIS2022 - SANTIAGO DE COMPOSTELA

4TH MAY 2022

OUTLINE

- Introduction:
 - ➔ Simultaneous fits of PDFs and physics parameters at the LHC

- The SimuNET methodology
(based on [S. Iranipour, MU, arXiv:2201.07240](#))
 - ➔ The approach
 - ➔ Application to the determination of PDFs and SMEFT coefficients

- Conclusions and outlook

INTRODUCTION

EXTRACTING PHYSICS PARAMETERS FROM LHC DATA

✓ Abundance of precise LHC data allows to extract information on SM and BSM parameters & non-perturbative objects such as PDFs with unprecedented precision

$$\chi^2 = \frac{1}{N_{\text{dat}}} \sum_{i=1}^{N_{\text{dat}}} (T_i(\{\theta\}, \{c\}) - D_i) \text{cov}_{ij}^{-1} (T_j(\{\theta\}, \{c\}) - D_j)$$

$$T_i(\{\theta\}, \{c\}) = \text{PDFs}(\{\theta\}, \{c\}) \otimes \hat{\sigma}_i(\{c\})$$

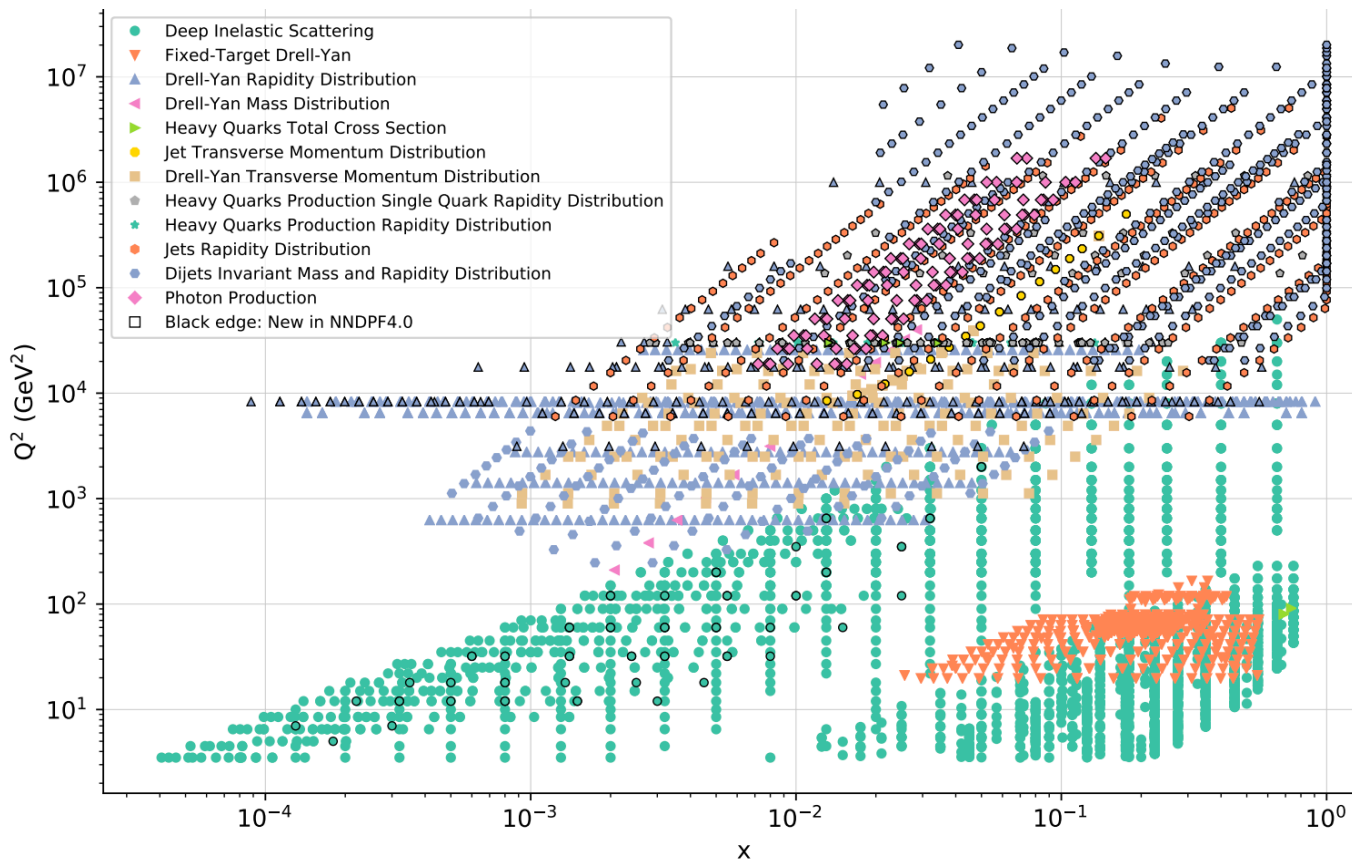


(B)SM parameters: $\alpha_s(M_z), M_w, \theta_w, \text{SMEFT WCs}, \dots$

Parameters determining PDFs at initial scale

✓ In a PDF fit typically

$$T_i(\{\theta\}) = \text{PDFs}(\{\theta\}, \{c = \bar{c}\}) \otimes \hat{\sigma}_i(\{c = \bar{c}\})$$



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(B)SM parameters: $\alpha_s(M_Z)$, M_W , θ_W , SMEFT WCs.....

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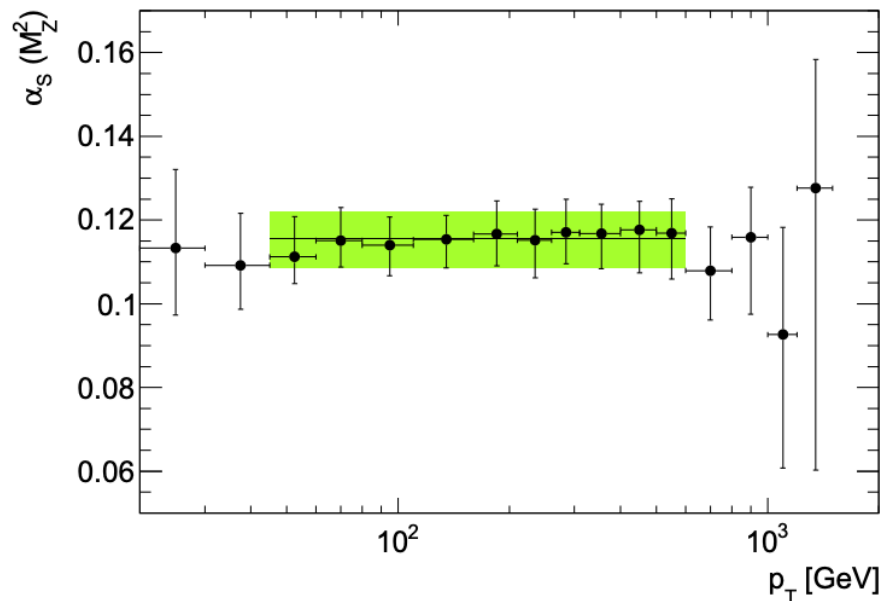
✓ In a fit of (B)SM parameters

$$T_i(\{c\}) = \text{PDFs}(\{\bar{\theta}\}, \{c\}) \otimes \hat{\sigma}_i(\{c\})$$

or - for example in case of $\alpha_s(M_Z)$ -

$$T_i(\{c\}) = \text{PDFs}(\{\bar{\theta}\}, \{c\}) \otimes \hat{\sigma}_i(\{c\})$$

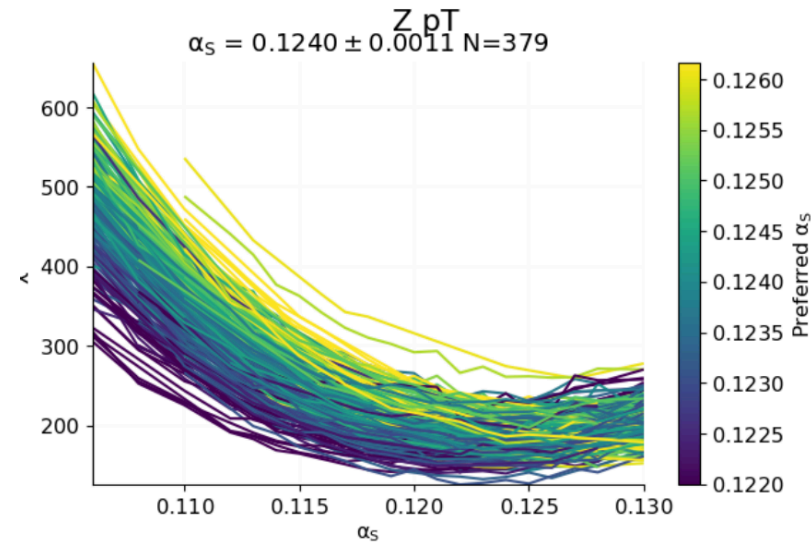
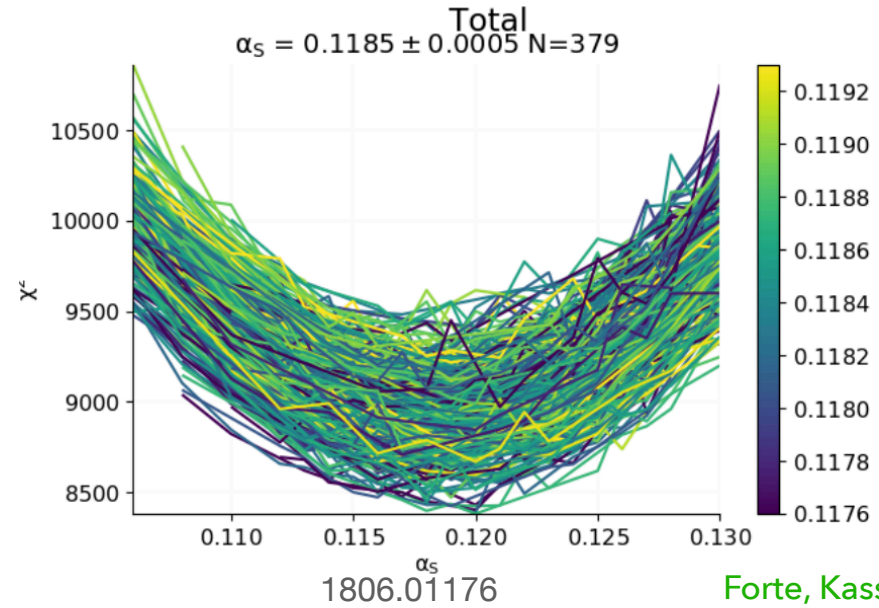
Extraction of $\alpha_s(M_Z)$ from inclusive jet xsec



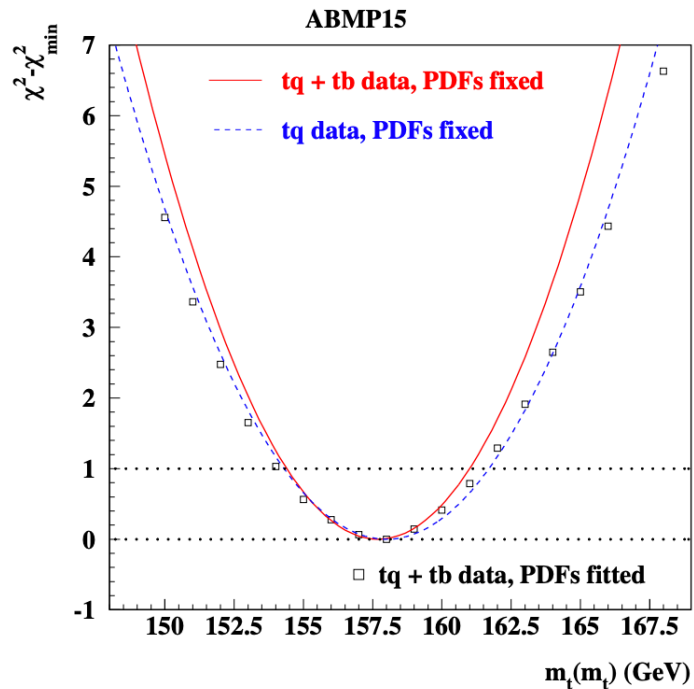
(a) $0 \leq |y| < 0.3$

SIMULTANEOUS FITS FOR SM PARAMETERS

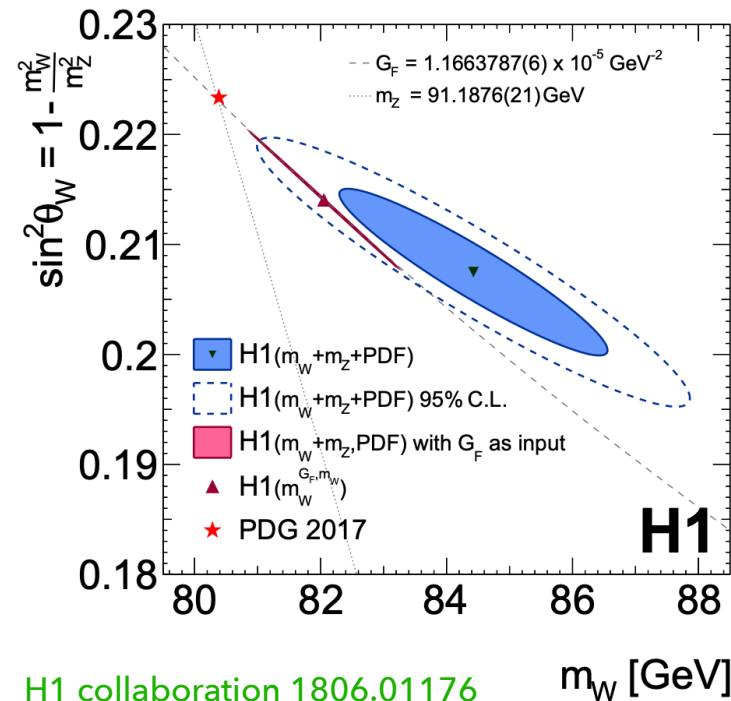
- ▶ Given the strong correlation between PDFs of the proton and α_s , a non simultaneous determination of α_s along with the PDFs from LHC processes might yield misleading results



