Profiling PDFs.

S.Glazov, xFitter workshop, 19 Feb 2016

PDF Profiling methodology

Predictions given for each PDF eigenvector can be included in χ^2 definition for comparisons with the data:

$$\chi^2(b,m) = \sum_i \left(\frac{\mu_i - m_i \left[1 - \sum_j b_j^{\mathrm{exp}} \gamma_{ji}^{\mathrm{exp}} + \sum_j b_j^{\mathrm{theo}} \gamma_{ji}^{\mathrm{theo}} \right]}{\Delta_i} \right)^2 + \sum_j (b_j^{\mathrm{exp}})^2 + \sum_j (b_j^{\mathrm{theo}})^2$$

Shifts of the theory nuisance parameters b_j^{theo} and reduction of their uncertainties affect the theory predictions. They also can be propagated to PDFs, to see the impact of the data on them. For asymmetric uncertainties, shifts are:

$$F = 0.5 \sum_j (\Delta F_j^{\mathrm{up}} - \Delta F_j^{\mathrm{down}}) b_j^{\mathrm{theo}} + (\Delta F_j^{\mathrm{up}} + \Delta F_j^{\mathrm{down}})(b_j^{\mathrm{theo}})^2$$

After profiling, the b_j^{theo} parameters are correlated to each other, must be diagonalized.

PDF rotation methodology

Using linear approximation, PDF dependence for N_{M} independent measurements can be described by the usual χ^2 function:

$$\chi^2(\beta) = \sum_{i=1}^{N_{\mathrm{M}}} \left(\frac{\sum_{j=1}^{N_{\mathrm{PDF}}} \Gamma_{ij}\beta_j}{\sigma_i} \right)^2 + \sum_{j=1}^{N_{\mathrm{PDF}}} \beta_j^2.$$

Here β are the nuisance parameters corresponding to each PDF eigenvector, $\Gamma_{ij} = 0.5(\Gamma_{ij}^{+} - \Gamma_{ij}^{-})$ are the symmetrized shifts of the measurement corresponding to each eigenvector, and σ_i are the expected uncertainties of the measurements (the value of σ_i does not matter if $N_{\mathrm{M}} < N_{\mathrm{PDF}}$, where N_{PDF} is the number of PDF eigenvectors). The corresponding covariance matrix is

$$C_{jk} = \frac{1}{2}\frac{d^2\chi^2}{\mathrm{d}\beta_j \mathrm{d}\beta_k} = \sum_i \frac{\Gamma_{ij}\Gamma_{ik}}{\sigma_i^2} + \delta_{ij}\,,$$

where δ_{ij} is the Kronecker symbol. The matrix C can be diagonalized using eigenvector decomposition (U), the eigenvectors corresponding to the largest eigenvalues (D) can be used to represent the bulk of PDF uncertainties.

$$\chi^2 = \beta^T C\beta = \beta^T U^T DU\beta = (\beta')^T D\beta',\;\; \beta' = U\beta\,,\;\; \Gamma' = U^T\Gamma\,.$$

Rotation for sets with asymmetric errors

For symmetric PDF uncertainties, the rotated eigenvectors shifts, $\Delta F'_i = F'_i - F'_0$, are linear combinations of the original shifts

$$\Delta F'_i = \sum U_{ij} \Delta F_j \, .$$

This rotation can be generalized to asymmetric uncertainties in several ways. E.g. the sum can be taken depending on the direction defined by U_{ij}:

$$\Delta^+ F'_i = \sum |U_{ij}| \begin{cases} \Delta^+ F_j, \text{ if } U_{ij} \geq 0 \\ \Delta^- F_j, \text{ if } U_{ij} < 0 \end{cases} \quad \Delta^- F'_i = \sum |U_{ij}| \begin{cases} \Delta^- F_j, \text{ if } U_{ij} \geq 0 \\ \Delta^+ F_j, \text{ if } U_{ij} < 0 \end{cases} \, .$$

