xFitter Tutorial

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xFitter tutorial

- Introduction: PDFs and the xFitter framework (formerly HERAFitter)
- An example of xFitter usage:

QCD analysis of W and Z boson production at the Tevatron

Exercises





PDFs in the LHC era

Factorisation theorem:

Partonic cross sections

 Cross section are calculated by convoluting short distance partonic reactions with Parton Distribution Functions (PDFs)

 $\sigma_{p p \to X} = \sum_{i, j} \int dx_1 dx_2 \left(f_i^p(x_1, \mu) \right)$

- Discovery of new exciting physics relies on precise knowledge of proton structure.
- PDFs are among the dominant uncertainties for the W mass measurement and gg → H production

xFitter provides a framework for

- Investigation of various methodologies in PDF fits
- Assess the impact of new data on PDF
- Help the experiments to improve the sensitivity of new measurements to PDF



PDFs

 $x_2, \mu \not \propto \sigma_i$

Schematic of PDF fits



Schematic of PDF fits



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QCD analysis of W and Z Tevatron data

arXiv:1503.05221

- This analysis provides an extensive example of usage of xFitter, and is a good reference for a typical phenomenological study that can be performed with xFitter
- Various PDF fitting techniques were used: MINUIT minimisation, Hessian profiling, Bayesian reweigthing
- The paper provides detailed descriptions of the settings of a QCD analysis and of the χ^2 definition
- Various PDF parametrisation forms are explored
- All the plots in the paper are produced with xFitter







Motivation

 Precise determination of the quark valence PDFs is essential for precision measurements at the LHC, like the W mass and the weak mixing angle, and also for searches of new physics



 The reason is the stronger coupling of photons to u-quark than d-quark

H1prelim-14-042,ZEUS-prel-14-007

Motivation

proton

U

d

u

đ

- In proton-antiproton collisions, DY processes of W and Z production are valence-quark dominated
- They can be used to improve quark valence PDFs, and especially the d-quark type, which is less constrained by DIS collider data

Ζ

W



u

Tevatron W and Z data sets

- 3 types of observables
 - Z do/dy (CDF and D0)
 - Lepton charge asymmetry in W \rightarrow I,v (D0)
 - W charge asymmetry (CDF and D0)

Fast theory predictions calculated with MCFM+APPLGRID



80

70

60

40

30

10

20 66 < M ... < 116 GeV/c² : measured o

0.5

NLO CTEQ6.1M prediction

1.5

2.5 2

lơ(ץ /Z)/dy (pb) 50

- Revised correlation model: uncertainties of data-driven corrections are treated as bin-to-bin uncorrelated (lepton ID, trigger, and charge efficiencies)
- Reasonable assumption: these corrections are influenced by stat noise

PDF fit of Tevatron W and Z production

QCD fit at NLO of HERA I and Tevatron W, Z data

The PDF parametrisation at the starting scale Q^2 = 1.7 GeV² is optimised through a χ^2 scan



Experiment	χ ² /points
H1 - ZEUS	516/550
D0	23/28
CDF	32/28
D0	12/10
CDF	14/13
D0	8/14
	606/628
	Experiment H1 - ZEUS D0 CDF D0 CDF D0

The optimal parametrisation has 15 parameters

Needed additional freedom in the valence PDFs to fit the W data, exp terms preferred



Impact on d-quark valence PDF

- The impact of the Tevatron W, Z data is assessed by comparing PDFs extracted from a fit to only HERA I data
- Observed large impact on d-quark valence PDF, mainly driven by the measurements of W charge asymmetry



Example of plots that can easily be produced with xFitter

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W charge asymmetry, D0 and CDF

Example of plots that can easily be produced with xFitter



 The results of the PDF fit are illustrated with data/theory comparison plots

Compatibility with global PDF sets



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Profiling global PDF sets

Assess the impact of the Tevatron data on the global PDF fits with a hessian profiling technique

