

Bayesian PDF fits to ZEUS high- x data

Michiel Botje for the Bayesian analysis team

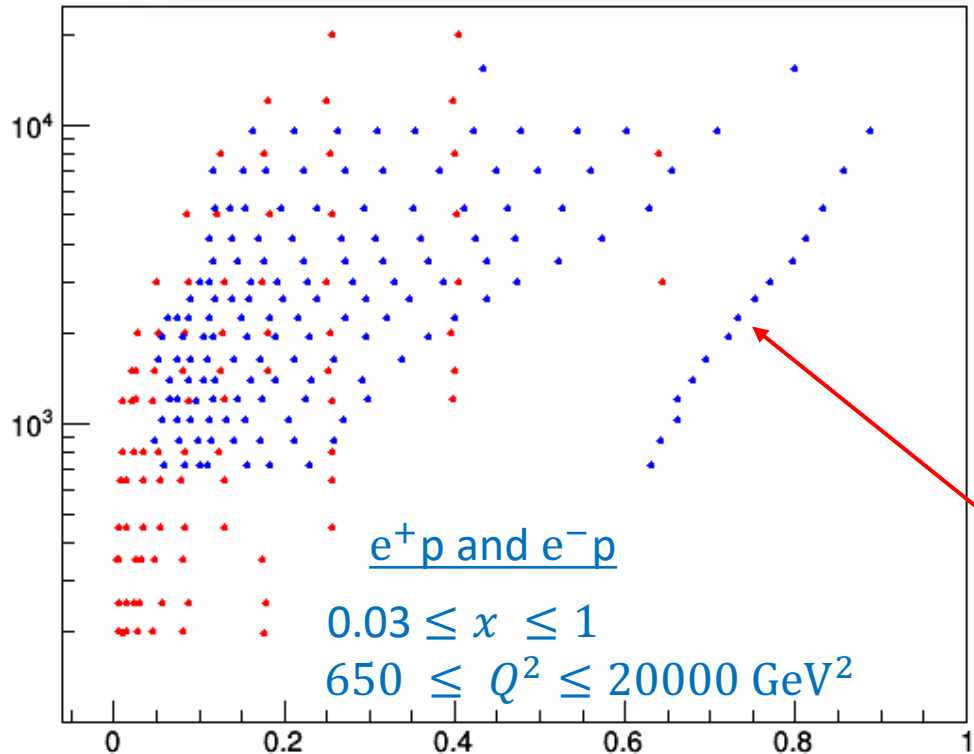
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Oliver Schulz	MPI Munich, Germany	BAT.jl framework
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Ritu Aggarwal	Pune University, India	Forward model
Michiel Botje	Nikhef Amsterdam, The Netherlands	QCDNUM/SPLINT

Phys.Rev.Lett. 130 (2023) 14, 141901, arXiv:2209.06571 [hep-ph]

xFitter External meeting, CERN, May 5, 2023

Measurement of neutral current $e^\pm p$ cross sections at high Bjorken x with the ZEUS detector

ZEUS collab., Phys.Rev. D **89**, 072007, hep-ex:1312.4438 (2014)



- Unique e^+p and e^-p data set extending to $x = 1$
- Data not used in any global pdf fit
- No higher twists which plague analysis of other high- x data
- Event numbers and differential cross-sections are given in 153 x - Q^2 bins for each data set
- At high x only integrated cross-sections are given

Use the full data set in a Bayesian pdf fit of bin-counts that can handle the Poisson statistics of low event numbers at very large x

Bayesian forward model approach

- Parameterise pdfs at some Q_0^2 and evolve at NNLO
- Compute at NNLO F_2 , F_L and xF_3 and Born neutral current $e^\pm p$ cross-sections
- Integrate x-sections over bins in x - Q^2 and compute event numbers
- Apply radiative and detector effects to get predictions for the observed events n
- Compute Poisson likelihood $P(n|\theta)$ for the set of fit parameters θ
- Define prior probabilities $P(\theta)$ for the fit parameters
- Get posterior from Bayes theorem

$$P(\theta|n, \text{model}) \propto P(n|\theta)P(\theta)$$

Posterior is also conditional on the choice of parameterisation

- Bayesian approach is very attractive because ...