Forte, Kassabov 2001.04986



Alekhin, Moch, Their 1608.05212



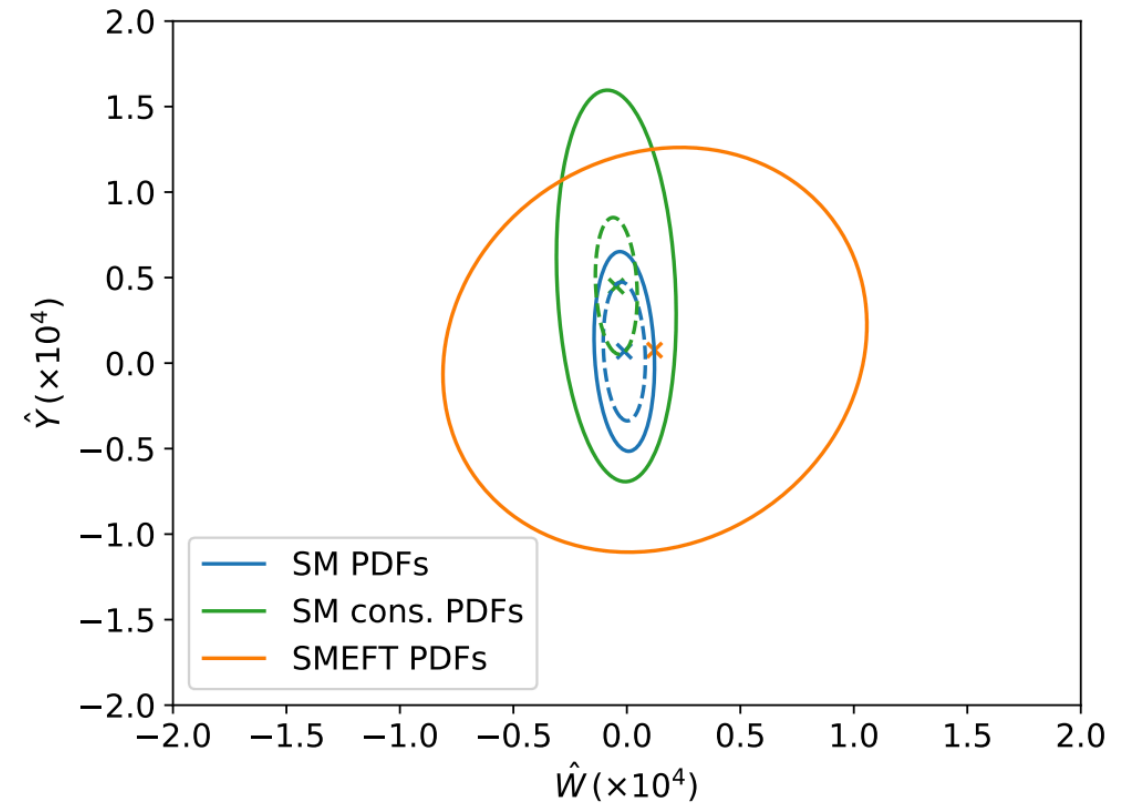
H1 collaboration 1806.01176

- ▶ Correlation of PDFs and the EW parameters or m_t weaker than in the case of α_s , but the very high accuracy which is sought suggests that the effect of simultaneous determination is not negligible
- ▶ Similar considerations for fits of polarised/unpolarised PDFs, proton/nuclear PDFs or PDFs and FFs (universal fits)

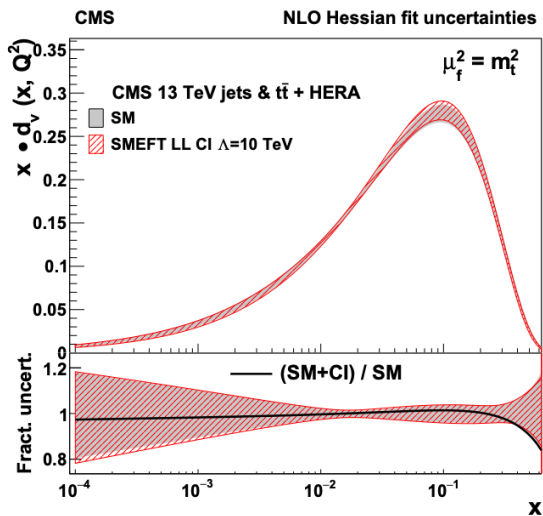
SIMULTANEOUS FITS FOR PDFS AND SMEFT

Greljo et al, 2104.02723

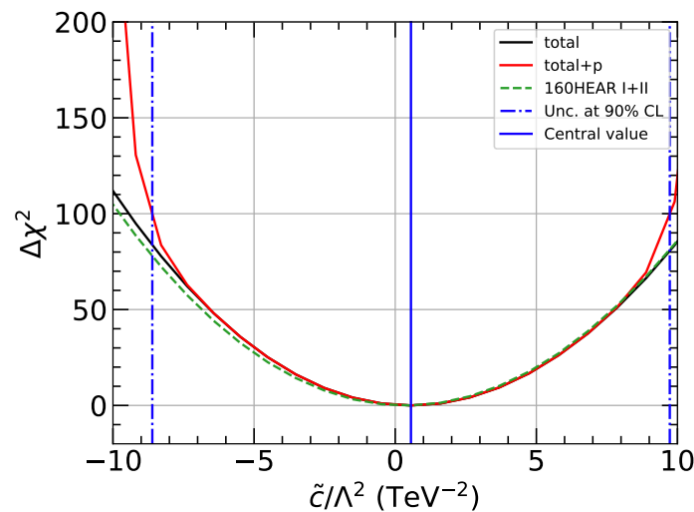
- ▶ Interplay between PDFs and new physics not negligible [Carrazza et al, 1905.05215][Greljo et al, 2104.02723] [Liu, Sun, Gao, 2201.06586] [CMS collaboration 2111.10431]
- ▶ Crucial to assess to what degree new physics might be absorbed in PDFs and how PDF treatment affects new physics bounds
- ▶ DY @ Run I+II: effect visible but within PDF uncertainties.
- ▶ DY @ HL-LHC not accounting for interplay leads to over-constrained bound [Greljo et al, 2104.02723]
- ▶ CMS analysis on inclusive jet cross section points to a non-negligible interplay [CMS collaboration, 2111.10431]



These results point towards the need of new generation of global fits, in which all ingredients that enter theoretical predictions are treated consistently.



CMS collaboration, 2111.10431



Liu, Sun, Gao, 2201.06586

THE SIMUNET METHODOLOGY

SIMUNET: A DEEP-LEARNING BASED SIMULTANEOUS FIT

- ▶ The idea: take a PDF fit based on NNPDF4.0 methodology [R. Stegeman's talk] and make dependence of observables on physics parameters $\{c_i\}$ explicit via fast interface before computing the loss function (e.g. adding SMEFT corrections, expanding observables in terms of SM precision parameters)

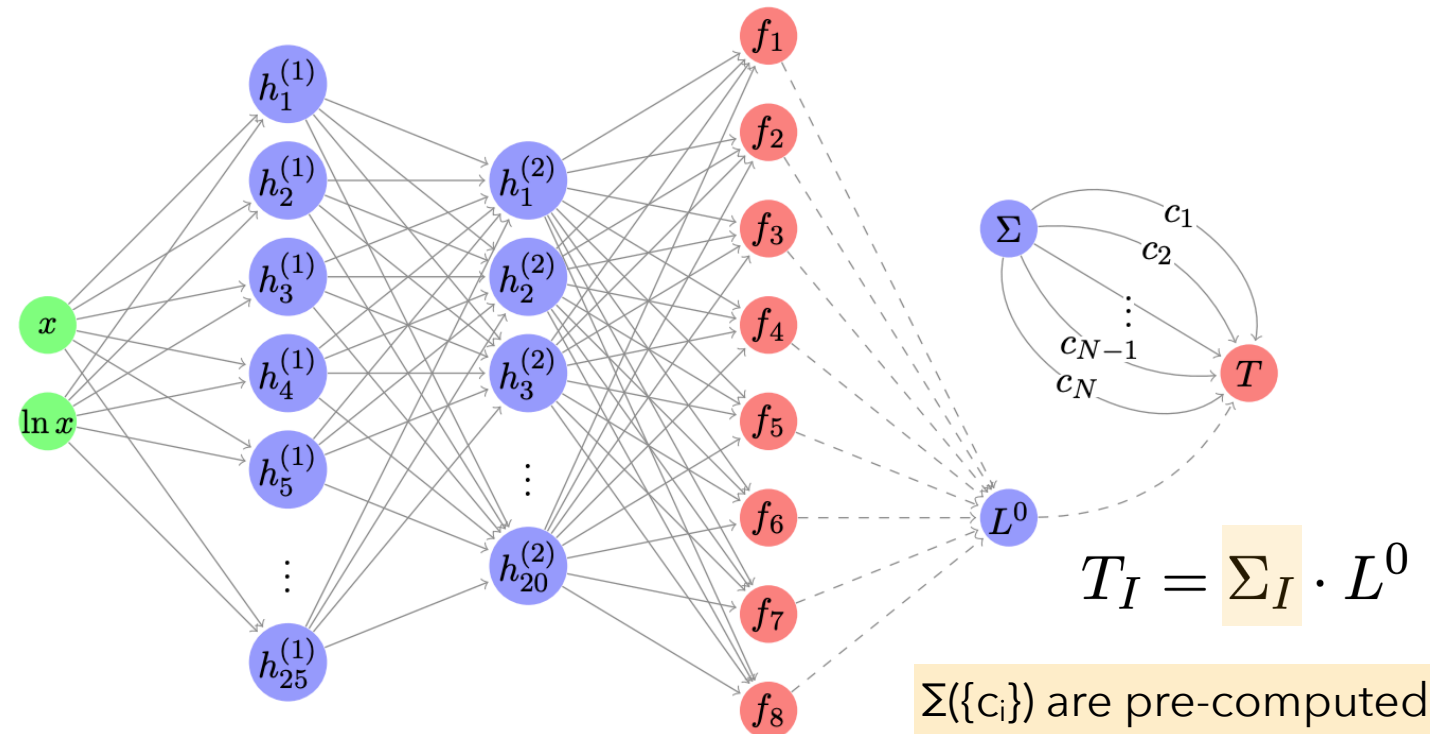
- ▶ Perform minimisation of loss function over

$$\hat{\theta} = \theta \cup \{c_i\}$$

- ▶ by adding new layer to the deep neural network used in NNPDF4.0

- ▶ Can expand dependence on c_i beyond linear terms in T (up to generic power in polynomial expansion) by adding non-trainable edges

Input layer Hidden layer 1 Hidden layer 2 PDF flavours Convolution step Theory prediction

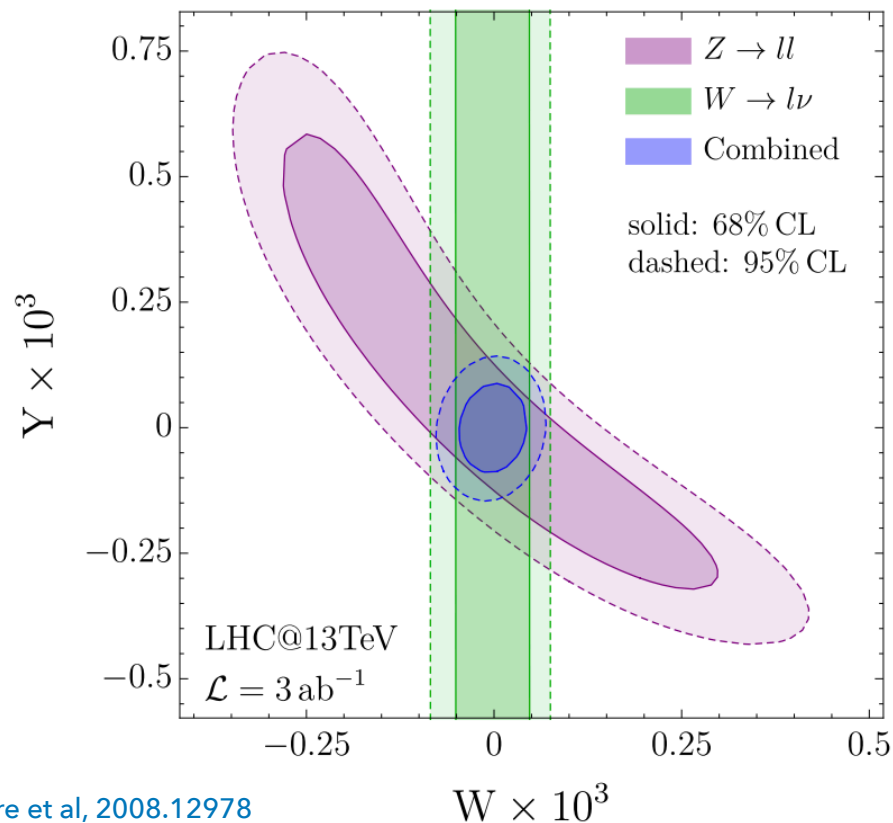


$\Sigma(\{c_i\})$ are pre-computed tables for fast interface accounting for PDF evolution and part. xsec

APPLICATION TO SIMULTANEOUS DETERMINATION OF PDFS AND SMEFT WC_s

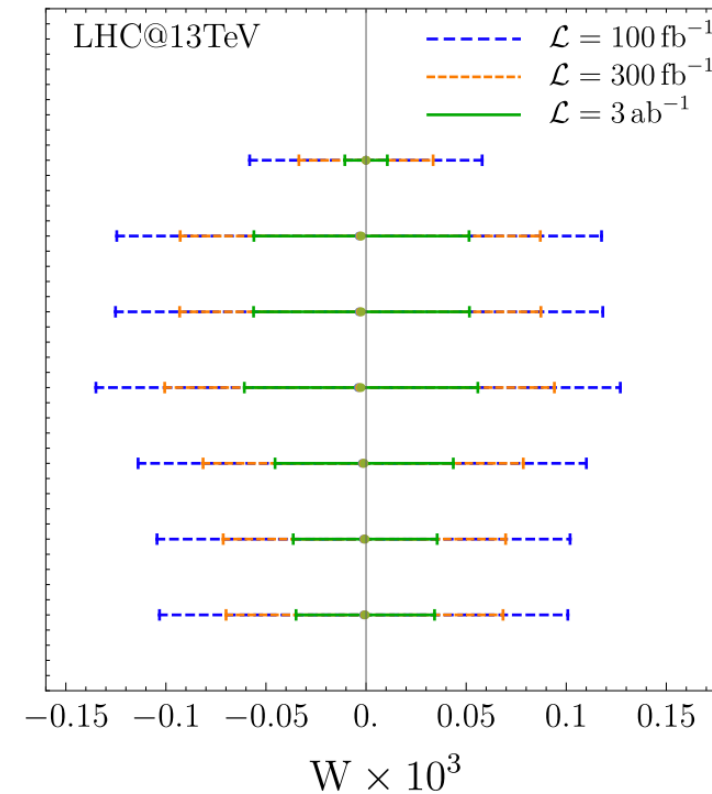
- Case study at higher energy: EW oblique corrections in high-mass NC and CC Drell-Yan tails.
- W and Y parametrise the self-energy of gauge bosons and are powerful probes of quark-lepton contact interactions that produce effects that grow with energy [Torre et al, 2008.12978]

$$\mathcal{L}_{\text{SMEFT}} \supset -\frac{\hat{W}}{4m_W^2}(D_\rho W_{\mu\nu}^a)^2 - \frac{\hat{Y}}{4m_W^2}(\partial_\rho B_{\mu\nu})^2$$