Alternatively, quadratic approximation can be used, which is also used for fits in `xFitter`: $\Gamma_i = (\Delta^+ F_i - \Delta^- F_i)/2$, $\Omega_i = (\Delta^+ F_i + \Delta^- F_i)/2$. In this case

$$\Delta^+ F'_i = \sum U_{ij} \left(\Gamma_i + U_{ij} \Omega_i \right) , \quad \Delta^- F'_i = \sum -U_{ij} \left(\Gamma_i - U_{ij} \Omega_i \right) .$$

Post-rotation after profiling

The diagonalization of the PDF eigenvectors after profiling aligns the resulting eigenvectors along the largest eigenvalues of the covariance matrix:

$$\beta^T C\beta = \beta^T G^T DG\beta = \beta^T(\sqrt{D}G)^T(\sqrt{D}G)\beta = \beta^T\Gamma^T\Gamma\beta = (\beta')^T\beta' \, .$$

It might be beneficial to restore the original directions of the eigenvectors, in particular in case of the asymmetric uncertainties. This can be achieved by first performing rotation to one selected original eigenvector in N_{PDF} space, when optimizing for another eigenvector in the orthogonal $N_{\mathrm{PDF}} - 1$ sub-space, etc. Since in the new basis the coordinates of the original eigenvectors are given by the Γ_{ij} matrix, the procedure can be described as

$$C^k = \Gamma_{ik}\Gamma_{jk} + \delta_{ij} \, , \quad C^k = G^T DG \, , \quad \Gamma' = G\Gamma \, ,$$

where there is no summation over index k and dimension of the matrices is reduced by one unit at each iteration. At the end of this procedure, the resulting profiling matrix Γ' takes triangular form. Finally, one can ensure that the directions of the profiled eigenvectors coincide with the original vectors by checking the sign of the diagonal elements Γ'_{ii}:

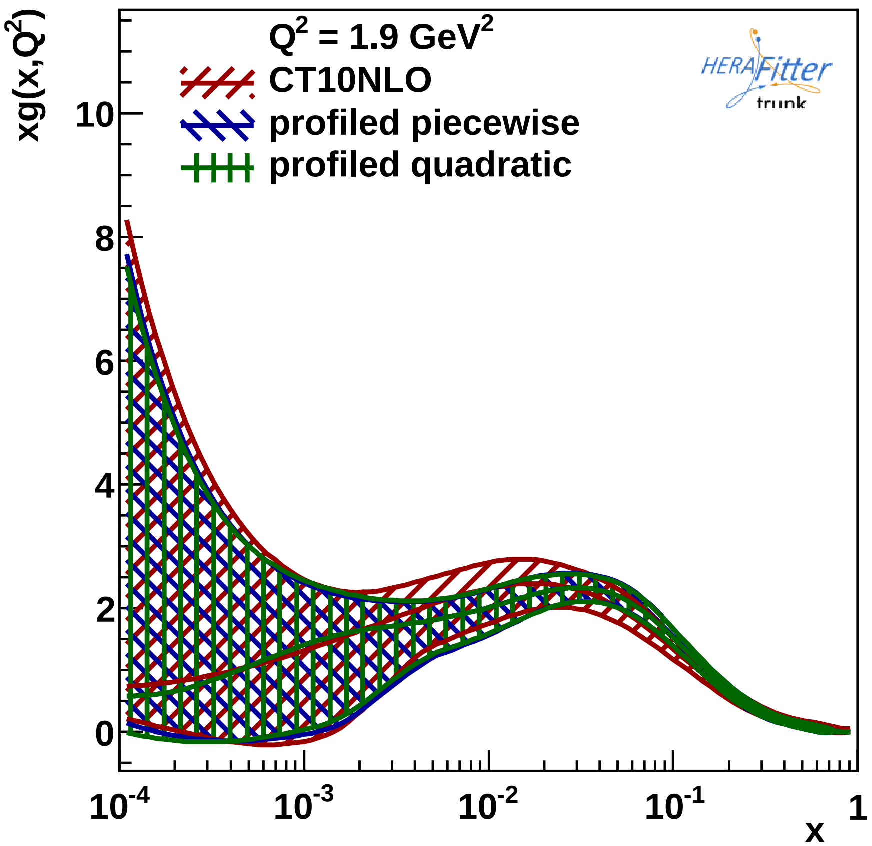
$$\Gamma''_{ij} = \begin{cases} \Gamma'_{ij} & \text{if} \quad \Gamma'_{ii} \geq 0 \\ -\Gamma'_{ij} & \text{if} \quad \Gamma'_{ii} < 0 \end{cases}$$