- No Gaussian assumptions
- Constraints are easily implemented (posterior cannot extend beyond prior range)
- Badly constrained parameters do not spoil the fit
- Uncertainties in badly constrained parameters (as encoded in the prior) are automatically propagated to the posterior of other parameters
- Can easily judge information content of the data by comparing posterior to prior
- Marginalisation of the posterior gives easy access to single-parameter distributions and correlations

- But also ...

- Priors should be chosen with care to not introduce bias in the posterior
- Need lots of CPU to map-out the posterior in multi-dimensional parameter space

For this analysis we use the Bayesian Analysis Toolkit and QCDNUM

- High-performance toolkit for Bayesian inference
 - Tools for definition of likelihoods, priors and posteriors
 - Provides MCMC sampling techniques to explore the posterior
 - Location and interval estimation, marginalisation, visualisation, *etc.*
 - And much more ...
- Written in Julia (with Julia interface to QCDNUM)

BAT.jl <https://bat.github.io>

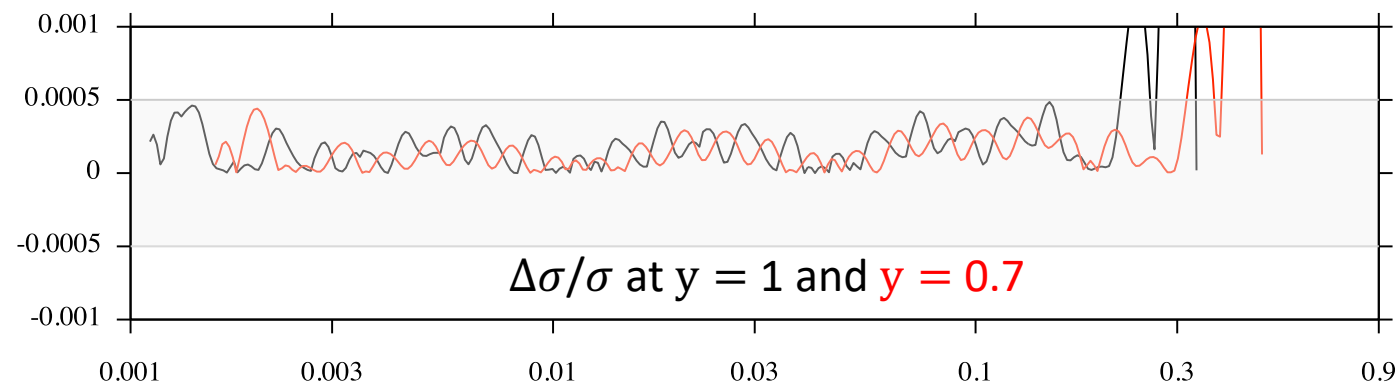
Analysis <https://github.com/cescalara/PartonDensity.jl>

- Use QCDNUM for evolution and structure functions at NNLO
- SPLINT add-on provides cubic spline interpolation and integration
 - Spline interpolation much faster than computing stfs and xsecs from scratch
 - Needs some tuning of spline-grid to balance speed vs accuracy
 - SPLINT provides fast integration over bins taking kinematic limit into account
 - SPLINT integration is factor 300 faster than 2-dim Gauss integration

Timing (MacBook Pro 2018)

	n_x	n_q	t [ms]
Evolution	100	50	3.6
6 Stf splines	22	7	2.9
Xsec spline	100	25	2.2
Integration	429 bins		0.8