Torre et al, 2008.12978

Combined bound



Only Stat

No Exp

No Syst

Baseline

Half PDF

No PDF

No TH

PDF set: PDF4LHC15_nlo_30_pdfas

APPLICATION TO SIMULTANEOUS DETERMINATION OF PDFS AND SMEFT WC_s

- We performed a similar analysis as in Torre et al, now with emphasis on PDF and their interplay with bounds on oblique operators

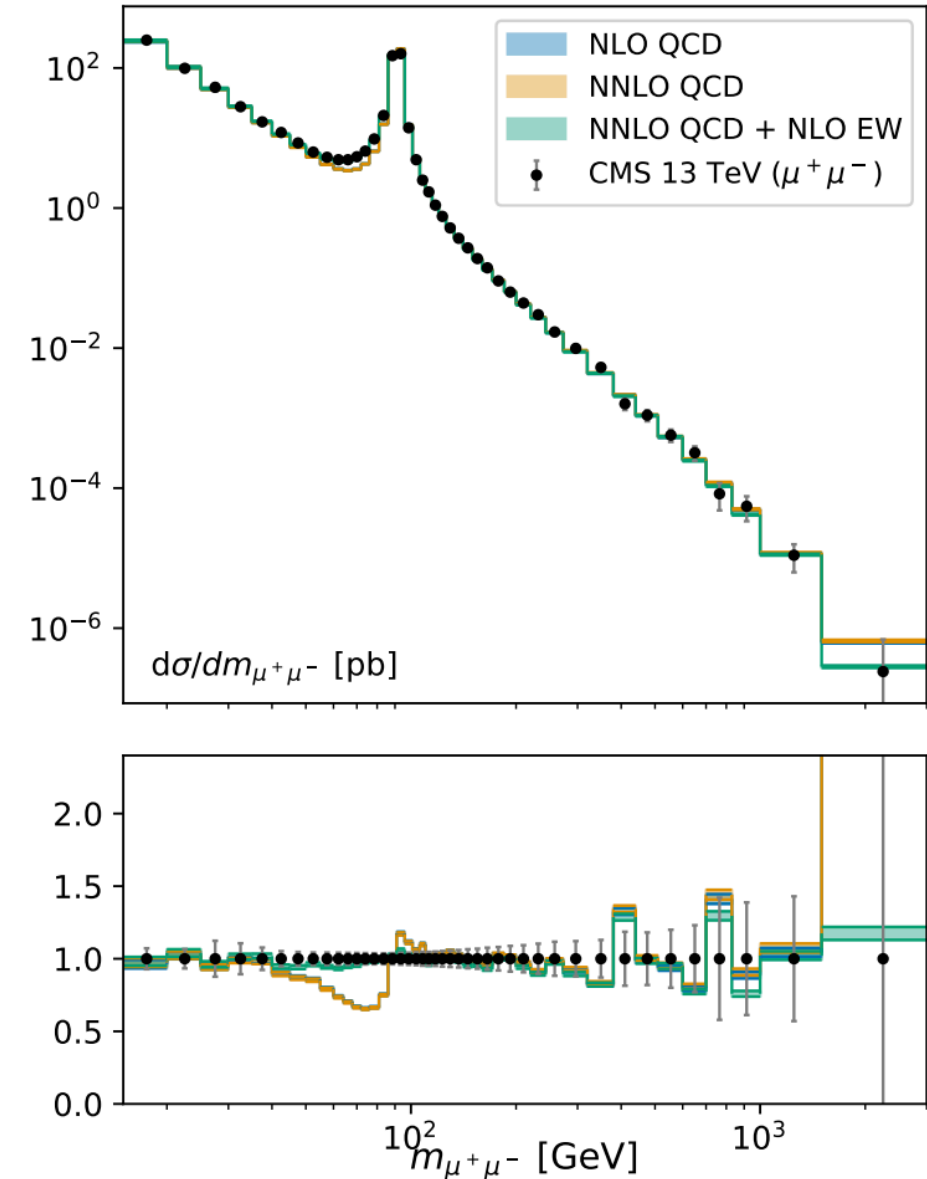
[Greljo, Iranipour, Kassabov, Madigan, Moore, Rojo, MU, Voisey: 2104.02723]

[Iranipour, MU, Voisey: 2201.07240]

- Settings:

- ➔ PDF fit based on DIS (~3000 data points), Drell-Yan on-shell and low-mass data from ATLAS, CMS and LHCb (~600 data points)
- ➔ + Run I and II ATLAS and CMS high mass NC Drell-Yan data (~300 data points)
- ➔ SM predictions at NNLO QCD + NLO EW

Exp.	\sqrt{s} (TeV)	Ref.	\mathcal{L} (fb $^{-1}$)	Channel	1D/2D	n_{dat}	$m_{\ell\ell}^{\text{max}}$ (TeV)
ATLAS	7	[117]	4.9	e^-e^+	1D	13	[1.0, 1.5]
ATLAS (*)	8	[83]	20.3	$\ell^-\ell^+$	2D	46	[0.5, 1.5]
CMS	7	[118]	9.3	$\mu^-\mu^+$	2D	127	[0.2, 1.5]
CMS (*)	8	[84]	19.7	$\ell^-\ell^+$	1D	41	[1.5, 2.0]
CMS (*)	13	[119]	5.1	$e^-e^+, \mu^-\mu^+$ $\ell^-\ell^+$	1D	43, 43 43	[1.5, 3.0]
Total						270 (313)	



APPLICATION TO SIMULTANEOUS DETERMINATION OF PDFS AND SMEFT WC_s

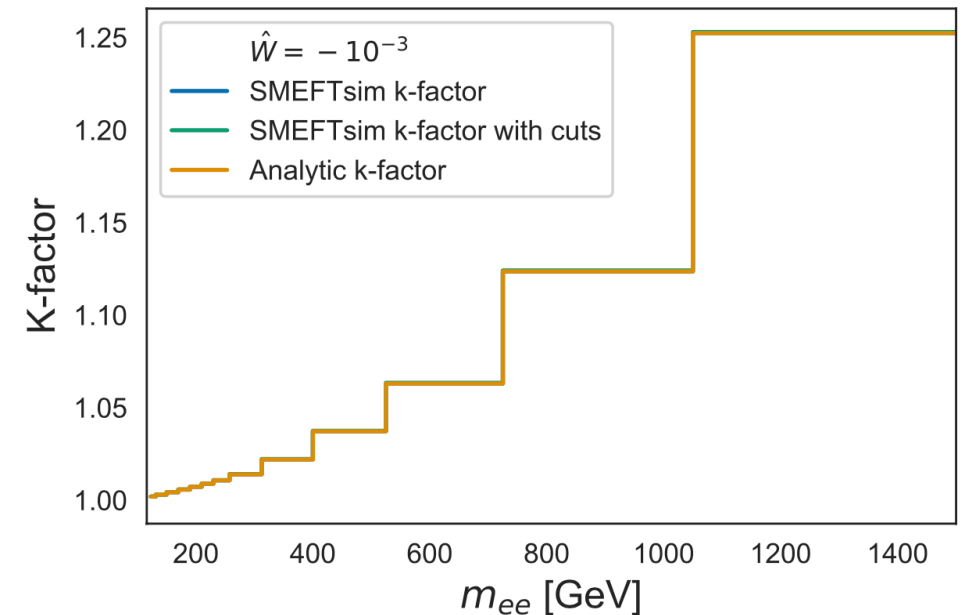
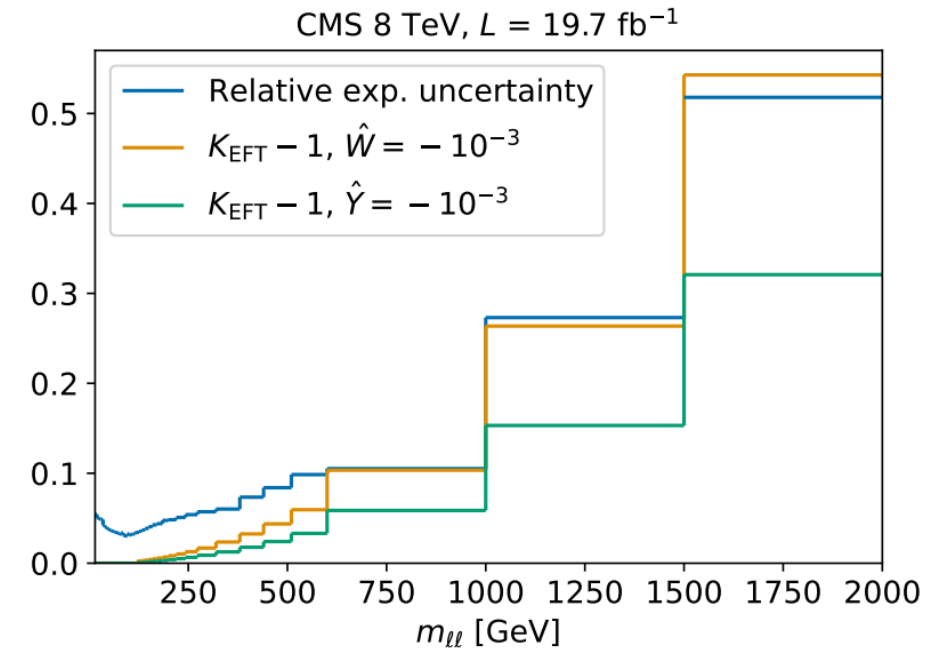
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 - ➔ SM predictions at NNLO QCD + NLO EW
 - ➔ SMEFT corrections added via local K-factors

$$d\sigma_{\text{SMEFT}} = d\sigma_{\text{SM}} \times K_{\text{EFT}}$$

$$K_{\text{EFT}} = 1 + \sum_{n=1}^{n_{\text{op}}} c_n R_{\text{SMEFT}}^{(n)} + \sum_{n,m=1}^{n_{\text{op}}} c_n c_m R_{\text{SMEFT}}^{(n,m)}$$

$$R_{\text{SMEFT}}^{(n)} \equiv \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SMEFT}}^{(n)} \right) / \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SM}} \right), \quad n = 1 \dots, n_{\text{op}}$$

$$R_{\text{SMEFT}}^{(n,m)} \equiv \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SMEFT}}^{(n,m)} \right) / \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SM}} \right), \quad n, m = 1 \dots, n_{\text{op}}$$



APPLICATION TO SIMULTANEOUS DETERMINATION OF PDFS AND SMEFT WC_s

- In the previous analysis, a scan in the (W,Y) parameter space was made
[Greljo, Iranipour, Kassabov, Madigan, Moore, Rojo, MU, Voisey: 2104.02723]

1. Take data, make theoretical predictions accounting for operator in **partonic cross section and PDFs**.
2. Compute chi2 as a function of WCs (Wilson Coefficients)
3. Minimise chi2 and find best-fit and C.L.s of WCs
4. Extract bounds

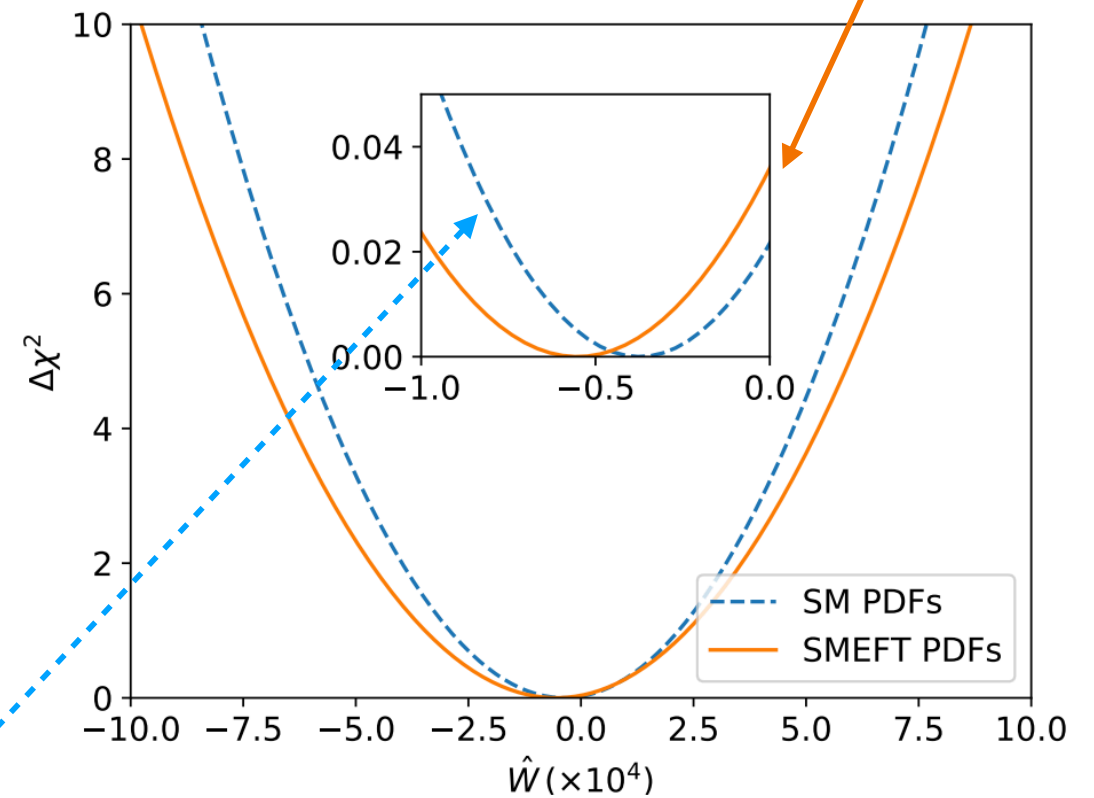
$$T = f_{1,\text{BSM}} \otimes f_{2,\text{BSM}} \otimes \hat{\sigma}_{\text{BSM}}$$

SMEFT PDFs / Simultaneous fit

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

$$T = f_1(\hat{W} = 0) \otimes f_2(\hat{W} = 0) \otimes \hat{\sigma}(\hat{W})$$

$$T = f_1(\hat{W}) \otimes f_2(\hat{W}) \otimes \hat{\sigma}(\hat{W})$$



THE SIMUNET ANALYSIS

- With SimuNET we can do a truly simultaneous fit, rather than a scan in benchmark point and it does not have limit in number of parameters that can be fitted alongside PDFs at the initial scale!

