On the Consistent Use of Scale Variations in PDF Fits and Predictions

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In collaboration with R. S. Thorne.

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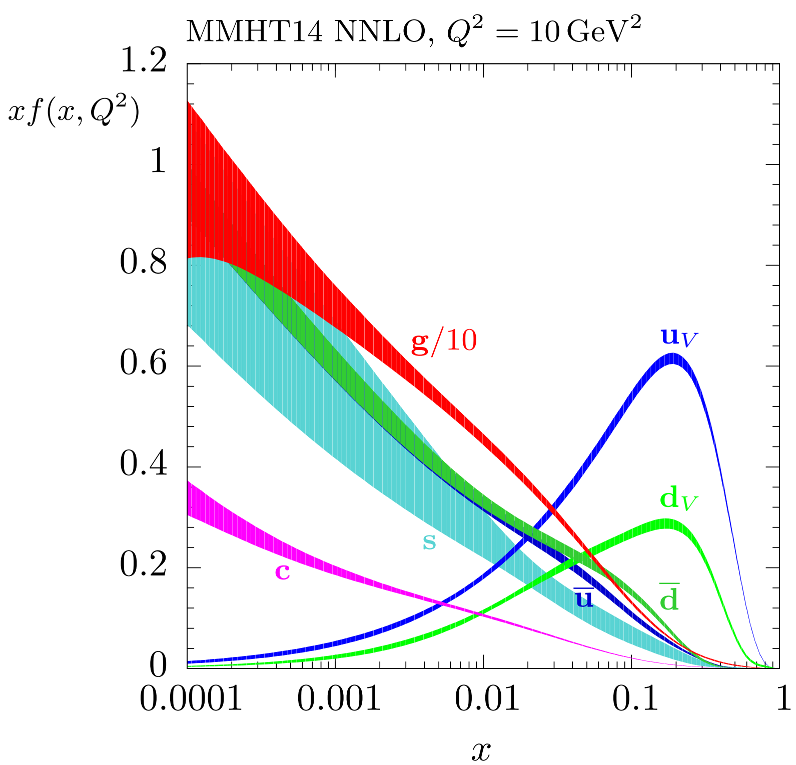
Theoretical Uncertainties in PDFs

- Treatment of PDF uncertainties well developed. Two established methods - Hessian and MC replicas - and procedures for converting between the two.
- However this only concerns 'experimental' uncertainties, due to propagation of data errors through to fit.
- Other sources of error, due in particular to 'theory' in fit:
    - Value of strong coupling α_S, quark masses $m_{c,b}$.
    - Treatment of heavy flavour in cross sections.
    - Higher twists effects.
    - Nuclear corrections
    - ...
- Sources of these numerous, and focus of many studies.
- One source until recently never touched on - what is uncertainty due to fact we are using approximate fixed-order theory in the fit?
- Increasingly relevant in high precision LHC era.



MHO Uncertainties

- Generically in fit relate observables O to PDFs f via (schematically):

$$O \sim f \otimes \sigma \sim f \otimes \left(\sigma^{(0)} + \alpha_S \sigma^{(1)} + \cdots\right)$$

- Function of PDF fit is to invert this relation, giving $f(O\,;\,\sigma)$.
- But σ and therefore $f(O\,;\,\sigma)$ not known exactly - source of uncertainty due to the missing higher orders (MHOs) in theory (the `…').
- Typically these MHOs are estimated via scale variations. First concrete study including these have been recently performed by NNPDF. **See Cameron's talk**
- Our aim is a little different - to try and consider from first principles how such uncertainties should/could be included in a fit.

LHL and R.S. Thorne, arXiv:1811.08434

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On the Consistent Use of Scale Variations in PDF Fits and Predictions

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Abstract

We present an investigation of the theoretical uncertainties in parton distribution functions (PDFs) due to missing higher–order corrections in the perturbative predictions used in the

Basic Idea

- PDFs themselves not observable. Can recast fit process purely in terms of **fit** and **predicted** observables, with no reference to PDFs.