Example: profiling HERAPDF15NLO

As an example, below are given the results of the HERAPDF15NLO profiling using the ATLAS 2010 W, Z data. Note e.g. that the original eigenvector 10 affects only the new eigenvector 10, its uncertainty is reduced to 0.6977

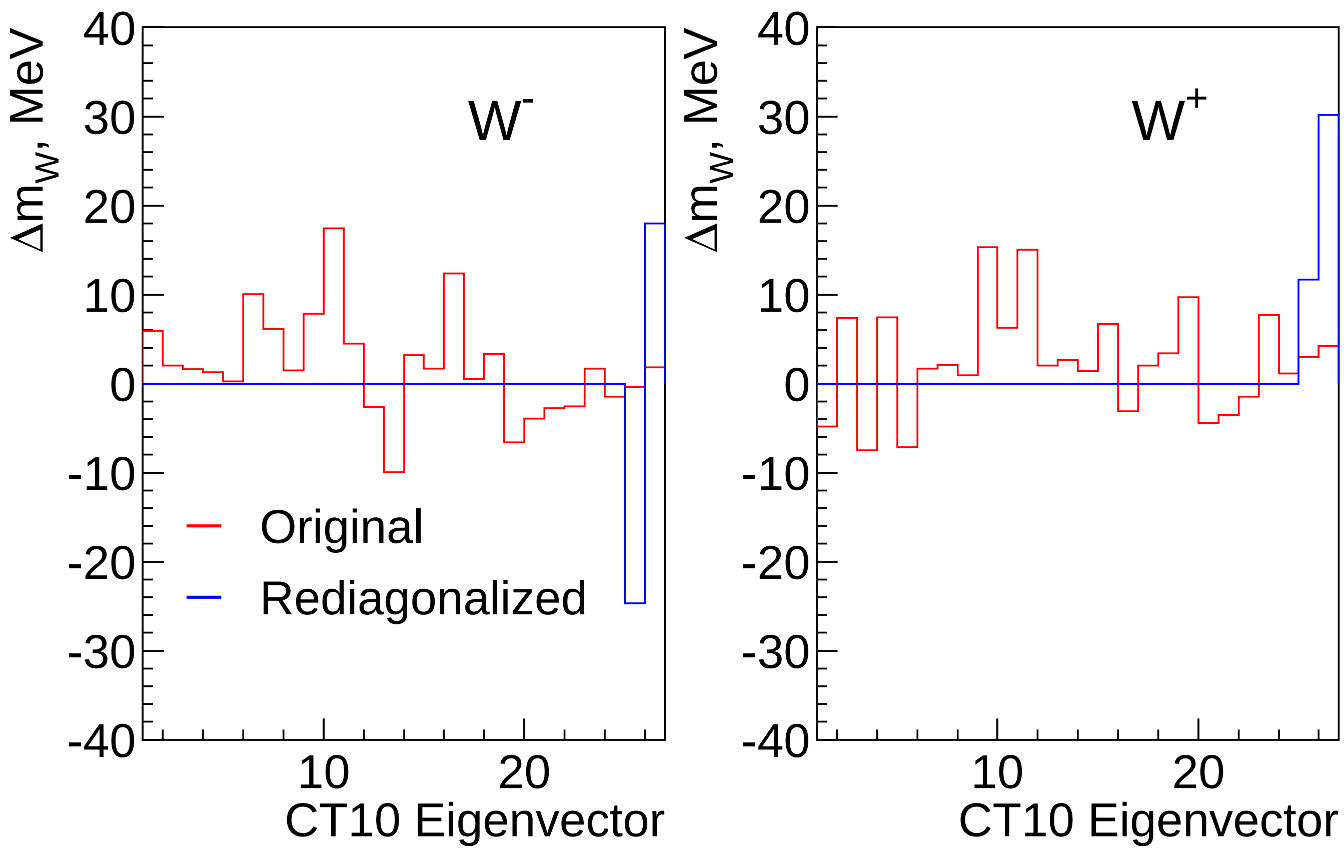
```
cat output/pdf_shifts.dat
LHAPDF set=                HERAPDF15NLO_EIG
 10
  1 -0.0064  0.9987
  2 -0.0838  0.9893
  3  0.0976  0.9756
  4 -0.3745  0.9630
  5 -0.0676  0.9831
  6  0.7334  0.9406
  7  0.2987  0.9634
  8 -0.3419  0.8767
  9  0.6662  0.9194
 10 -0.7011  0.6977
cat output/pdf_rotation.dat
LHAPDF set=                HERAPDF15NLO_EIG
  10
    1  0.998494  0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
    2 -0.006112  0.984912  0.000000  0.000000 -0.000000  0.000000  0.000000 -0.000000 -0.000000 -0.000000
    3  0.009619  0.038416  0.971351 -0.000000 -0.000000  0.000000 -0.000000  0.000000  0.000000  0.000000
    4 -0.003520 -0.046477  0.046229  0.938295 -0.000000 -0.000000  0.000000  0.000000  0.000000 -0.000000
    5 -0.003507  0.003023  0.010990  0.025255  0.970369 -0.000000 -0.000000 -0.000000  0.000000 -0.000000
    6  0.001223  0.002171  0.006016  0.049349  0.018796  0.934258 -0.000000  0.000000 -0.000000  0.000000
    7 -0.000364  0.017446  0.001635  0.085343 -0.054907 -0.038960  0.931616 -0.000000 -0.000000  0.000000
    8 -0.012431 -0.049505  0.071189 -0.057106 -0.039412  0.010774 -0.021346  0.868702  0.000000 -0.000000
    9  0.001634  0.039591 -0.029444  0.129510 -0.033428 -0.093207 -0.109898  0.082426  0.894731 -0.000000
   10  0.002466 -0.026666 -0.009489 -0.129140  0.137537  0.039995  0.218584  0.084169  0.211688  0.697666
```