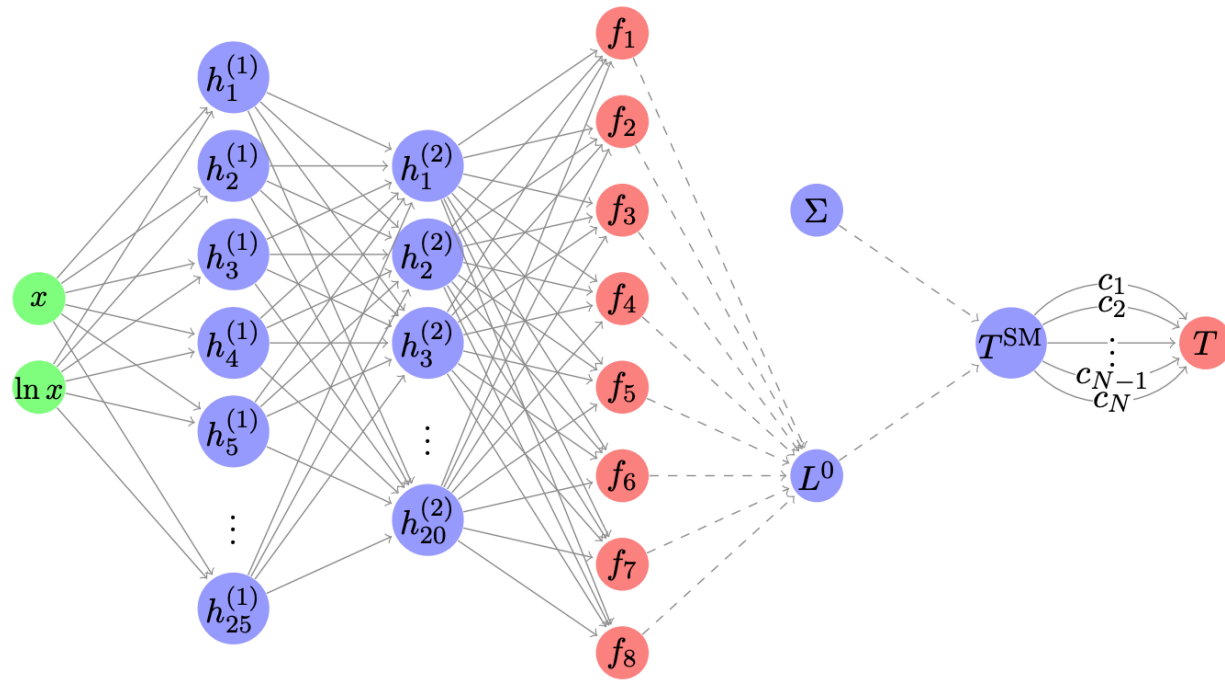
[Iranipour, MU, Voisey: 2201.07240]

Linear dim-6 operator

Input layer	Hidden layer 1	Hidden layer 2	PDF flavours	Convolution step	SM Observable	SMEFT Observable
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$$T(\hat{\theta}) = \Sigma(\{c_n\}) \cdot L^0(\theta) = T^{\text{SM}}(\theta) \cdot \left(1 + \sum_{n=1}^N c_n R_{\text{SMEFT}}^{(n)} \right)$$

$$T^{\text{SM}}(\theta) = \Sigma^{\text{SM}} \cdot L^0(\theta)$$

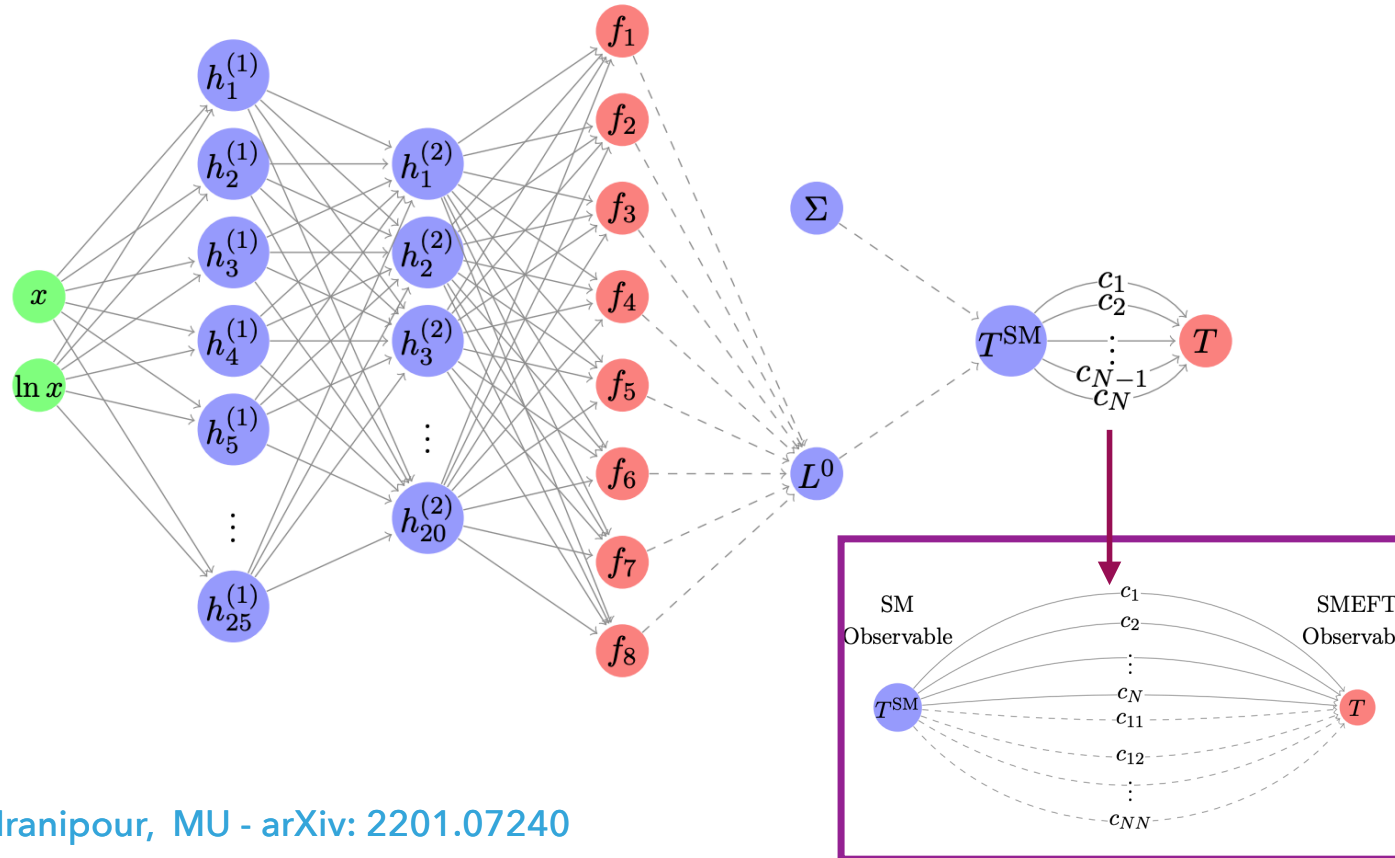


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[Iranipour, MU, Voisey: 2201.07240]

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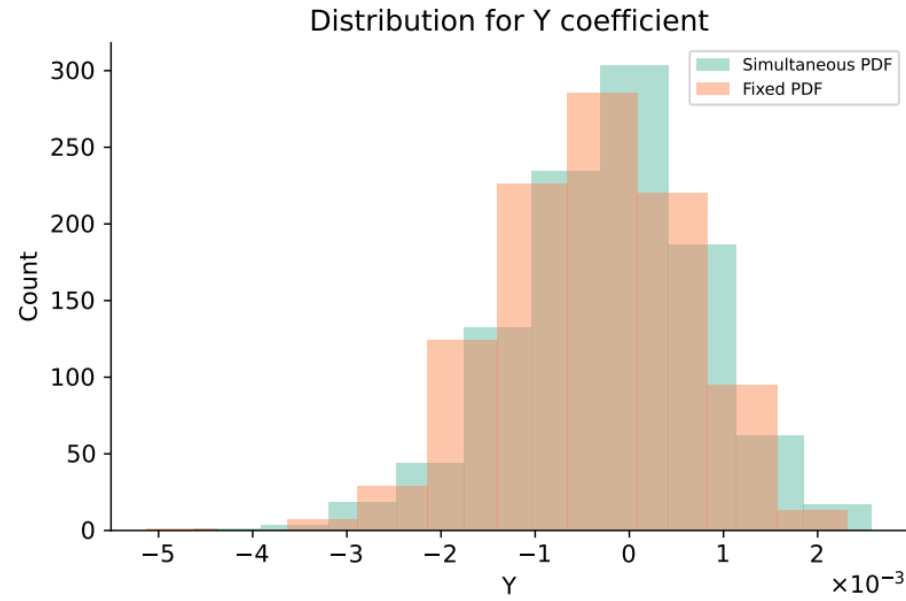
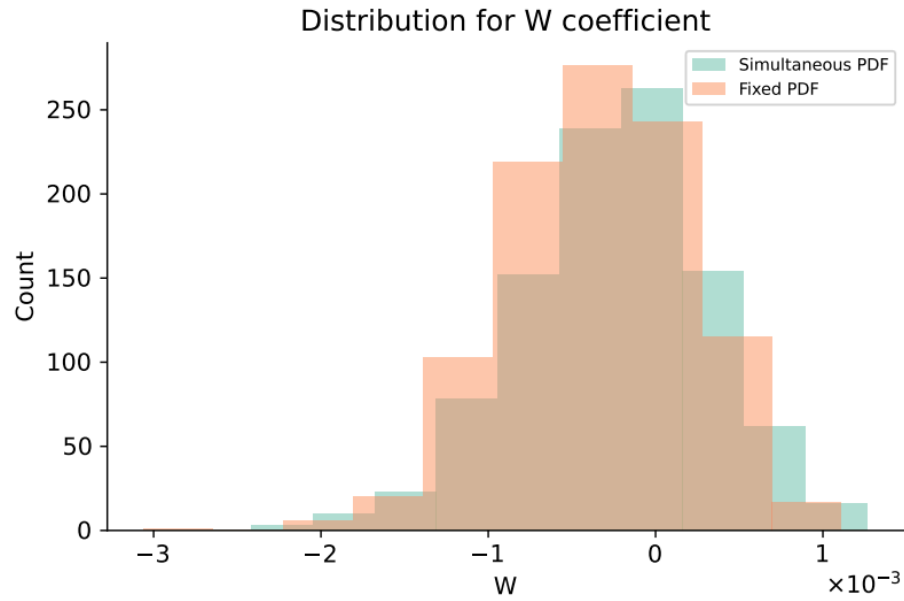
$$T^{\text{SM}}(\theta) = \Sigma^{\text{SM}} \cdot L^0(\theta)$$

Quadratic dim-6 operator

$$T(\hat{\theta}) = T^{\text{SM}}(\theta) \cdot \left(1 + \sum_{n=1}^N c_n R_{\text{SMEFT}}^{(n)} + \sum_{1 \leq n \leq m \leq N} c_{nm} R_{\text{SMEFT}}^{(n,m)} \right)$$

$c_n c_m$

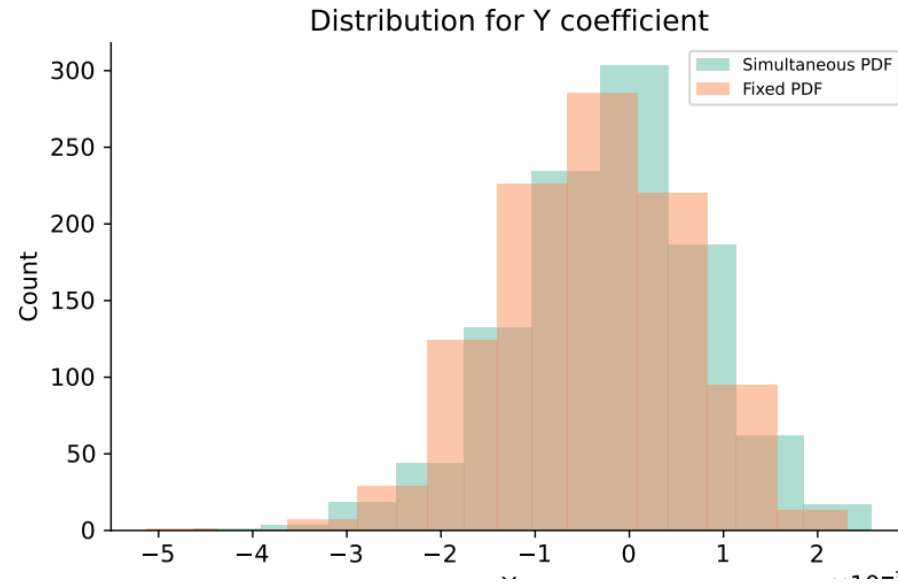
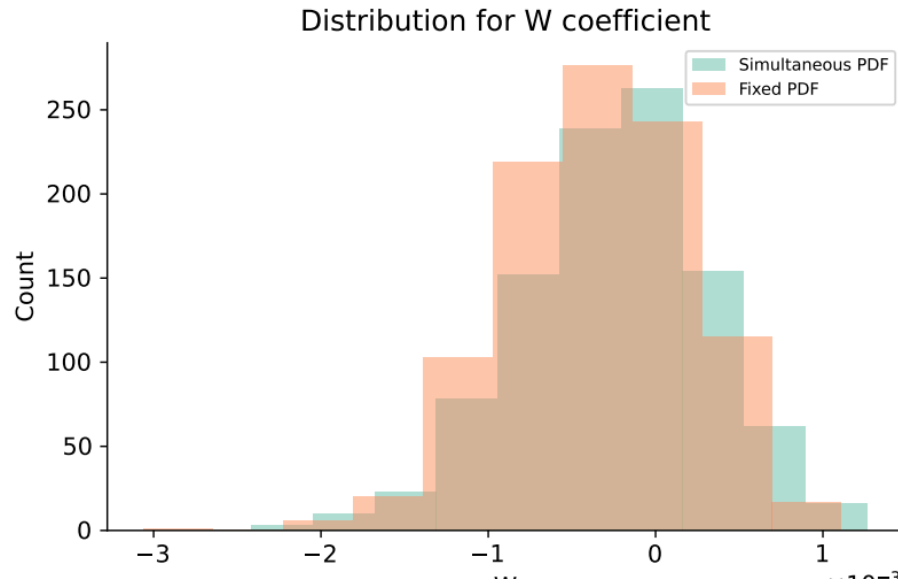
RESULTS: DRELL-YAN DATA @RUN1 AND RUN2