Fit $$O_{\rm fit} \sim f_i(\mu^2) \otimes \sigma_i(\mu^2) \sim f_i(\mu^2) \otimes \left(\sigma_i^{(0)}(\mu^2) + \alpha_S\, \sigma_i^{(1)'}(\mu^2) + \cdots\right)$$

A $\downarrow$ $\qquad$ **B** $\downarrow$ f_i $\downarrow$ **C** $\qquad$ $i:$ PDF type

Prediction $$O_{\rm pred} \sim f_i(\mu^2) \otimes \sigma'_i(\mu^2) \sim f_i(\mu^2) \otimes \left(\sigma_i^{(0)'}(\mu^2) + \alpha_S\, \sigma_i^{(1)'}(\mu^2) + \cdots\right)$$

- Rule of thumb: vary scale $\mu \in \left(\frac{\mu_0}{2}, 2\mu_0\right)$. Can propagate through to PDFs. However, will traditionally then include such a variation **again** in prediction.
- If we interpret 'theory uncertainty' as that inherent in expressing predicted quantity in terms of measured one then varying at both **B** and **C** not obviously the right procedure.
- Recasting in terms of $O_1 \leftrightarrow O_2$ via **A** makes this concrete.

Simple Model

- Simplest thing we can consider- fit to non-singlet structure function $F_{\rm NS}$ and prediction of another $F'_{\rm NS}$. At NLO:

$$g \otimes f(x) = \int_x^1 \frac{{\rm d}z}{z} f(z) g\left(\frac{x}{z}\right) \, ,$$

Fit $$F_{\rm NS}(x,Q^2) = xq_{\rm NS}(x,a_iQ^2) + \tilde{\alpha}_S C_q^{(1)} \otimes xq_{\rm NS}(x,a_iQ^2) - \tilde{\alpha}_S \ln a_i P_{qq}^{(0)} \otimes xq_{\rm NS}(x,a_iQ^2)$$

B

q_{NS}

C

A

Prediction $$F'_{\rm NS}(x,Q^2) = xq_{\rm NS}(x,a_fQ^2) + \tilde{\alpha}_S C_q^{(1)} \otimes xq_{\rm NS}(x,a_fQ^2) - \tilde{\alpha}_S \ln a_f P_{qq}^{(0)} \otimes xq_{\rm NS}(x,a_fQ^2)$$

- Here $a_{i,f} = \mu^2_{i,f}/Q^2$ reflects relative variation of factorization scale μ (renormalization scale fixed), so that rule of thumb variation is $a_{i,f} \in \left(\frac{1}{4}, 4\right)$
- '**Standard**' fit - fix $a_i = 1$: $\quad xq_{\rm NS}(x,\mu^2) = F_{\rm NS}(x,\mu^2) - \tilde{\alpha}_S C_q^{(1)} \otimes F_{\rm NS}(x,\mu^2) \, ,$

To $O(\alpha_S)$ throughout

- This is step **B**, to be used in **C**. However can just as well substitute in expression for F'_{NS} to get direct relation **A**.

Standard Fit

- Simplest thing we can consider- fit to non-singlet structure function F_{NS} and prediction of another F'_{NS}. At NLO:

$$g \otimes f(x) = \int_x^1 \frac{\mathrm{d}z}{z} f(z) g\left(\frac{x}{z}\right) ,$$

Fit $$F_{\mathrm{NS}}(x,Q^2) = xq_{\mathrm{NS}}(x,a_iQ^2) + \tilde{\alpha}_S C_q^{(1)} \otimes xq_{\mathrm{NS}}(x,a_iQ^2) - \tilde{\alpha}_S \ln a_i P_{qq}^{(0)} \otimes xq_{\mathrm{NS}}(x,a_iQ^2)$$

A ↓ B ↓ q_{NS} C ↓

Prediction $$F'_{\mathrm{NS}}(x,Q^2) = xq_{\mathrm{NS}}(x,a_fQ^2) + \tilde{\alpha}_S C_q^{(1)} \otimes xq_{\mathrm{NS}}(x,a_fQ^2) - \tilde{\alpha}_S \ln a_f P_{qq}^{(0)} \otimes xq_{\mathrm{NS}}(x,a_fQ^2)$$

- Predict:

$$F'_{\mathrm{NS}}(x,Q^2) = F_{\mathrm{NS}}(x,a_fQ^2) + \tilde{\alpha}_S \left(C_q'^{(1)} - C_q^{(1)}\right) \otimes F_{\mathrm{NS}}(x,a_fQ^2) - \tilde{\alpha}_S \ln a_f P_{qq}^{(0)} \otimes xF_{\mathrm{NS}}(x,a_fQ^2) ,$$

$\longrightarrow$ Direct $F_{\mathrm{NS}} \leftrightarrow F'_{\mathrm{NS}}$ relation, with MHO uncertainty on $\delta F'_{NS} : a_f \in \left(\frac{1}{4}, 4\right)$

- Straightforward to now consider MHO at fit stage - vary a_i . What do we find?