Add the hessian PDF uncertainties as nuisance parameters β in the χ^2

Minimise the χ^2 and profile the PDF shifts β to the data

 $\chi^2(\boldsymbol{\beta}_{\mathrm{exp}}) \to \chi^2(\boldsymbol{\beta}_{\mathrm{exp}}, \boldsymbol{\beta}_{\mathrm{th}})$

xFitter is used to asses the impact of new data on already existing PDF sets





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- PDF fit to HERA I+II data
- **2** PDF fit and α_s extraction from HERA jets data
- LHAPDF analysis: PDF profiling
- Plotting of LHAPDF6 files
- **9** Equivalence of χ^2 definitions

xFitter tutorial loading...

Open a shell and do:

student@mcnet:~\$ cd tutorial/xfitter
student@mcnet:~/tutorial/xfitter\$ svn up

• Each of the five exercise is in a separate directory:

```
exercise1/
exercise2/
exercise3/
exercise4/
exercise5/
```

 You can find the xFitter manual, the README file, and this tutorial in doc/

doc/manual.pdf
doc/README
doc/tutorial.pdf

As a general rule, each exercise has:

- A README file, which contains all the commands to perform the exercise
- A input/ directory, with all the necessary input settings for running xFitter
- During the exercise, we will create a run/ directory, where we will run xFitter
- The results will be saved in the output/ directory, for further manipulation

On a shell type xfitter and press the Tab character twice

- xfitter: The main xFitter program, to perform PDF fits
- xfitter-draw: Graphical visualisation of the results
- xfitter-process: Post-fit or pre-fit manipulation of LHAPDF files
- xfitter-config: Provide compiler options to link xFitter as an external library

In general, each time we want to run xFitter, we need to care about three configuration files:

- steering.txt
 - Running mode: PDF fit or LHAPDF analysis
 - List of data sets
 - PDF parametrisation
 - QCD Order, heavy flavour scheme
 - χ^2 settings
- ewparam.txt
 - EW and SM parameters (mainly used for the DIS cross section)
- minuit.in.txt
 - Settings and commands for minuit
 - Fix and free parameters of the PDF parametrisation

Exercise 1 PDF fit

cd exercise1

- purpose: Learn the basic settings of a QCD analysis
- data set: HERA I+II inclusive DIS data
- QCD order: NNLO



The HERA I+II data sets are set in input/steering.txt

```
&InFiles
```

```
! Number of intput files
NInputFiles = 7
```

```
! Input files:
```

```
InputFileNames(1) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_920.dat'
InputFileNames(2) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_820.dat'
InputFileNames(3) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_675.dat'
InputFileNames(4) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_460.dat'
InputFileNames(5) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCem.dat'
InputFileNames(6) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCem.dat'
InputFileNames(6) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_CCem.dat'
InputFileNames(7) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_CCem.dat'
InputFileNames(7) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_CCem.dat'
```

We will use the option RunningMode = 'Fit' in input/steering.txt

```
&xFitter
RunningMode = 'Fit'
    'Fit' -- standard MINUIT-minimization of PDF and other parameters
    'LHAPDF Analysis' -- Evalutate input LHAPDF set uncertaitnies, chi2, profiling or reweig
    Requires &LHAPDF namelist to specify the set name. If PDFSTYLE is set to LHAPDFQ0, LHAPDF or LHAPDFNATIVE, sets it to LHAPDF
    'PDF Rotate' -- performs PDF re-diagonalization. Requires theo.in files to operate
```

&End

The order in perturbative QCD is set in input/steering.txt

&xFitter

... Order = 'NNLO' ! 'LO', 'NLO' or 'NNLO', used for DGLAP evolution. ... &End

the starting scale Q02 of the PDF parametrisation is set in <code>input/steering.txt</code>