Distribution of W & Y best fits over MC reps with fixed SM PDFs (baseline)

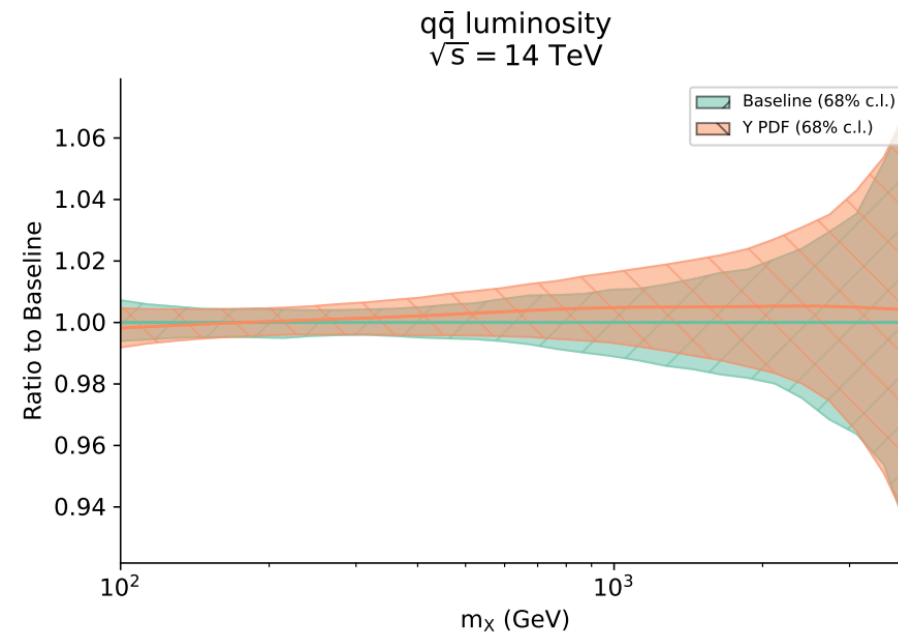
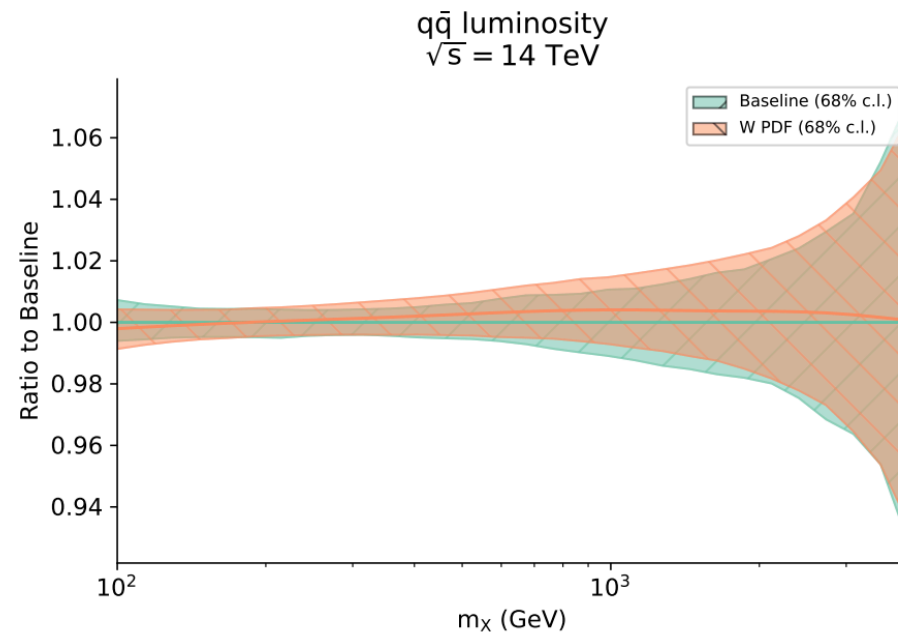
Distribution of W & Y best fits over MC reps with PDFs fitted alongside them

RESULTS: DRELL-YAN DATA @RUN1 AND RUN2



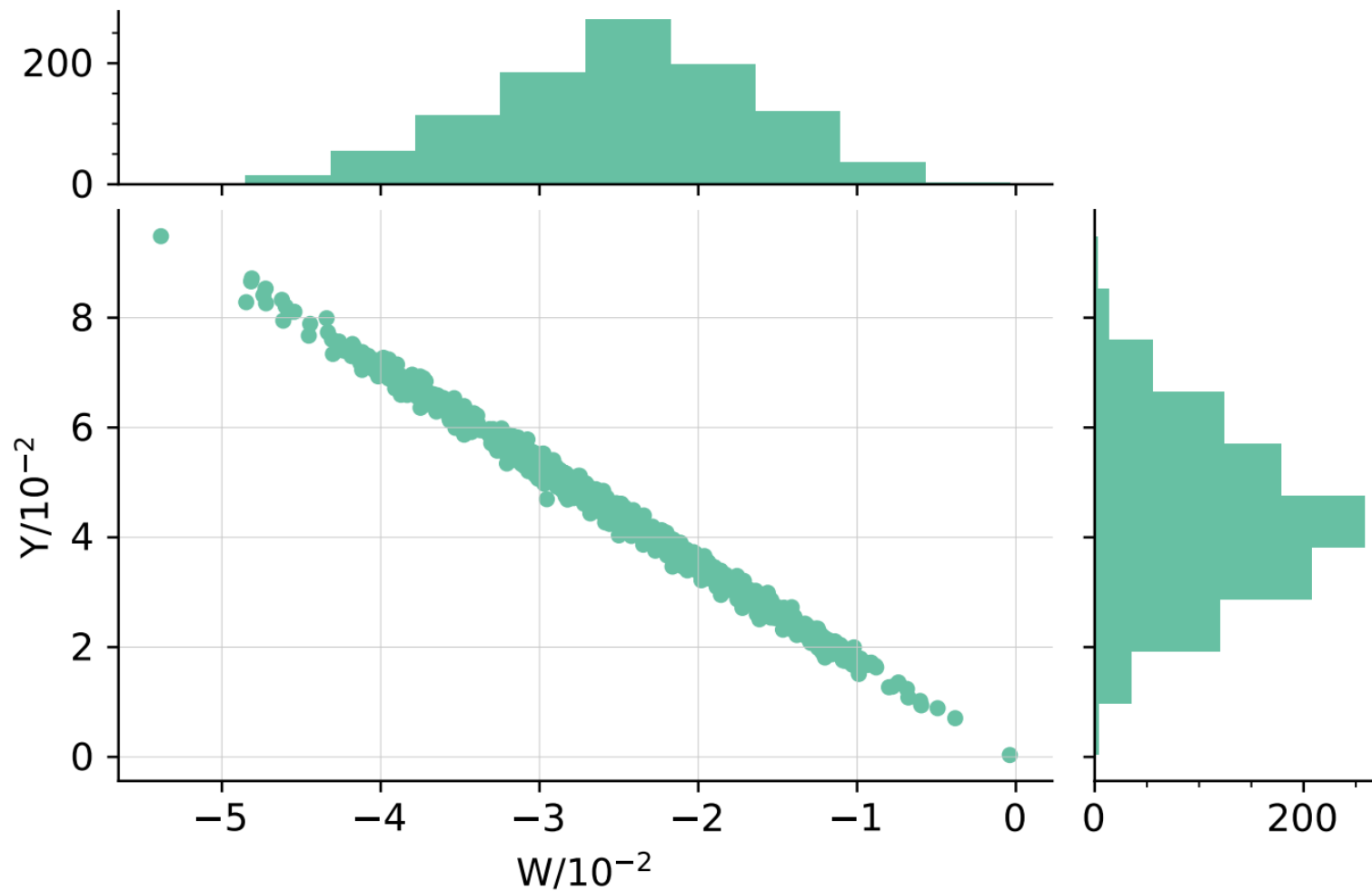
Distribution of W & Y best fits over MC reps with fixed SM PDFs (baseline)

Distribution of W & Y best fits over MC reps with PDFs fitted alongside them



Same comparison for quark-antiquark luminosity

RESULTS: DRELL-YAN DATA @RUN1 AND RUN2



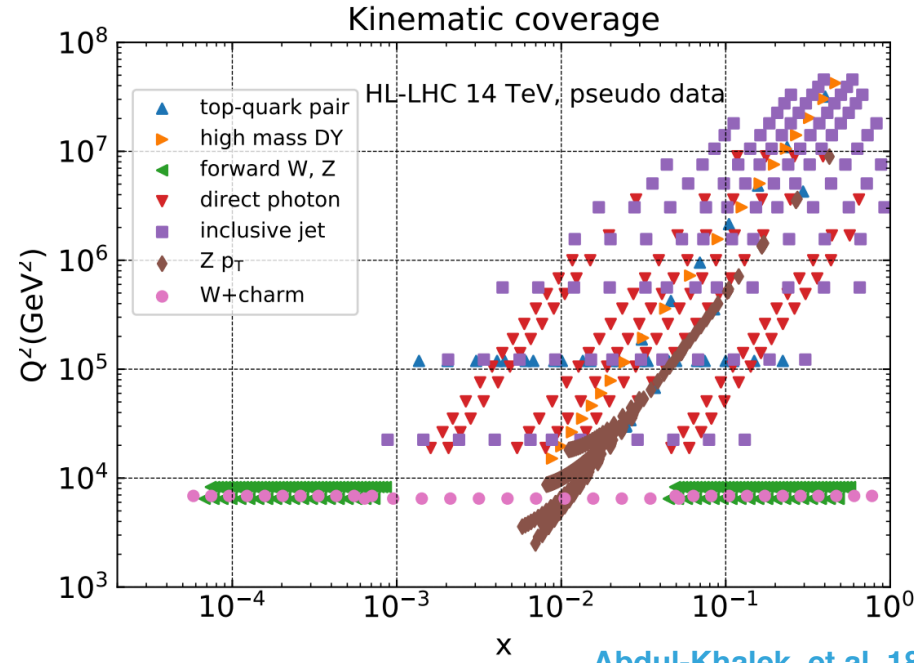
- ✓ Simultaneous analysis confirms results of previous study based on scan on benchmark points in the SMEFT space: with current data effect is not-negligible but small compared to PDF uncertainties
- ✓ Methodology able to find flat direction in W-Y parameter space
- ✓ To eliminate it, need Drell-Yan charged current data

RESULTS: DRELL-YAN DATA @HL-LHC

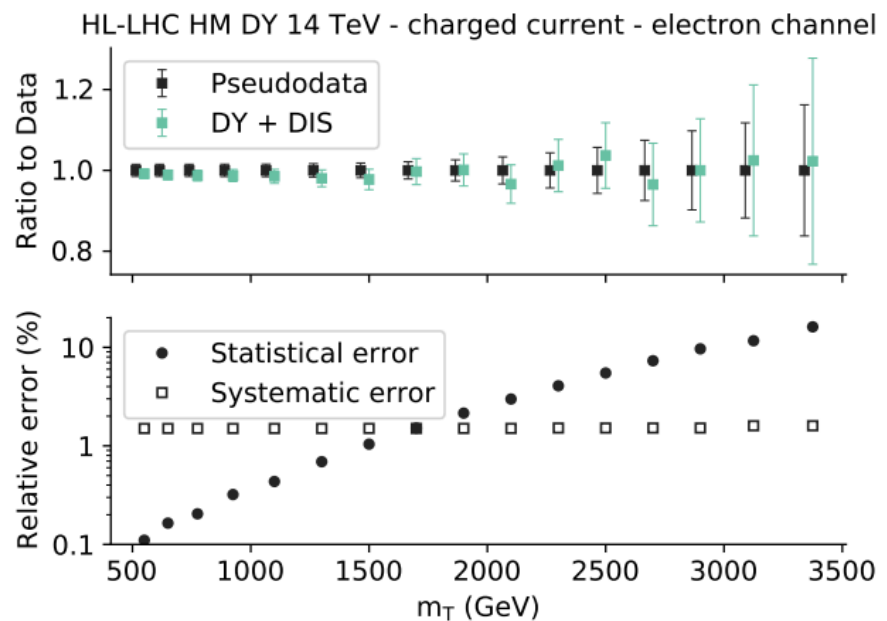
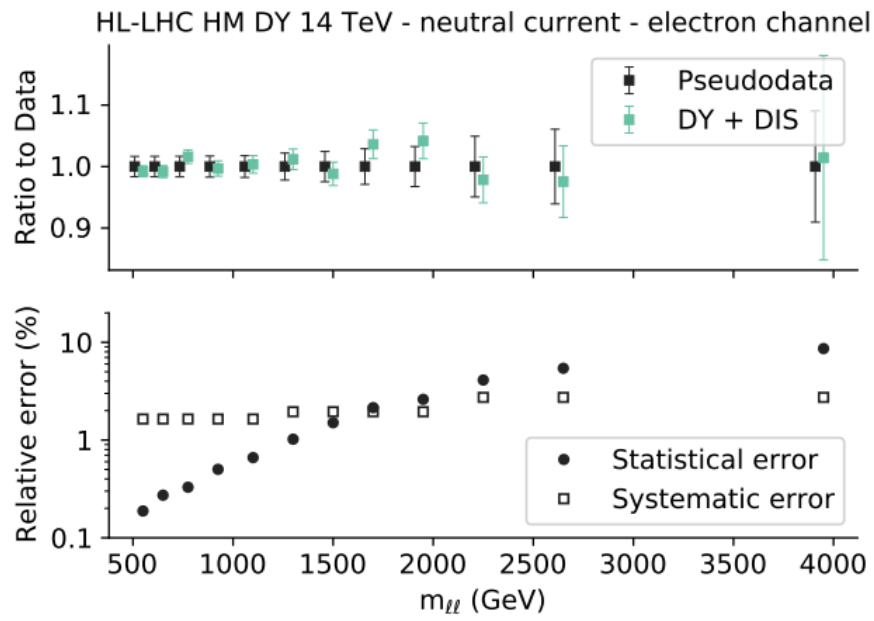
- Add HL-LHC projections for both NC and CC in PDF fit

$$\sigma_i^{\text{hllhc}} \equiv \sigma_i^{\text{th}} \left(1 + \lambda \delta_{\mathcal{L}}^{\text{exp}} + r_i \delta_{\text{tot},i}^{\text{exp}} \right), \quad i = 1, \dots, n_{\text{bin}}$$

$$\delta_{\text{tot},i}^{\text{exp}} = \left((\delta_i^{\text{stat}})^2 + \sum_{j=1}^{n_{\text{sys}}} \left(f_{\text{red},j} \delta_{i,j}^{\text{sys}} \right)^2 \right)^{1/2}$$