$\Delta\sigma/\sigma \lesssim 5 \times 10^{-4}$ along the kinematic cut



Parameterisation

- Parameterise pdf as beta distribution $xf(x) = Ax^\lambda(1-x)^K$
- Integrable for $\lambda > -1$ $\Delta \equiv \int_0^1 xf(x)dx = A \frac{\Gamma(\lambda+1)\Gamma(K+1)}{\Gamma(\lambda+K+2)}$
- Replacement $\lambda \rightarrow \lambda - 1$ for valence pdf gives number density
- Integrable for $\lambda > 0$ giving $A_i = N_i^v \frac{\Gamma(\lambda_i + K_i + 1)}{\Gamma(\lambda_i)\Gamma(K_i + 1)}$ with $\begin{cases} N_d^v = 1 \\ N_u^v = 2 \end{cases}$
- Can fix valence λ for given N and Δ through $\Delta_i = N_i^v \frac{\lambda_i}{\lambda_i + K_i + 1}$
- Easy to control low- x behaviour
 - Integrable and decreasing towards low x for $\lambda > 0$ (valence)
 - Integrable and increasing towards low x for $-1 < \lambda < 0$ (sea, gluon)

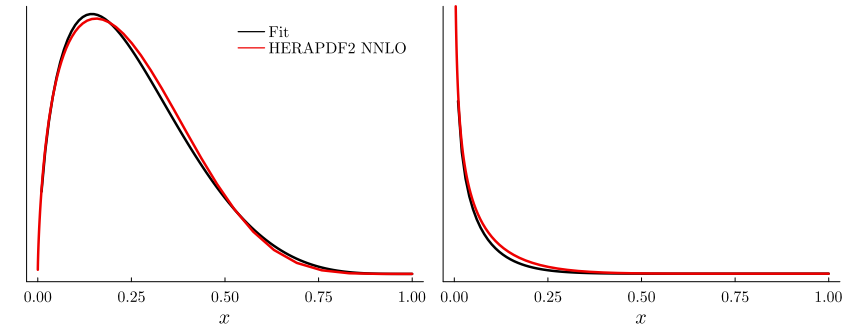
Parameterise 5 flavours at input scale $Q_0^2 = 100 \text{ GeV}^2$

$$x d^v(x) = A_d x^{\lambda_d} (1-x)^{K_d}$$

$$x u^v(x) = A_u x^{\lambda_u} (1-x)^{K_u}$$

$$x \bar{q}(x) = A_i x^{\lambda_{\bar{q}}} (1-x)^{K_{\bar{q}}} \quad i = \{\bar{d}, \bar{u}, \bar{s}, \bar{c}, \bar{b}\}$$

$$x g(x) = A_g^v x^{\lambda_g^v} (1-x)^{K_g} + A_g^s x^{\lambda_g^s} (1-x)^{K_{\bar{q}}}$$



Parameterise HERAPDF at $Q^2 = 100 \text{ GeV}^2$ to check flexibility as shown here for u^v and \bar{u}

- Gluon with a valence and sea component
- Fix λ_d and λ_u via the quark counting rules
- All $x \bar{q}$ have the same shape but different normalisations
- Gluon sea component has same high- x power as the anti-quarks
- Do not fit normalisation constants but momentum fractions Δ which are more meaningful
- Momentum sum constraint $\Delta_u + \Delta_d + 2 \sum_{\bar{q}} \Delta_{\bar{q}} + \Delta_g^v + \Delta_g^s = 1$

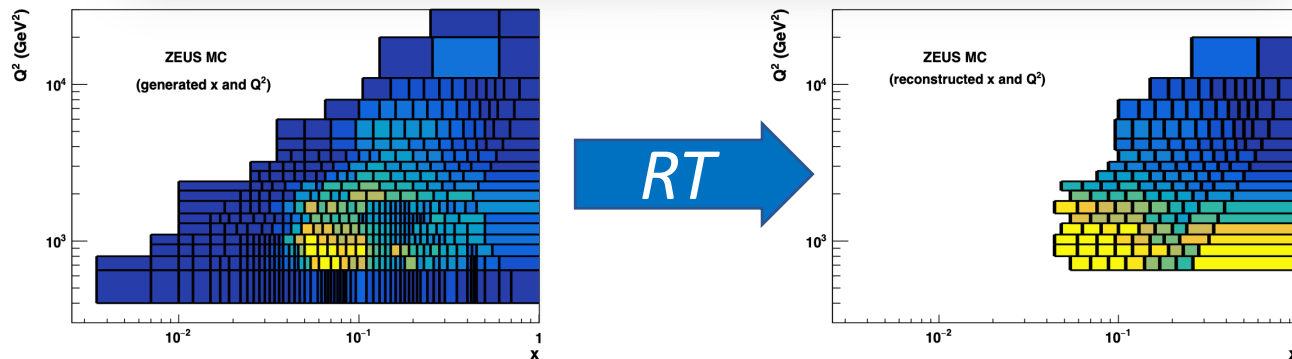
7 shape parameters + 9 momentum fractions with sum rule constraint contribute 15 degrees of freedom to the fit