- Doing this we find for relation **A**: $a_{i,f} = \mu_{i,f}^2/Q^2$

Scale var. - prediction:

$$F'_{\rm NS}(x,Q^2) = F_{\rm NS}(x,a_f Q^2) + \tilde{\alpha}_S \left(C_q'^{(1)} - C_q^{(1)}\right) \otimes F_{\rm NS}(x,a_f Q^2) - \tilde{\alpha}_S \ln a_f P_{qq}^{(0)} \otimes x F_{\rm NS}(x,a_f Q^2)\ ,$$

Scale var. - prediction & fit:

$$F'_{\rm NS}(x,Q^2) = F_{\rm NS}(x,a_{fi} Q^2) + \tilde{\alpha}_S \left(C_q'^{(1)} - C_q^{(1)}\right) \otimes F_{\rm NS}(x,a_{fi} Q^2) - \tilde{\alpha}_S \ln a_{fi} P_{qq}^{(0)} \otimes x F_{\rm NS}(x,a_{fi} Q^2)\ ,$$

where: $a_{fi} \equiv a_f/a_i$

$\longrightarrow$ **Identical** up to $a_f \to a_{fi}$ replacement!

- Thus in this case effect of varying scale in prediction and fit is **completely equivalent** to variation in prediction alone (or fit):

$$\delta F'_{NS}: \quad a_i \in \left(\frac{1}{4}, 4\right) \sim a_f \in \left(\frac{1}{4}, 4\right) \qquad\qquad a_i \in \left(\frac{1}{4}, 4\right) \,\&\, a_f \in \left(\frac{1}{4}, 4\right) \sim a_{fi} \in \left(\frac{1}{16}, 16\right)$$

- Indeed in terms of fundamental $F_{\rm NS} \leftrightarrow F'_{\rm NS}$ relation:

$$F'_{\rm NS}(x,Q^2) = F_{\rm NS}(x,aQ^2) + \tilde{\alpha}_S \left(C_q'^{(1)} - C_q^{(1)}\right) \otimes F_{\rm NS}(x,aQ^2) - \tilde{\alpha}_S \ln a P_{qq}^{(0)} \otimes x F_{\rm NS}(x,aQ^2)$$

there is only one d.o.f. ('a'), corresponding to difference in (squared) scale at which we evaluate $F_{\rm NS}$ and $F'_{\rm NS}$.

Interpretation

$$F'_{\rm NS}(x,Q^2) = F_{\rm NS}(x,aQ^2) + \tilde{\alpha}_S \left(C_q'^{(1)} - C_q^{(1)}\right) \otimes F_{\rm NS}(x,aQ^2) - \tilde{\alpha}_S \ln a P_{qq}^{(0)} \otimes x F_{\rm NS}(x,aQ^2)$$

- ‘Rule of thumb’ variation: one varies logarithms in a within specified range, to keep track of decreasing dependence with order, but keeping $a \sim O(1)$.
- Within context of basic $F_{\rm NS} \leftrightarrow F'_{\rm NS}$ relation, this leads to $a \in \left(\frac{1}{4}, 4\right)$. MHO uncertainty in PDF should reflect this.
- In this example: either vary in **fit** or **prediction** by set amount, but **not in both**.
- If one wished to argue for larger variation, this could still be performed with larger range in either fit or prediction - complete overlap between these.
- Note: can also extend idea to higher orders straightforwardly in Mellin space, and extension to DY cross section works in same way.

$$F'_{\rm NS}(j,Q^2) = \frac{f'_q(j,\tilde{\alpha}_s)}{f_q(j,\tilde{\alpha}_s)} \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_s \gamma_{qq}(j,\tilde{\alpha}_s)} F_{\rm NS}(j,\mu^2)$$

- Clearly **global PDF** fit much more complex. Can we take this idea further?