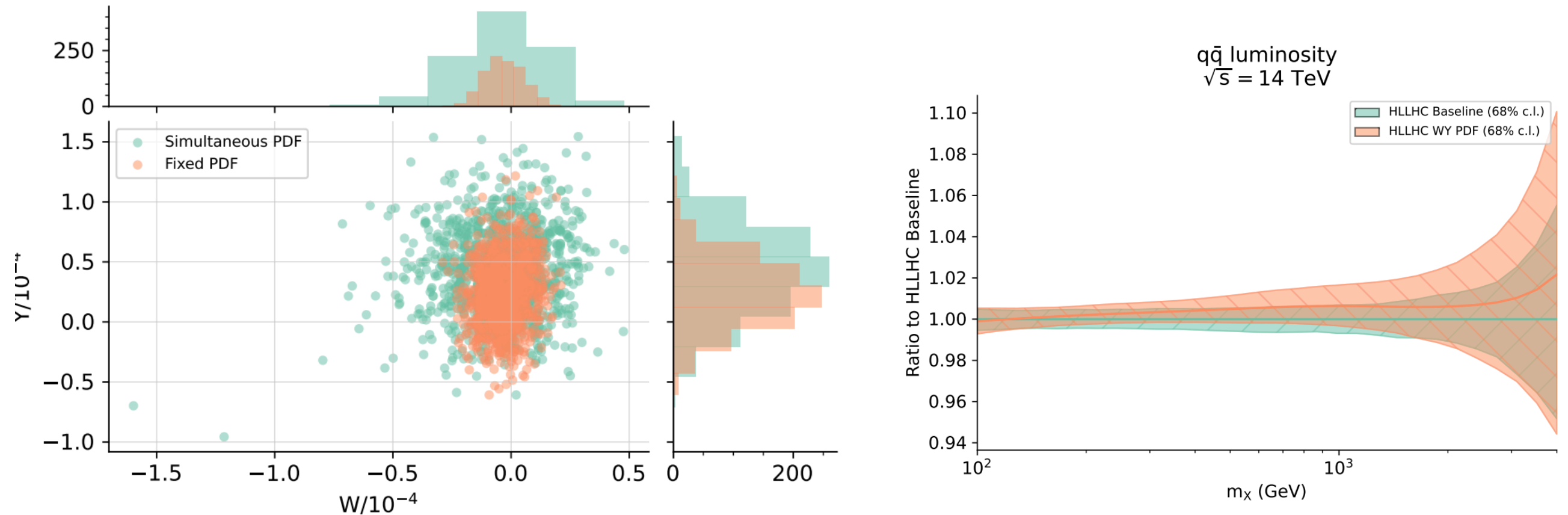


Abdul-Khalek et al, 1810.03639



+ muon channel

RESULTS: DRELL-YAN DATA @HL-LHC



- ✓ Simultaneous analysis confirms results of previous study based on scan on benchmark points in the SMEFT space: at HL-LHC the effect of interplay becomes important as WCs bounds broaden and PDFs change significantly once SMEFT effects allowed in theory predictions entering PDF fit
- ✓ Stress-tested and shown robustness with closure tests

CONCLUSIONS AND OUTLOOK

- While huge progress made in determining key ingredients of theoretical predictions from the data, PDFs, α_s , SMEFT WCs coefficients, it is not yet evident how to combine all these partial fits into a global interpretation of the LHC data
- Time to work on new generation of global fits, in which all ingredients that enter theoretical predictions are treated consistently.
- SimuNET methodology based on an extension of the NNPDF4.0 NN architecture, allows the addition of an extra layer to simultaneously determine PDFs alongside an arbitrary number of physics parameters that enter predictions.
- Proof-of-concept on simultaneous determination of W and Y oblique parameters and PDFs from DIS+DY fit
- Lots of exciting avenues being explored:
 - ➔ Determination of PDFs and α_s (Stegeman et al)
 - ➔ Determination of PDFs and SMEFT coefficients in the top sector (Kassabov, Madigan, Mantani, Moore, Morales, Rojo, MU)
 - ➔ Systematic study of new physics contamination in PDF fits
 - ➔ Determination of PDFs and electroweak parameters

THANK YOU FOR YOUR ATTENTION!

EXTRA MATERIAL

FAST INTERFACE FOR THEORETICAL PREDICTIONS

$$T_I = \Sigma_I \cdot L^0$$

$$\Sigma_I(c) = [\hat{\sigma}(c) \otimes \Gamma(c)]_I$$

T_I: Theoretical prediction for experimental measurement I in a fit

Σ_I: Pre-computed FK-tables (including both partonic cross section and evolution kernel from Q₀ to Q)

Depending on parameter to fit alongside PDFs, its dependence might appear in either/both σ and Γ

$$\Sigma_I = \Sigma_I \begin{pmatrix} \alpha_s(M_Z) = 0.118 \\ \sin^2 \theta_W(M_Z) = 0.23 \\ M_W = 80.4 \text{ GeV}/c^2 \\ M_Z = 91.2 \text{ GeV}/c^2 \\ \vdots \\ c_i = 0 \end{pmatrix}$$

- ▶ Need to include a fast interface to parameter dependence to the fast interface of initial scale PDFs

$$T(\hat{\theta}) = T^{\text{SM}}(\theta) \cdot \left(1 + \sum_{n=1}^N c_n R_{\text{SMEFT}}^{(n)} + \sum_{1 \leq n \leq m \leq N} c_n c_m R_{\text{SMEFT}}^{(n,m)} \right)$$

$$R_{\text{SMEFT}}^{(n)} \equiv \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SMEFT}}^{(n)} \right) / \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SM}} \right), \quad n = 1 \dots, N$$

$$R_{\text{SMEFT}}^{(n,m)} \equiv \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SMEFT}}^{(n,m)} \right) / \left(\mathcal{L}_{ij}^{\text{NNLO}} \otimes d\hat{\sigma}_{ij,\text{SM}} \right), \quad n, m = 1 \dots, N$$

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$$\Sigma_I(c) = [\hat{\sigma}(c) \otimes \Gamma(c)]_I$$

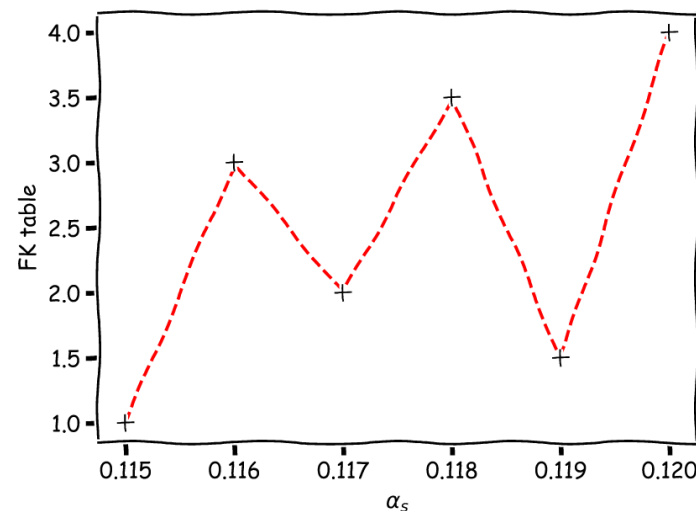
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- We performed a similar analysis as in Torre et al, now with emphasis on PDF and their interplay with bounds on oblique operators

[Greljo, Iranipour, Kassabov, Madigan, Moore, Rojo, MU, Voisey: 2104.02723]

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

1. Take data, make theoretical predictions accounting for operator in partonic cross section **with fixed SM PDFs**.
2. Compute chi2 as a function of WCs (Wilson Coefficients)
3. Minimise chi2 and find best-fit and C.L.s of WCs
4. Extract bounds

$$T = f_{1,\text{SM}} \otimes f_{2,\text{SM}} \otimes \hat{\sigma}_{\text{BSM}}$$

SM PDFs

1. Take data, make theoretical predictions accounting for operator **in partonic cross section and PDFs**.
2. Compute chi2 as a function of WCs (Wilson Coefficients)
3. Minimise chi2 and find best-fit and C.L.s of WCs
4. Extract bounds

$$T = f_{1,\text{BSM}} \otimes f_{2,\text{BSM}} \otimes \hat{\sigma}_{\text{BSM}}$$

SMEFT PDFs / Simultaneous fit

ANALYSIS METHODOLOGY

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- Methodology for simultaneous fit is similar to the one adopted in fits of α_s from a global fit of PDFs

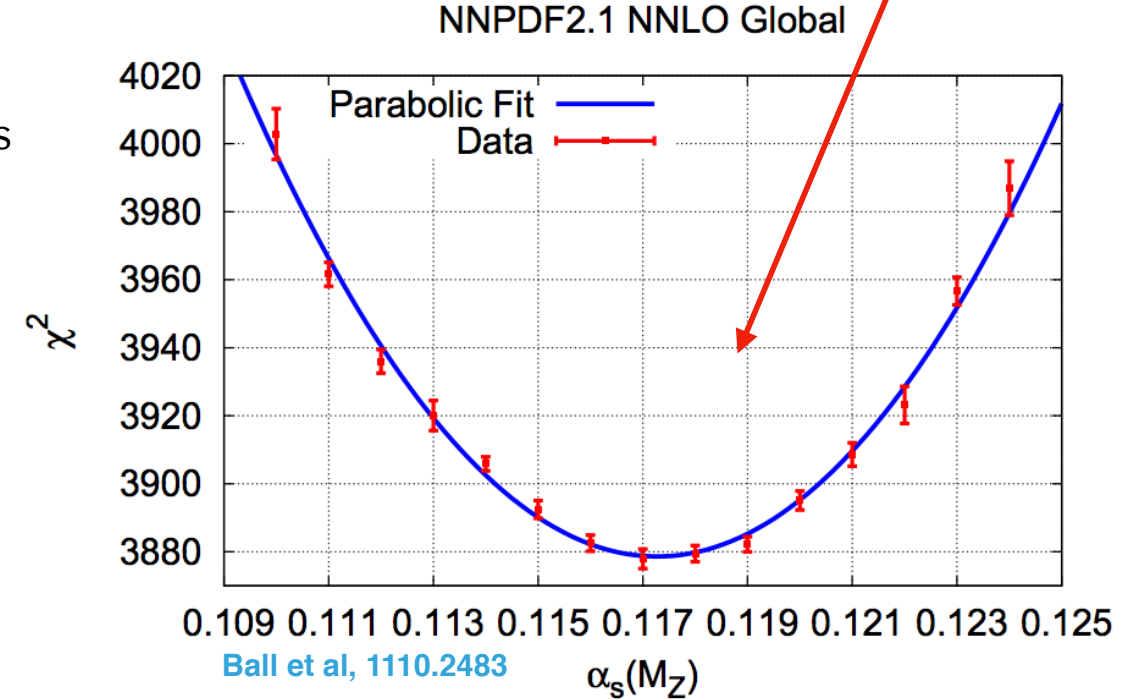
$$\chi^2 = \frac{1}{n_{\text{dat}}} \sum_{i,j=1}^{n_{\text{dat}}} (D_i - T_i) (\text{cov}^{-1})_{ij} (D_j - T_j)$$

1. Take data, make theoretical predictions accounting for operator in partonic cross section **with fixed SM PDFs**.
2. Compute chi2 as a function of WCs (Wilson Coefficients)
3. Minimise chi2 and find best-fit and C.L.s of WCs
4. Extract bounds

$$T = f_{1,\text{SM}} \otimes f_{2,\text{SM}} \otimes \hat{\sigma}_{\text{BSM}}$$

SM PDFs

$$T = f_1(\alpha_s) \otimes f_2(\alpha_s) \otimes \hat{\sigma}(\alpha_s)$$



1. Take data, make theoretical predictions accounting for operator **in partonic cross section and PDFs**.
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SMEFT PDFs / Simultaneous fit

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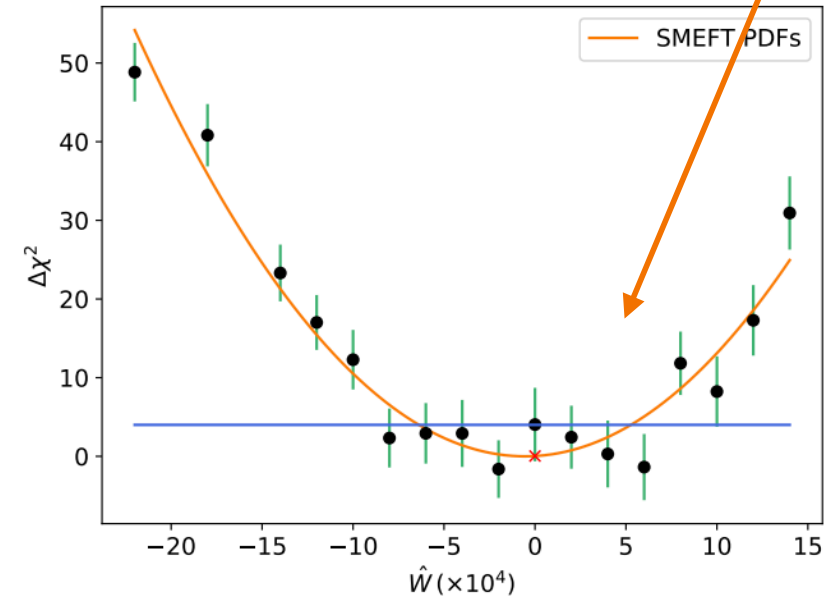
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SM PDFs