&xFitter ... QO2 = 1.9 ! Evolution starting scale ... &End

Exercise 1 - settings

the Heavy flavour scheme is set in input/steering.txt

&xFitter

!	 Scheme for heavy flavors		
!	 HF_SCHEME = 'ZMVFNS'	:	ZM-VFNS (massless) from QCDNUM,
!	 HF_SCHEME = 'ZMVFNS MELA'	:	ZM-VFNS (massless) from MELA (N-space),
!	 HF_SCHEME = 'RT'	:	Thorne-Roberts VFNS (massive)
!	 HF_SCHEME = 'RT FAST'	:	Fast approximate TR VFNS scheme, usign k-factor
!	 HF_SCHEME = 'RT OPT'	:	Thorne-Roberts VFNS (massive)
!	 HF_SCHEME = 'RT OPT FAST'	:	Fast approximate TR VFNS scheme, usign k-factor
!	 HF_SCHEME = 'ACOT Full'	:	ACOT - F.Olness Version (massive), using k-factors
!	 HF_SCHEME = 'ACOT Chi'	:	ACOT - F.Olness Version (massive), using k-factors
!	 HF_SCHEME = 'ACOT ZM'	:	ACOT - F.Olness Version (massless), using k-factors
!	 HF_SCHEME = 'FF'	:	Fixed Flavour Number Scheme (qcdnum)
!	 HF_SCHEME = 'FF ABM'	:	Fixed Flavour Number Scheme (ABM)
!	 HF_SCHEME = 'FF ABM RUNM'	:	Fixed Flavour Number Scheme (ABM) using run mass def
!	 HF_SCHEME = 'FONLL-A'	:	FONLL-A mass scheme provided by APFEL with pole masses (available
!	 HF_SCHEME = 'FONLL-A RUNM OFF'	:	FONLL-A mass scheme provided by APFEL with MSbar masses running (
!	 HF_SCHEME = 'FONLL-A RUNM ON'	:	FONLL-A mass scheme provided by APFEL with MSbar masses running (
!	 HF_SCHEME = 'FONLL-B'	:	FONLL-B mass scheme provided by APFEL with pole masses (available
!	 HF_SCHEME = 'FONLL-B RUNM OFF'	:	FONLL-B mass scheme provided by APFEL with MSbar masses running (
!	 HF_SCHEME = 'FONLL-B RUNM ON'	:	FONLL-B mass scheme provided by APFEL with MSbar masses running (
!	 HF_SCHEME = 'FONLL-C'	:	FONLL-C mass scheme provided by APFEL with pole masses (available
!	 HF_SCHEME = 'FONLL-C RUNM OFF'	:	FONLL-C mass scheme provided by APFEL with MSbar masses running (
!	 HF_SCHEME = 'FONLL-C RUNM ON'	:	FONLL-C mass scheme provided by APFEL with MSbar masses running
		!	(Any of the FONLL schemes at LO is equivalent to the ZM-VFNS)

HF_SCHEME = 'RT OPT'

• • •

the PDF parametrisation is set in input/steering.txt

&xFitter

• •								
ŗ.	PDF parameteris	ation style. Possible styles are currently available:						
ŗ.	'HERAPDF' H	CRAPDF-like with uval, dval, Ubar, Dbar, glu evolved pdfs						
!	'CTEQ'	CTEQ-like parameterisation						
!	'CTEQHERA'	Hybrid: valence like CTEQ, rest like HERAPDF						
!	, CHEB,	CHEBYSHEV parameterisation based on glu,sea, uval,dval evolved pdfs						
ŗ.	'LHAPDFQO'	use lhapdf library to define pdfs at starting scale and evolve with local qcdnum p	ara					
!	'LHAPDF'	use lhapdf library to define pdfs at all scales						
!	'LHAPDFNATIVE'	use lhapdf library to access pdfs and alphas						
ŗ.	'DDIS'	use Diffractive DIS						
!	'BiLog'	bi-lognormal parametrisation						
F	PDFStyle = 'HERAPDF'							