Event predictions

- Evolve at NNLO with QCDNUM and compute neutral current $e^\pm p$ cross-sections
- Integrate over 429 bins and compute vector of event predictions \vec{v}
- Multiply by matrix RT to correct for radiative and detector effects: $\vec{u} = RT\vec{v}$
- This gives the observed event predictions \vec{u} in 153 ZEUS bins for each data set
- For parameters θ the predictions $\vec{u}(\theta)$ give for the likelihood of observing the events \vec{n} :

$$P(\mathbf{n}|\boldsymbol{\theta}) = \prod_{\text{bins}} \frac{u^n e^{-u}}{n!}$$

ZEUS, Phys. Rev. D **101**, 11209, hep-ex:2003.08732 (2020)



- Added to RT is the weighted sum of 10 systematic matrices
- The 10 weights δ_i are left free parameters in the fit giving a total of 16+10=26 parameters

Priors

M. Betancourt, Proc. AIP
Conf., **1443**, 157 (2012)

- Take 9-dimensional Dirichlet distribution for momentum prior
 - $\text{dir}(\vec{\alpha})$ with 9 shape parameters α is multivariate extension of beta distribution
 - Lives on an 8-dimensional manifold in the space $\Delta_i \in [0,1]$ with $\sum \Delta_i = 1$
- Set Dirichlet shape parameters $\vec{\alpha}$ according to asymptotic expectations
 - $\Delta(\text{gluon}) \approx \Delta(\text{quarks})$, $\Delta(u^V) \approx 2\Delta(d^V)$, $\Delta(s, c, b) \sim \text{small}$
- Pdf shape priors set to truncated Normal or Uniform such that the pdfs are integrable and have the required low- x behaviour
- Priors of systematic δ parameters set to truncated Normal with zero mean and unit width

	Prior	Range
α	Dir(20, 10, 20, 20, 5, 2.5, 1.5, 1.5, 0.5)	[0, 1]
K_u	Normal(3.5, 0.5)	[2, 5]
K_d	Normal(3.5, 0.5)	[2, 5]
λ_g^v	Uniform	[0, 1]
λ_g^s	Uniform	[-1, -0.1]
K_g	Normal(4, 1.5)	[2, 7]
$\lambda_{\bar{q}}$	Uniform	[-1, -0.1]
$K_{\bar{q}}$	Normal(4, 1.5)	[3, 10]
δ	Normal(0, 1)	[-5, 5]

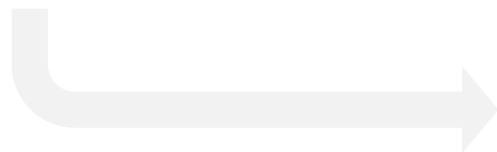
Performance

- Analysis results based on 2 MCMC chains of 500k samples each
- On a 2021 MacBook Pro (M2 processor) the 1M samples take
 - About 1 hr burn-in time
 - About 3 hrs running time
- Smaller samples already give good results but less smooth posterior
- After burn-in the chains could be farmed-out on different machines
- Did not yet exploit the potential for threaded computing in QCDNUM

Much room for increased performance ...