Extension

- Next step towards generality, included coupled q, g evolution. Toy model - fit to two structure function observables:

$$F(Q^2) = \Sigma_+(\mu^2)\left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S\gamma_+} F_+ + \Sigma_-(\mu^2)\left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S\gamma_-} F_- \;,$$

$$H(Q^2) = \Sigma_+(\mu^2)\left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S\gamma_+} H_+ + \Sigma_-(\mu^2)\left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S\gamma_-} H_- \;,$$

1 quark flavour

and prediction of a third, $K(Q^2)$. Effect of coupled DGLAP simplified here by moving to diagonal basis. $\Sigma_\pm$: DGLAP eigenvectors

- Leaving details to our paper, varying in fit ($a_{f,h}$) and prediction (a_k), get:

$$K(Q^2) \sim \left(K_1 + \tilde{\alpha}_S \ln\left(\frac{a_f}{a_k}\right) K_2 + \tilde{\alpha}_S \ln\left(\frac{a_h}{a_f}\right) K_3\right) F\left(\frac{a_k}{a_f}Q^2\right) + F \leftrightarrow H$$

$$a_f \leftrightarrow a_h$$

- Situation no longer so simple - have introduced **completely new** logarithmic dependence on a_h/a_f . Variation in prediction alone would instead give:

$$K(Q^2) \sim (K_1 - \tilde{\alpha}_S \ln(a_k) K_2)\, F\left(a_k Q^2\right) + F \leftrightarrow H$$

- What does this tell us?

Prediction only:

$$K(Q^2) \sim (K_1 - \tilde{\alpha}_S \ln(a_k) K_2)\, F\left(a_k Q^2\right) + F \leftrightarrow H$$

Fit & prediction:

$$K(Q^2) \sim \left(K_1 + \tilde{\alpha}_S \ln\left(\frac{a_f}{a_k}\right) K_2 + \tilde{\alpha}_S \ln\left(\frac{a_h}{a_f}\right) K_3\right) F\left(\frac{a_k}{a_f} Q^2\right) + F \leftrightarrow H$$

- Including MHO uncertainty in fit has introduced genuinely new d.o.f. in $K \leftrightarrow F, H$ relation - **cannot** in general include via variation in **fit/prediction alone**.
- We find if one assumes variations fully correlated in fit could equally include in prediction (but implicitly assumes correlated there as well).

Backup

- However, things do simplify if one considers low/high x regions:

$$F(Q^2) = \Sigma_+(\mu^2) \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S \gamma_+} F_+ + \Sigma_-(\mu^2) \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S \gamma_-} F_- \; ,$$

★ High x : $\Sigma_+(j,\mu^2) = g(j,\mu^2)$, $\Sigma_-(j,\mu^2) = \Sigma_q(j,\mu^2)$

★ Low x : $g(j,\mu^2) \sim q(j,\mu^2) \sim \Sigma_+(j,\mu^2)$

- That is, certain eigenvectors dominate, with consequences for our results…

Low/High x limits

- In both cases, dominance of single eigenvector/separation of q, g means that we revert back to original 'non-singlet' case.
- Consider e.g. fit to processes sensitive to high x gluon (jets, $t\bar{t}$ ...). Then:

$$F(Q^2) = \underset{\sim g}{\Sigma_+(\mu^2)} \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S \gamma_+} F_+ + \underset{\sim \Sigma_q}{\Sigma_-(\mu^2)} \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S \gamma_-} F_- \quad \longrightarrow \quad F(Q^2) = \Sigma_+(\mu^2) \left(\frac{Q^2}{\mu^2}\right)^{\tilde{\alpha}_S \gamma_+} F_+$$

$$\text{and :} \quad K(Q^2) = \frac{K_+}{F_+} \left\{1 + \tilde{\alpha}_S \ln\left(\frac{a_f}{a_k}\right) \gamma_+\right\} F\left(\frac{a_k}{a_f} Q^2\right)$$

one scale d.o.f, i.e. vary in fit/prediction but not both, as in simple case.