&End

Convention for the HERAPDF-like PDF parametrisation

$$Ax^{B}(1-x)^{C}(1+Dx+Ex^{2})-A'x^{B'}(1-x)^{C'}$$

Exercise 1 - settings

the starting values of the parameters are set in input/minuit.in.txt

set title new 14p HERAPDF parameters 2 'Bg' -0.061953 0.027133 3 'Cg' 5.562367 0.318464 'Aprig' 0.166118 7 0.028009 8 'Bprig' -0.383100 0.009784 'Cprig' 25.000000 9 0.000000 12 0.810476 0.016017 'Buv' 'Cuv' 4.823512 0.063844 13 15 'Euv' 9.921366 0.835891 22 'Bdv' 1.029995 0.061123 23 'Cdv' 4.846279 0.295439 33 'CUbar' 7.059694 0.809144 1.548098 34 'DUbar' 1.096540

41	'ADbar'	0.268798	0.008020
42	'BDbar'	-0.127297	0.003628
43	'CDbar'	9.586246	1.448861

call fcn 3 *migrad 200000 *hesse set print 3

return

The first number is the starting value, if the second number is set to 0, the parameter is fixed July 8, 2016 Stefano Camarda To do a real MINUIT minimisation fit (about 1000-10000 iterations):

*call fcn 3 migrad 200000 hesse

To run only 3 iterations:

call fcn 3 *migrad 200000 *hesse # Setup a run directory

mkdir run
cp input/* run
ln -s ~/xfitter/xfitter-1.2.2/datafiles run/datafiles

 $\# \operatorname{Run} \mathtt{xfitter}$

cd run xfitter cd .. (or cd tutorial/xfitter/exercise1)

xfitter-draw output
evince output/plots.pdf

To see the full list of plotting options do:

xfitter-draw --help

Exercise 2

Simultaneous PDF fit and α_s extraction from HERA jets data

cd exercise2

- \bullet $\mathit{purpose:}$ Learn the basics of an α_{s} extraction
- data set: H1 jets data
- QCD order: NLO

We add the H1 jets data to the list of data sets in input/steering.txt

```
&InFiles
```

- ! Number of intput files NInputFiles = 12
- ! Input files:

```
InputFileNames(1) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_920.dat'
InputFileNames(2) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_820.dat'
InputFileNames(3) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_875.dat'
InputFileNames(4) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_460.dat'
InputFileNames(5) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_460.dat'
InputFileNames(6) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_de0.dat'
InputFileNames(6) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_de1'
InputFileNames(7) = 'datafiles/hera/h1zeusCombined/inclusiveDis/1506.06042/HERA1+2_NCep_dat'
InputFileNames(8) = 'datafiles/hera/h1/jets/0706.3722/H1_InclJets_HighQ2_99-00.dat',
InputFileNames(8) = 'datafiles/hera/h1/jets/0911.5678/H1_InclJets_LighQ2_99-00.dat',
InputFileNames(10) = 'datafiles/hera/h1/jets/1406.4709/H1_NormTrijets_HighQ2_03-07.dat'
InputFileNames(11) = 'datafiles/hera/h1/jets/1406.4709/H1_NormTrijets_HighQ2_03-07.dat'
InputFileNames(12) = 'datafiles/hera/h1/jets/1406.4709/H1_NormDrijets_HighQ2_03-07.dat'
```

For the H1 jets data we need to add also the files containing the uncertainty correlation matrices in

input/steering.txt

The highest order in perturbative QCD for which the jets data are available is NLO, and is set in input/steering.txt

&xFitter ... Order = 'NLO' ! 'LO', 'NLO' or 'NNLO', used for DGLAP evolution. ... &End

We have to free the $\alpha_s(m_Z)$ parameter input/steering.txt

&ExtraMinimisationParameters name = 'alphas', 'fs', 'fcharm' value = 0.118 , 0.4, 0. step = 0.001 , 0.0 , 0. ! set to 0 to avoid minimisation &End To do a real MINUIT minimisation fit (about 1000-10000 iterations):