Example: profiling, asymmetric uncertainties



The quadratic propagation is default, the piecewise-linear is activated by the `--piecewise-linear` option.

Example: Optimizing W^+ and W^- mass measurement



Use PDF uncertainty estimation using MCFM+CUTE predictions (ATL-PHYS-PUB-2014-015), directly for W mass measurement using lepton p_T. The rediagonalization procedure reduces the number of relevant eigenvectors to just $N_\mathrm{M} = 2$.

xFitter implementation: LHAPDF6 manipulation

The operations on LHAPDF files are performed using standalone executable `xfitter-process` which is shipped with the xFitter package.

Symmetrisation:

```
xfitter-process symmetrize pdf_dir_in pdf_dir_out
```

Rotation:

```
xfitter-process rotate [--piecewise-linear] pdf_rotation pdf_dir_in pdf_di

Options are
  --piecewise-linear: use piecewise linear approximation
   (default: quadratic approximation )
```

Profiling:

```
xfitter-process profile [--piecewise-linear] pdf_shifts pdf_rotation \
                                     pdf_dir_in pdf_dir_out
Options are
```

The `pdf_rotation` and `pdf_shifts` files can be produced by xFitter, their format is given on slide 5

xFitter implementation: profiling

The `pdf_shifts.dat` and `pdf_rotation.dat` files are produced automatically for evaluations of the predictions using LHAPDF, with uncertainties included:

```
*
* Main steering cards
*
&xFitter
  RunningMode = 'LHAPDF Analysis'
                ! 'LHAPDF Analysis' -- Evalutate input LHAPDF set uncertaitnies, chi2, profilin
                !                      Requires &LHAPDF namelist to specify the set name. If PD
                !                      set to LHAPDFQ0, LHAPDF or LHAPDFNATIVE, sets it to LHAP

  PDFStyle = 'LHAPDF'
  ...
&End
*
* (Optional) LHAPDF sttering card
*
&lhapdf
  LHAPDFSET   = 'CT10nlo' ! LHAPDF grid file
  LHAPDFERRORS = T
&End
```

xFitter implementation: rotation

The rotation is defined by the text-based theory predictions (central, plus variations due to each PDF eigenvector), weighted according to the importance of the observable. The text-based predictions can be produced using `LHAPDFERRORS = T` option (`theo_0X.dat` files). The weights are introduced by hand, as an extra column with a predefined name "stat" or "uncor" (weight = 1/stat$\hat{2}$). The evaluation of rotation vectors is activated by 'PDF ROTATE' mode:

```
&InTheory
    InputTheoNames = 'theo_01.dat'
&End
...
*
* Main steering cards
*
&xFitter
  RunningMode = 'PDF Rotate'
  ...
&End
```

PDF plus model uncertainties

- QCD analysis of the data depends not only on PDFs but also other parameters, such as α_S and heavy flavour masses m_c, m_b.
- Usual way to estimate uncertainties due to these external parameters is to repeat PDF fits with the parameters varied within their uncertainties.
- It can be shown (CTEQ:PRD82:054021,2010 and also backup slides) that the uncertainty resulting from these "model variation" sets can be added in quadrature to the PDF uncertainties to get the total PDF plus model uncertainty; e.g. PDF+model variation set is orthogonal.
- Talk from Pavel Shvydkin tomorrow will discuss improved user interface for this procedure.

Extra slides

Motivation

Eigenvector representation of PDF sets with uncertainties allow for a number of useful operations. They are based on

- linearity of the evolution equation
- "zero" sum rules for $\Delta F_i = F_i - F_0$, the difference between a PDF eigenvector and the central PDF ("eigenvector shift").

That guarantees that any linear combination of ΔF_i is a valid ΔF_i which can be added to a central PDF set to provide a valid central PDF set.

Uniformity of the `LHAPDF6` library makes possible to perform operations such as rotation and profiling in a uniform way. In this representation, the central PDF set is a vector of values of all 13 PDFs at all Q^2, x grid points. The results stay in `LHAPDF6` format, represented as vectors in this space, without need for additional interpolation, without any loss of accuracy.

(see also
https://indico.cern.ch/event/357157/contribution/6/material/slides/0.pdf and
https://indico.cern.ch/event/354731/contribution/5/material/slides/0.pdf)

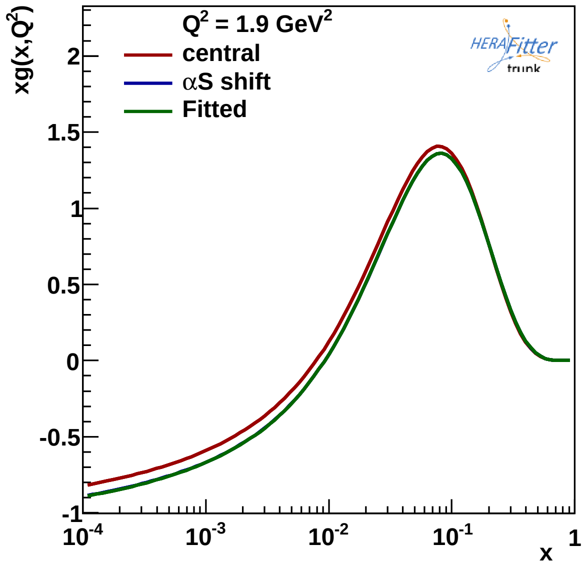
PDF+α_S studies: test setup

The decorrelation is illustrated using a toy $13p$ fit to the HERA-I data, at NLO, using ZMVFNS. The model variation under study is the α_S variation of $\delta\alpha_S(M_Z) = 0.0005$. The ZMVFNS fit requires a large value of $m_C = 1.8$ GeV. To avoid threshold effects, the data are required to be at $Q^2 \geq 7$ GeV^2.