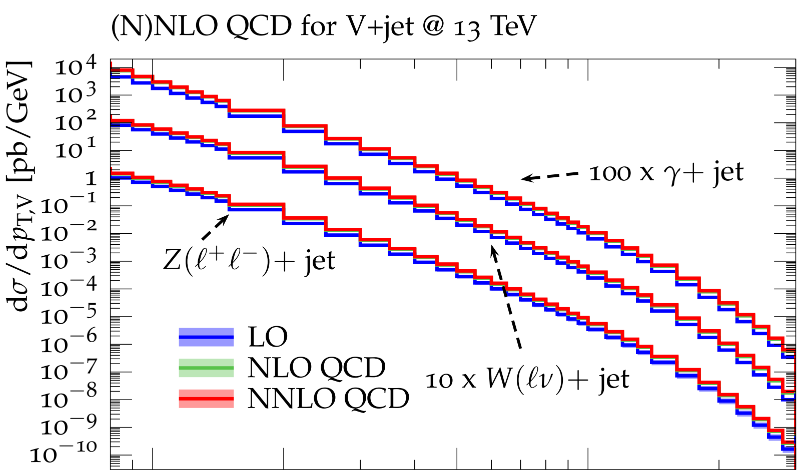
Renormalization Scale

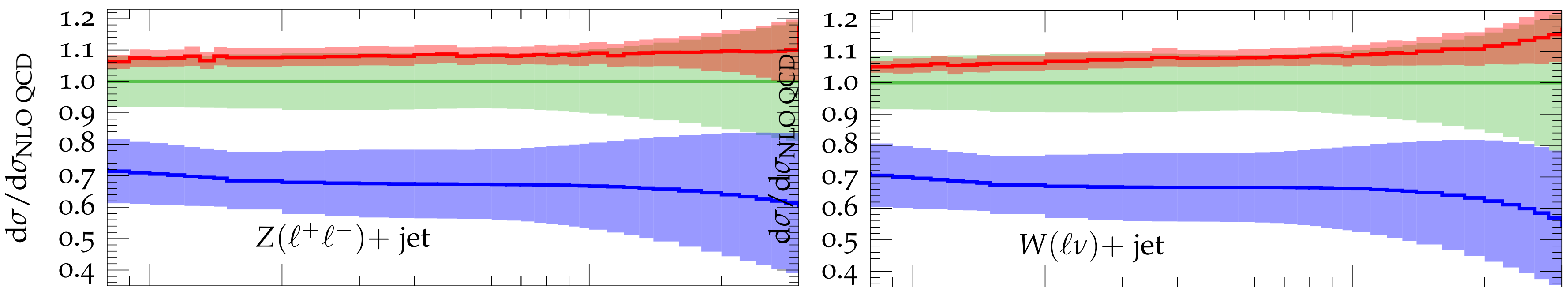
- Consider within very simple toy model, fit to $A(Q^2)$ and predict $B(Q^2)$:

$$A(Q^2) = \tilde{\alpha}_S(\mu_i^2) A_1 \left[1 + \frac{\tilde{\alpha}_S(\mu_i^2)}{A_1} \left(A_2 + \beta^{(0)} A_1 \ln a_i \right) \right] q(Q^2) \; .$$

$$B(Q^2) = \tilde{\alpha}_S(\mu_f^2) B_1 \left[1 + \frac{\tilde{\alpha}_S(\mu_f^2)}{B_1} \left(B_2 + \beta^{(0)} B_1 \ln a_f \right) \right] q(Q^2)$$

- If we write $\alpha_S \leftrightarrow A(Q^2)$, then in fact find similar situation to factorization scale. But not what we are interested in here, i.e. a fit to PDFs.
- In that case, no simple breakdown of scales as before. However, what if we consider two related processes (e.g. W, Z)?





J. M. Lindert et al., Eur. Phys. J. C77 (2017) no.12, 829

Related Processes

- On the other hand for two related processes (e.g. W, Z):

$$\frac{A_2}{A_1} \sim \frac{B_2}{B_1} \equiv C_{\rm NLO}$$

our fit results in the relation:

$$B(Q^2) \ = \frac{B_1 A(Q^2)}{A_1} \frac{\tilde{\alpha}_S(\mu_f^2)}{\tilde{\alpha}_S(\mu_i^2)} \left[1 + \beta^{(0)} \left(\tilde{\alpha}_S(\mu_f^2) \ln a_f - \tilde{\alpha}_S(\mu_i^2) \ln a_i\right) + \frac{B_2}{B_1} \tilde{\alpha}_S(\mu_f^2) - \frac{A_2}{A_1} \tilde{\alpha}_S(\mu_i^2)\right] .$$

$$\downarrow$$

$$\frac{B(Q^2)}{A(Q^2)} = \frac{B_1}{A_1} \left[1 + \beta^{(0)} \left(\tilde{\alpha}_S(\mu_f^2) \ln a_f - \tilde{\alpha}_S(\mu_i^2) \ln a_i\right) + C_{\rm NLO} \left(\tilde{\alpha}_S(\mu_f^2) - \tilde{\alpha}_S(\mu_i^2)\right)\right]$$

- Thus, to maintain consistency with requirement that this ratio $A(Q^2)/B(Q^2)$ should be ~ constant under inclusion of higher-order QCD corrections, need to take $\mu_i \sim \mu_f$ in relation between fit/predicted observables.