$$T = f_1(\hat{W}) \otimes f_2(\hat{W}) \otimes \hat{\sigma}(\hat{W})$$



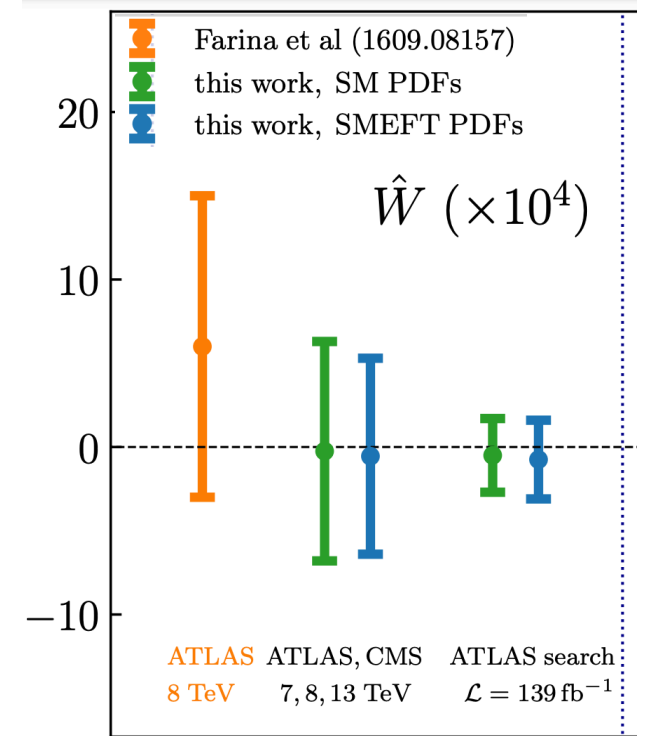
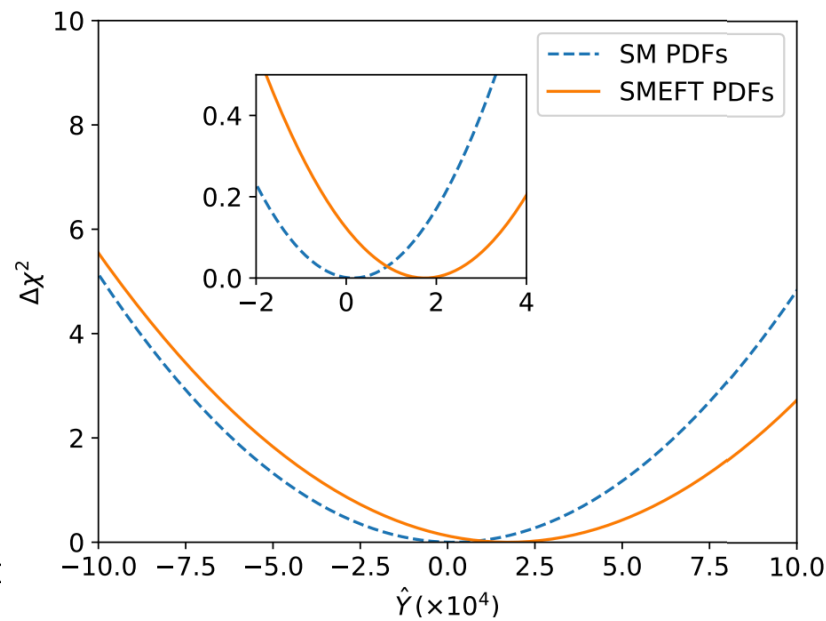
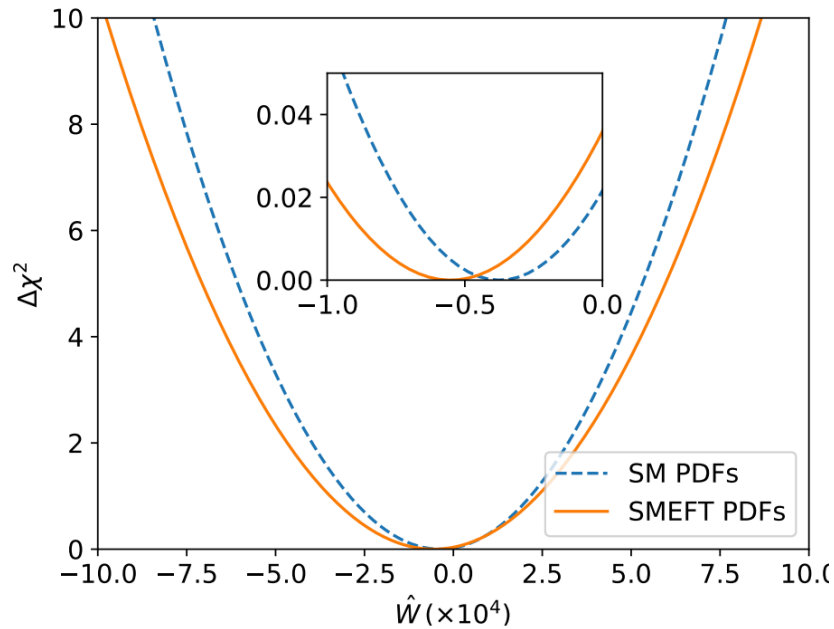
Greljo et al, 2104.02723

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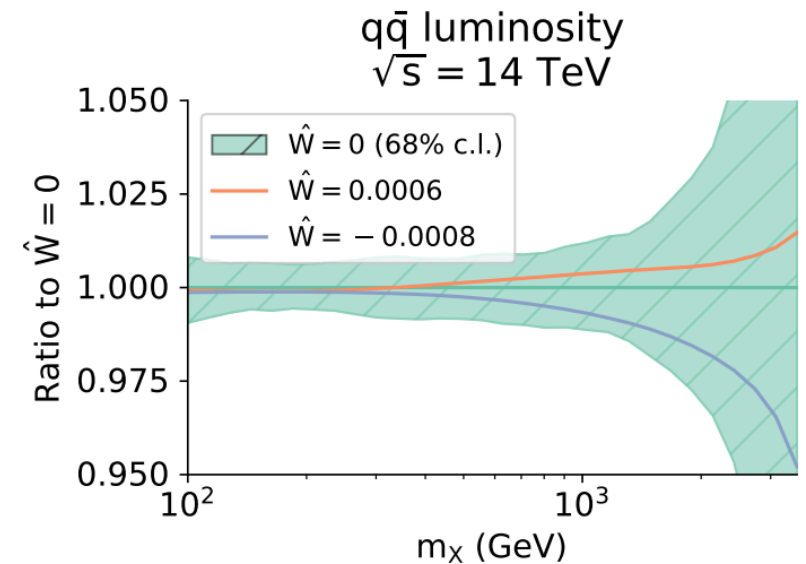
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SMEFT PDFs / Simultaneous fit

INTERPLAY @ RUN I AND RUN II



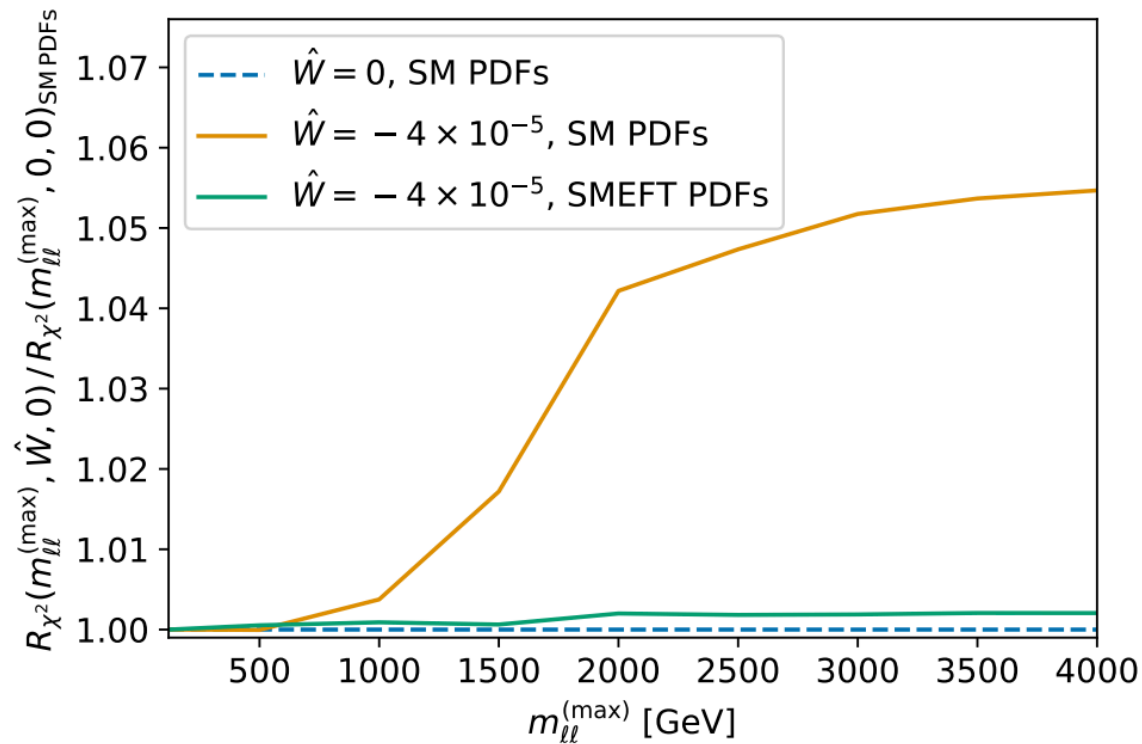
- With current data, PDFs are moderately affected by inclusion of non-zero W and Y coefficients in the fit, mostly quark-antiquark luminosity within uncertainties
- Broadening of individual bounds on W and Y once SMEFT PDFs are used (i.e. PDFs that have been fitted with consistent values of W and Y) is not negligible, but still within PDF uncertainties
- If SMEFT PDFs are used in determining bounds from ATLAS search same mild broadening (larger than PDF uncertainties)



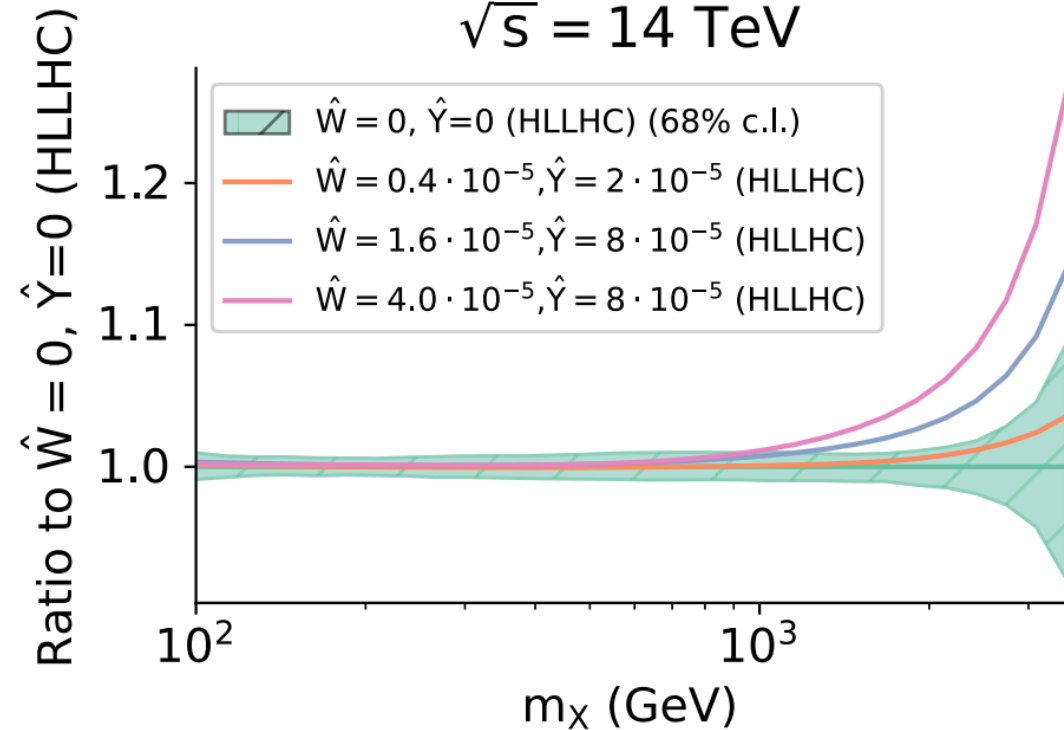
INTERPLAY @ HL-LHC

- Compare Wilson coefficients bounds from HL-LHC projections assuming SM PDFs (that include NC+CC data) to the bounds on the same Wilson coefficients obtained from a simultaneous fit of PDFs and Wilson coefficients
- Not accounting for interplay (using PDFs as a black box) leads to over-constrained bounds
- PDFs do absorb effect of new physics in this case!

$$R_{\chi^2(m_{\ell\ell}^{(\max)}, \hat{W}, \hat{Y})} \equiv \frac{\chi^2(m_{\ell\ell}^{(\max)}, \hat{W}, \hat{Y})}{\chi^2(120 \text{ GeV}, \hat{W}, \hat{Y})}$$