*call fcn 3 migrad 200000 hesse

To run only 3 iterations:

call fcn 3 *migrad 200000 *hesse # Setup a run directory

mkdir run
cp input/* run
ln -s ~/xfitter/xfitter-1.2.2/datafiles run/datafiles

 $\# \operatorname{Run} \mathtt{xfitter}$

cd run xfitter cd .. (or cd tutorial/xfitter/exercise2)

xfitter-draw output
evince output/plots.pdf

Exercise 3 LHAPDF analysis

cd exercise3

- *purpose:* Learn how to include a new data set into an existing PDF set, without redoing a PDF fit
- *data set:* Tevatron *W*-boson charge asymmetry
- QCD order: NLO

Download PDF sets from LHAPDF

cd ~/tutorial/xfitter/pdfsets

LHAPDF is a convenient library for the generic interpolation of PDFs as functions of x and q^2 . PDFs are saved as tables of PDF values at fixed points in x and q^2 , and fast interpolation functions allow to access the PDFs at any other value.

```
cd ~/tutorial/xfitter/pdfsets
lhapdf --pdfdir=./ install CT14nlo
export LHAPATH='pwd'/:$LHAPATH
```

Exercise 3 - Profiling methodology

The inclusion of new data into an existing PDF set can be done with a Hessian profiling technique We define a χ^2 with theory uncertainties ($\beta_{\rm th}$ are the PDF uncertainties)

$$\chi^{2}(\boldsymbol{\beta_{exp}}, \boldsymbol{\beta_{th}}) = \chi^{2}_{exp} + \chi^{2}_{th} = \sum_{i=1}^{N_{data}} \frac{\left(\sigma^{exp}_{i} + \sum_{j} \Gamma^{exp}_{ij} \beta_{j,exp} - \sigma^{th}_{i} - \sum_{k} \Gamma^{th}_{ik} \beta_{k,th}\right)^{2}}{\Delta^{2}_{i}} + \sum_{j} \beta^{2}_{j,exp} + \sum_{k} \beta^{2}_{k,th}$$

• Find the $\beta_{k,{
m th}}$ which minimised the χ^2 on the new data

- The fit is done by solving a system of linear equations
- Reinterpret the $\beta_{k,{
 m th}}^2$ shifts as optimisation of the PDFs

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The Tevatron W asymmetry data sets and correlation files are set in input/steering.txt

&End

```
&InCorr
    ! Number of correlation (statistical, systematical or full) files
    NCorrFiles = 1
    ! Correlation files:
        CorrFileNames(1) = 'datafiles/tevatron/d0/wzProduction/1312.2895/D0_W_asymmetry.corr'
```

We will use the option RunningMode = 'LHAPDF Analysis' in input/steering.txt

&End

```
PDFs are taken from LHAPDF, so there is no need to specify a parametrisation in input/steering.txt
```

We also enable the treatment of asymmetric PDF uncertainties with an iterative procedure

```
&xFitter
   PDFStyle = 'LHAPDFNATIVE'
   ...
   AsymErrorsIterations = 20
   ...
&End
```

Setup a run directory

mkdir run
cp input/* run
ln -s ~/xfitter/xfitter-1.2.2/datafiles run/datafiles

 $\# \operatorname{Run} \mathtt{xfitter}$

cd run xfitter cd .. (or cd tutorial/xfitter/exercise3)

```
cp -r run/output .
xfitter-draw output:CT14nlo profile:output:CT14nlo-profile@
evince plots/plots.pdf
```

to produce a new PDF in Ihapdf6 format

xfitter-process profile output/pdf_shifts.dat output/pdf_ro

save the new PDF set into our lhapdf6 collection

cp -r CT14nlo-TEVW/ ../pdfsets/

Exercise 4 Plotting LHAPDF files

cd exercise4

- purpose: Direct visualisation of PDFs from LHAPDF6
- language: Python

Take an output PDF from a previous exercise

cp -r ../exercise1/output .