- In practice, keeping track of such fit/prediction correlations impossible. However can enter at same level as correlations between related processes in fit $\Rightarrow$ (open) question of whether it makes sense to include one when ignoring the other.

In Summary

- By considering PDF fit as a relation between different observables we find that:
  - ★ Including factorization scale variation in both fit and prediction leads to overestimate of error in certain regimes (simplified model - low/high x).
  - ★ Only varying in predictions does not fully account for theory error inherent in the relationship between observables.
  - ★ Assuming a full correlation between factorization scales at the fit stage also misses this (and if fully correlated in fit, why not in prediction as well?).

- A possible route forward (future work):
  - ★ Vary factorization scale at fit stage.
  - ★ Do not vary factorization scale at prediction stage.
  - ★ Apply a phenomenological approach for dealing with correlation between different processes entering fit.

Caveats

- ★ **Caveat 1** : This all relies on us trusting scale variation as the correct approach. Our results might even be taken as indication that it is not. But result of working in physical basis should apply in any case.

- ★ **Caveat 2** : Only applies to factorization scale. We find renormalization scale is different, with no clear fit/prediction overlap (i.e. should include both). However correlations between related processes (e.g. W, Z) in fit/prediction in principle as important as in fit.

Thank you for listening!

Backup

Correlated Scale Variations

$$K(Q^2) \sim \left(K_1 + \tilde{\alpha}_S \ln\left(\frac{a_f}{a_k}\right) K_2 + \tilde{\alpha}_S \ln\left(\frac{a_h}{a_f}\right) K_3\right) F\left(\frac{a_k}{a_f} Q^2\right) + F \leftrightarrow H$$

- If one assumes all factorization scale variation is correlated across observables, have $a_f = a_h$, and:

$$K(Q^2) \sim (K_1 - \tilde{\alpha}_S \ln(a_{kf}) K_2)\, F\left(a_{kf} Q^2\right) + F \leftrightarrow H$$

compare with variation in prediction alone:

$$K(Q^2) \sim (K_1 - \tilde{\alpha}_S \ln(a_k) K_2)\, F\left(a_k Q^2\right) + F \leftrightarrow H$$

- Thus again we reduce back to case where variation could be included in either fit or prediction, but not both (n.b. correlation in fit observables $\Rightarrow$ correlation in predicted ones).
- However such an assumption appears to be overly strong, missing some of the genuine d.o.f inherent in the $K \leftrightarrow F, H$ relation.

Renormalization Scale

- Consider within very simple toy model, fit to $A(Q^2)$ and predict $B(Q^2)$:

$$A(Q^2) = \tilde{\alpha}_S(\mu_i^2) A_1 \left[1 + \frac{\tilde{\alpha}_S(\mu_i^2)}{A_1}\left(A_2 + \beta^{(0)} A_1 \ln a_i\right)\right] q(Q^2) \,.$$

$$B(Q^2) = \tilde{\alpha}_S(\mu_f^2) B_1 \left[1 + \frac{\tilde{\alpha}_S(\mu_f^2)}{B_1}\left(B_2 + \beta^{(0)} B_1 \ln a_f\right)\right] q(Q^2)$$

- If we write $\alpha_S \leftrightarrow A(Q^2)$, then in fact find similar situation to factorization scale. But not what we are interested in here, i.e. a fit to PDFs.

- In that case, no simple breakdown of scales as before (fact. scale fixed here):

$$a_{i,f} = \mu_{i,f}^2/Q^2$$

$$B(Q^2) = \frac{B_1 A(Q^2)}{A_1}\frac{\tilde{\alpha}_S(\mu_f^2)}{\tilde{\alpha}_S(\mu_i^2)}\left[1 + \beta^{(0)}\left(\tilde{\alpha}_S(\mu_f^2)\ln a_f - \tilde{\alpha}_S(\mu_i^2)\ln a_i\right) + \frac{B_2}{B_1}\tilde{\alpha}_S(\mu_f^2) - \frac{A_2}{A_1}\tilde{\alpha}_S(\mu_i^2)\right] \,.$$

e.g. if we take $\mu_f = \mu_i$ ($a_{fi} = 1$) and vary renormalization scales, this is not the same as taking $a_i = a_f = 1$ ($\mu_{i,f} = Q$), as in case of factorisation scale - due to 3rd/4th terms which depend on absolute scales $\mu_{i,f}$.