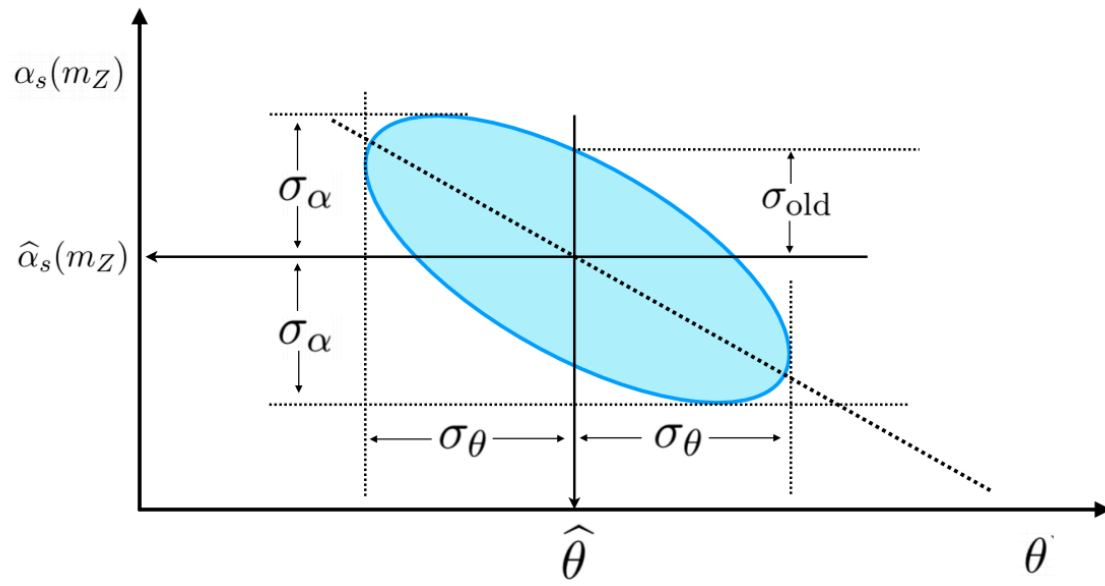


q \bar{q} luminosity
 $\sqrt{s} = 14 \text{ TeV}$

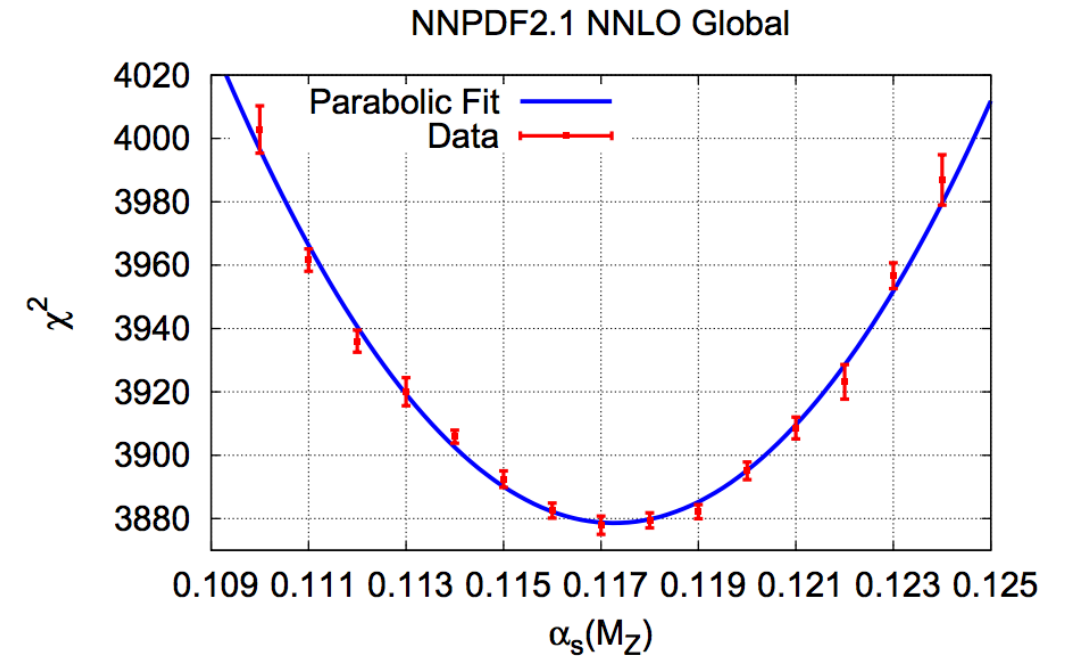


PDFs AND α_s

- PDFs and α_s strongly correlated (PDF evolution with the scale and hard cross sections)
- Cleanest determinations of α_s from processes that do not require knowledge of the PDFs
- A determination of α_s jointly with the PDFs has advantage that it is driven by the combination of many experimental measurements from several different processes.



Ball, Carrazza, Del Debbio, Forte, Kassabov, Rojo, Slade, MU 1802.03398

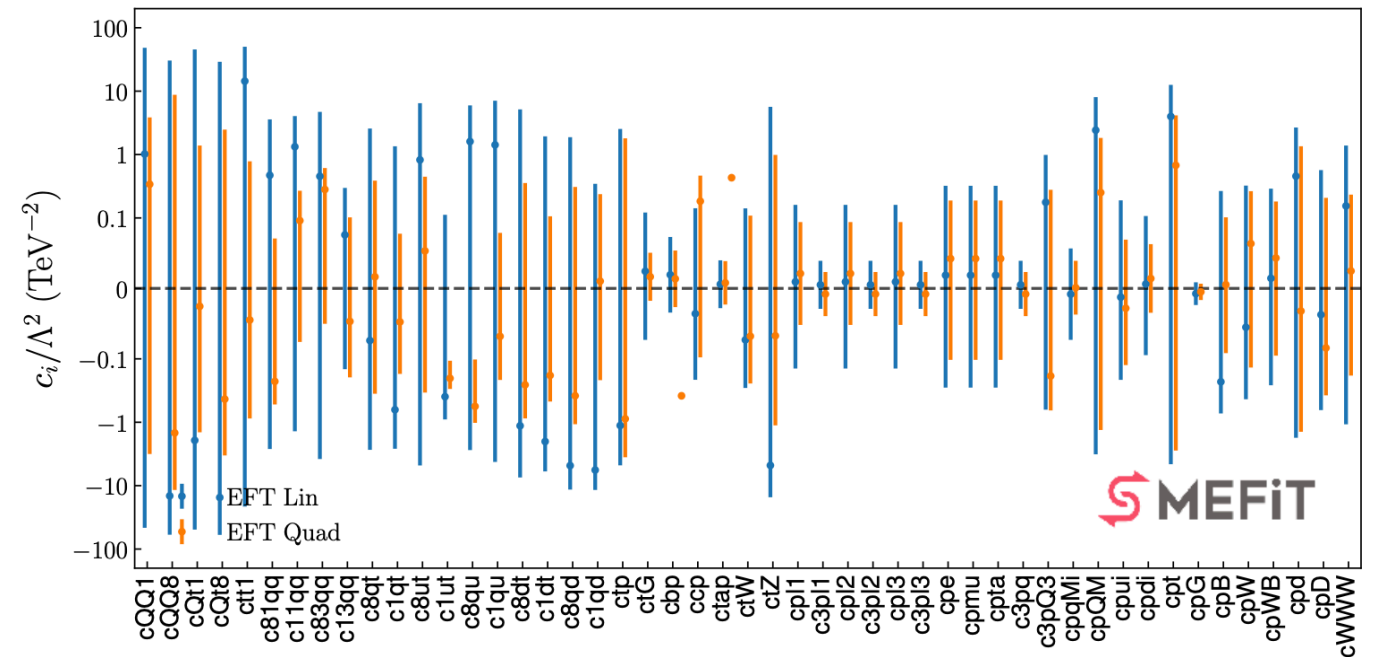
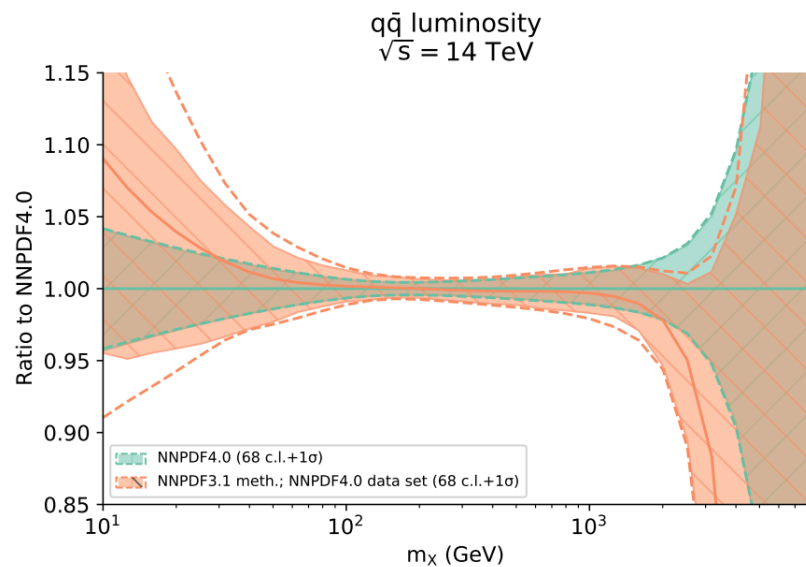


Ball et al, 1110.2483

- Early determinations involve a scan over α_s and ignored PDF and α_s correlation in the fit
- Recent simultaneous determination of PDF and α_s using correlated replica method
- Many determination of α_s from analyses of specific LHC processes have been published recently (from $tt\bar{t}$, Z and W production, jets)
- How reliable are such partial determination of α_s ?

PDFS AND NEW PHYSICS

- In principle low-scale physics is separable from high-scale physics, BUT the complexity of the LHC environment might well intertwine them.
- PDFs are low-scale quantities extracted from experimental data at all scales, without considering any potential high-scale contamination due to new physics.
- (SM)EFT fits are performed by assuming a priori that PDFs are SM-like.



PDFS AND NEW PHYSICS

- From the point of view of PDF fits:
 - ➔ How to make sure that new physics effects are not inadvertently fitted away in a PDF fit?
- From the point of view of SMEFT fits:
 - ➔ Should I make sure I am using a clean set of PDFs in a SMEFT analysis? How to define it? Is it enough?
 - ➔ How would the bounds change if I was consistently using PDFs that include in the fit the same operators that I am fitting?

T

$$\boxed{d\sigma^{pp \rightarrow ab}} = \sum_{i,j} \boxed{f_i \otimes f_j \otimes d\hat{\sigma}^{ij \rightarrow ab}} + \dots$$

↑

 $f(\{\theta_k\})$

↑

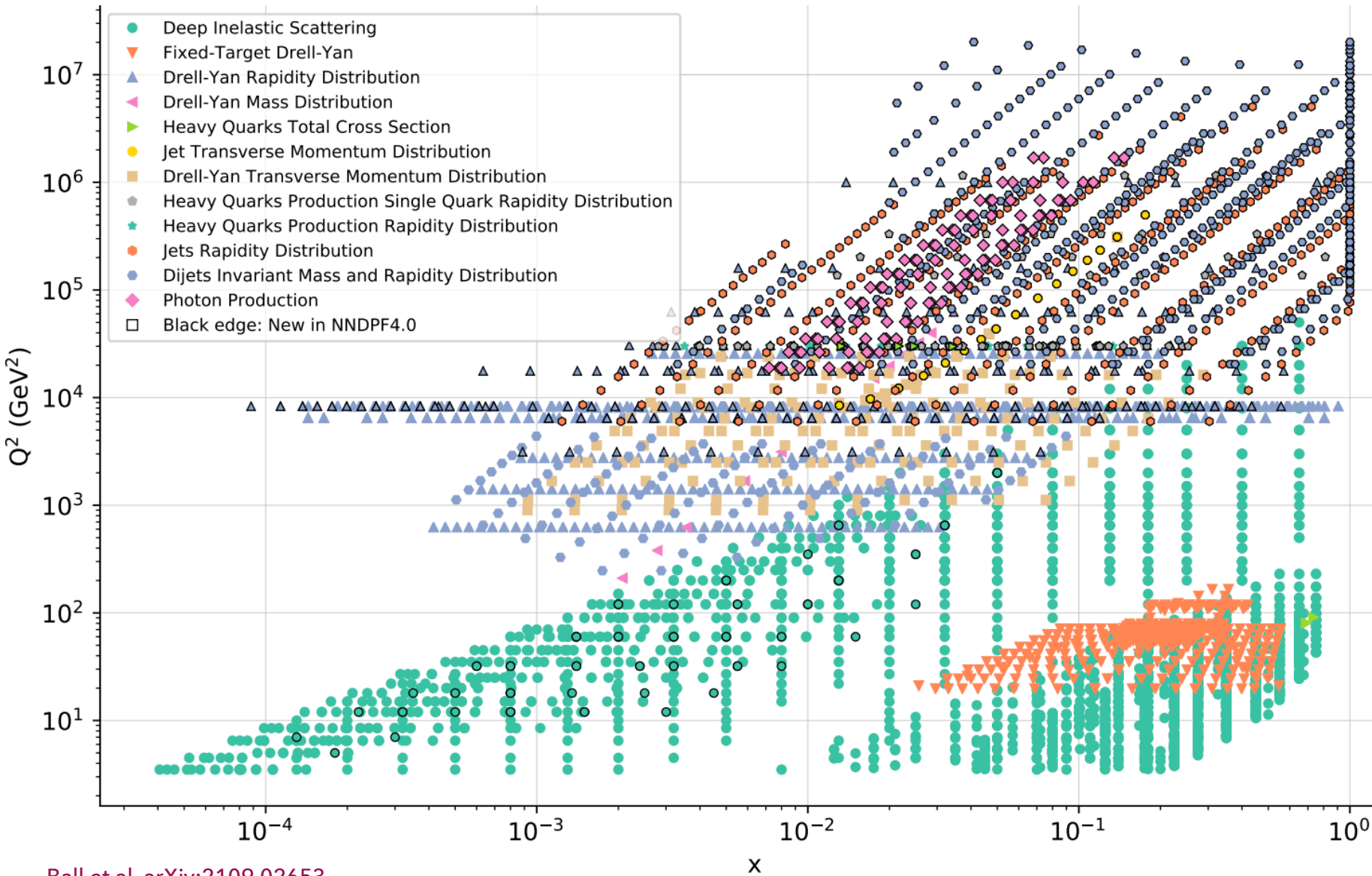
 $\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_i \frac{c_i}{\Lambda^2} \mathcal{O}_i^{(6)} + \dots$

➔

Simultaneous fits can shed light on their interplay

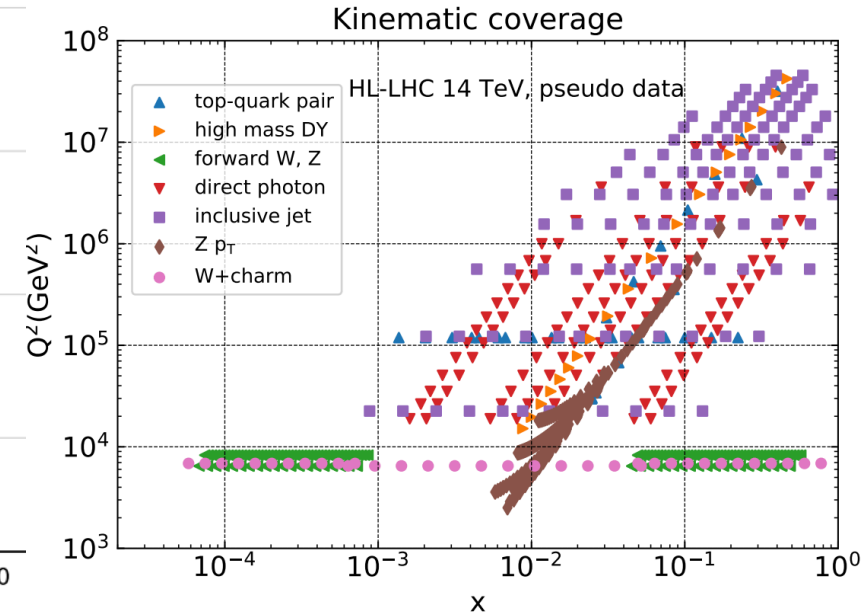
$T(\{\theta_k\}, \{c_i\})$

PDFS AND NEW PHYSICS



Ball et al, arXiv:2109.02653

- Top pair production and single top data included in SMEFT analysis
[Hartland et al 1901.05965] [Ellis et al 2012.02779]
- Dijets data in [Bordone et al 2103.10332]
[Alioli et al 1706.03068]
- Drell-Yan data in [Farina et al 1609.08157]
[Torre et al 2008.12978]
- Inclusive jets in [Alte et al 1711.07484]
- Overlap enhanced in HL-LHC projections [Abdul Khalek et al, 1810.03639]



Abdul Khalek et al, arXiv:1810.03639

Input layer	Hidden layer 1	Hidden layer 2	PDF flavours	Convolution step	Theory prediction
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