In this setup, an $\alpha_S(M_Z)$ scan has been performed. The data prefers large value of $\alpha_S(M_Z) = 0.1294$ with a large uncertainty (~ 0.005). The χ^2/dof value at the minimum is $\chi^2/dof = 499.52/537$

The 13-PDF eigenvectors are determined using the standard procedure by Jon Pumplin. The uncertainties are checked using toy-MC method.

Step 1: decomposing model variation with eigenvectors



← for the two example, the main impact of the α_S variation is for the gluon density and it can be described by the PDF eigenvector decomposition pretty accurately.

First we want to represent the model variation in terms of eigenvector decomposition. Since the baseline PDF parameterisation is the same, it can be always done in the PDF parameter space in a unique way. However it is more practical to perform the decomposition in the PDF-space, at the evolution starting scale. In this case LHAPDF6 grid files can be used directly:

$$\chi^2(\Gamma_j) = \sum_{f,x_i} \left(\delta P^f_{\delta\alpha_S}(x_i) - \sum \Gamma_j P_f^{\mathrm{eig},j}(x_i)\right)^2 .$$

Here the sum is performed over all PDF flavours f and grid points x_i.

The PDF + model χ^2

The correlation of the PDF and model uncertainties can be represented by a covariance matrix of

$$\chi^2(\beta_i^{\rm PDF}, \beta^m) = \sum_{i=1}^{N_{\rm eig}} \left(\beta_i^{\rm PDF} - \Gamma_i \beta^m\right)^2 + (\beta^m)^2 \ .$$

Here β^m corresponds to the vector $(0 \ldots 0, 1)$ in PDF/model variation space. To check the χ^2 function, one can vary β by one unit and verify that it changes by one unit too, for a correspondig variations of PDFs. The inverse covariance matrix of the χ^2 function is

$$C = \begin{pmatrix} 1. & 0 & \ldots & -\Gamma_1 \\ 0. & 1. & \ldots & -\Gamma_2 \\ \ldots & \ldots & \ldots & \ldots \\ -\Gamma_1 & -\Gamma_2 & \ldots & 1 + \sum \Gamma_j^2 \end{pmatrix} .$$

Properties of the matrix C

It is easy to show that $\det C = 1$. The diagonal elements of the covariance matrix C^{-1} are $1 + \Gamma_j^2$ for PDF eigenvector j and 1 for the model variation, meaning that adding in quadrature rule is Ok for the PDFs themselves.

The characteristic polynomial of C is

$$f(t) = \det(C - I \cdot t) = (1-t)^{N_{\text{eig}}-1}\left[1 - \left(2 + \sum \Gamma_j^2\right) t + t^2\right] .$$

That means that $N_{\text{eig}} - 1$ eigenvalues of C are equal to unity while the remaining two eigenvalues are equal to $A = 1 + \frac{\sum \Gamma_j^2 + \sqrt{4 \sum \Gamma_j^2 + \left(\sum \Gamma_j^2\right)^2}}{2}$ and $1/A$. The eigenvectors corresponding to unit eigenvalues are orthogonal rotations in PDF space while the remaining two are the hyperbolic rotations (“squeeze mapping”) in PDF/model variation space.

→ after diagonalization of C^{-1} the PDF plus model variation uncertainties are represented by $N_{\text{eig}} - 1$ pure PDF variations and 2 mixed PDF-model variations.

Finally, the resulting set can be rotated such that model variation direction is orthogonal to the rest, restoring the original form of the eigenvector set. The result of this operation coincides with the original PDF plus model variation set.