Start the jupyter notebook

jupyter notebook

In the browser, select new \rightarrow Python2 # cut and paste from testPlot.py into the browser # execute commands with Alt+Enter

Exercise 5 Equivalence of χ^2 representations

cd exercise5

- $\bullet \ purpose:$ Test the equivalence of the nuisance parameters and covariance matrix χ^2 formulas
- data set: Tevatron W asymmetries

Nuisance parameters representation of the χ^2

$$\begin{split} \chi^{2}(\boldsymbol{\beta}) &= \\ \sum_{i=1}^{N_{\text{data}}} \frac{\left(\sigma_{i}^{\text{exp}} + \sum_{j} \Gamma_{ij}^{\text{exp}} \beta_{j} - \sigma_{i}^{\text{th}}\right)^{2}}{\Delta_{i}^{2}} + \sum_{j} \beta_{j}^{2} \end{split}$$

Covariance matrix representation of the χ^2

$$\chi^{2}(C) = \sum_{ij}^{N_{\text{data}}} (\sigma_{i}^{\text{exp}} - \sigma_{i}^{\text{th}}) C_{\text{tot } ij}^{-1} (\sigma_{j}^{\text{exp}} - \sigma_{j}^{\text{th}}).$$

The two representations are matematically equivalent. In xFitter we can switch from one to the other.

To convert a covariance matrix into nuisance parameters representation:

```
&CovarToNuisance
  ! Global switch for using nuisance param representation for covariance mat.
  ! ----> change this setting
  LConvertCovToNui = .true.
  ! Tolerance -- zero means exact transformation
  Tolerance = 0.0
  ! The following lines allow to adjust error scaling properties (default: :M)
  DataName = 'DO W asymmetry 2013'
  DataSystType = ':A'
  &End
```

To convert a nuisance parameters (correlated systematic uncertainties) into covariance matrix representation:

```
&xFitter
...
CHI2SettingsName = 'StatScale', 'UncorSysScale', 'CorSysScale', 'UncorChi2Type', 'CorChi2Type'
! ----> change this setting
! Chi2Settings = 'Poisson', 'Linear', 'Linear', 'Diagonal', 'Hessian'
Chi2Settings = 'Poisson', 'Linear', 'Linear', 'Diagonal', 'Matrix'
...
&End
```

First dataset: covariance matrix provided, and converted to nuisance parameter representation

diff input1-cov input1-nui

run chi2 test

ln -s ~/xfitter/xfitter-1.2.2/datafiles/ input1-cov/datafiles ln -s ~/xfitter/xfitter-1.2.2/datafiles/ input1-nui/datafiles cd input1-cov && xfitter && cd .. cd input1-nui && xfitter && cd ..

compare results

xfitter-draw input1-cov/output:covariance input1-nui/output:nuisance --outdir plots1

Second dataset: nuisance parameters provided and converted to covariance matrix representation

diff input2-nui input2-cov

run chi2 test

ln -s ~/xfitter/xfitter-1.2.2/datafiles/ input2-nui/datafiles ln -s ~/xfitter/xfitter-1.2.2/datafiles/ input2-cov/datafiles cd input2-nui && xfitter && cd .. cd input2-cov && xfitter && cd ..

compare results

xfitter-draw input2-nui/output:nuisance input2-cov/output:covariance

Summary

- xFitter is a framework for QCD analyses. It allows to perform PDF fits, sensitivity studies to PDFs, extraction of fundamental SM parameters, inclusion of new data on already existing PDF, and a variety of other phenomenological studies involving QCD and EW physics
- The program has many settings to address very different problems, nevertheless big efforts are made to keep the user interface accessible for simple and basic usage
- In this tutorial we have learned how to
 - Perform a PDF fit
 - Extract the value of the strong-coupling constant $\alpha_s(m_Z)$
 - Include new data sets into existing PDF sets by mean of Hessian profiling
 - Perform basic manipulation and plotting of PDF sets
 - Test the equivalence of the χ^2 representations