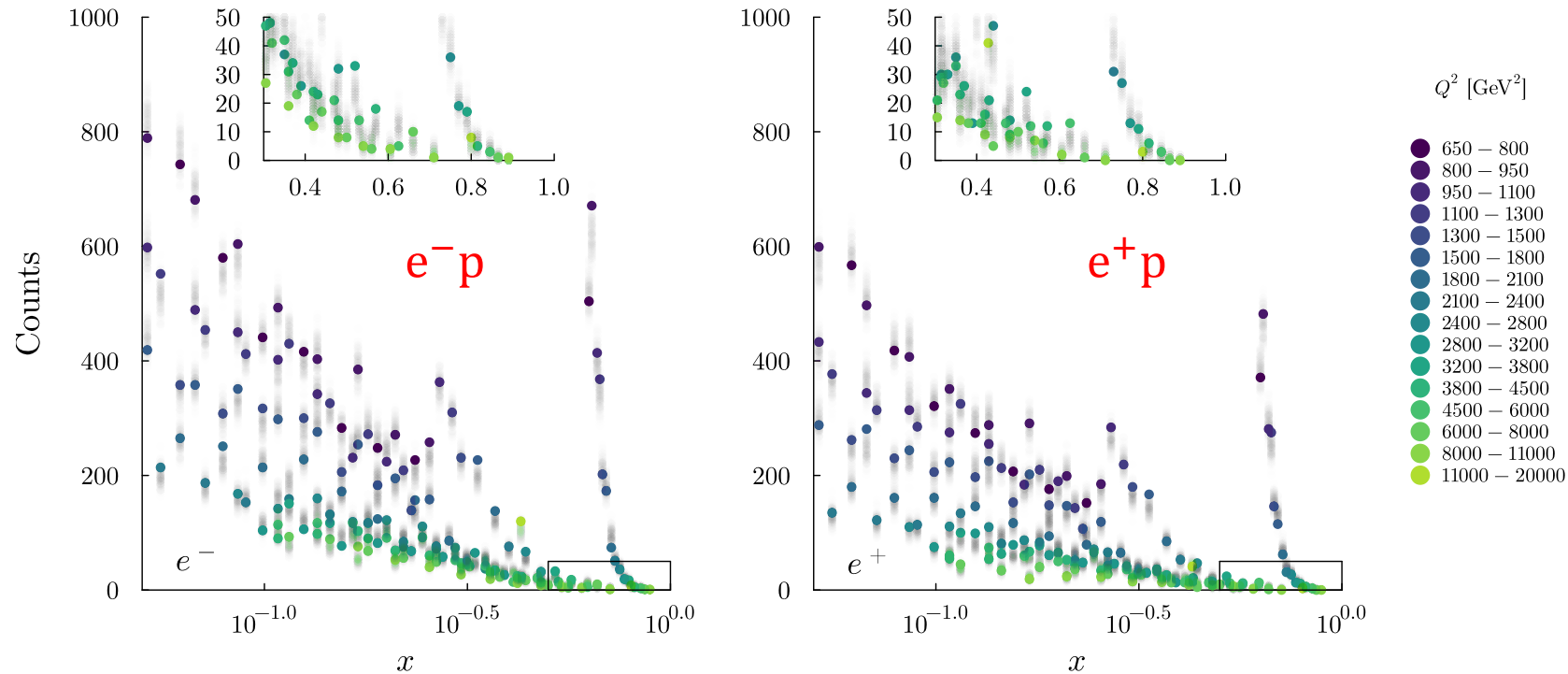
Results

- The real result of the analysis is the 26-dim posterior in parameter space
- Parameter values and errors are defined in two ways as
 - Position of the mode of the posterior in parameter space
 - Mode of the marginal parameter distribution with error corresponding to the smallest credible interval around the mode that contains 68% probability
- Here are the parameters that are reasonably well constrained by the data



	Global mode	Marginal mode		Global mode	Marginal mode
Δ_u	0.219	$0.219^{+0.008}_{-0.010}$	K_u	3.76	$3.78^{+0.14}_{-0.17}$
Δ_d	0.099	$0.088^{+0.028}_{-0.020}$	K_d	3.66	$3.69^{+0.33}_{-0.60}$
$\lambda_{\bar{q}}$	-0.55	$-0.52^{+0.06}_{-0.11}$	$K_{\bar{q}}$	6.01	$6.38^{+1.13}_{-1.40}$
K_g	4.92	$5.22^{+0.91}_{-1.57}$			
$2\Delta_{\bar{u}}$	0.126	$0.104^{+0.022}_{-0.027}$	$2\Delta_{\bar{d}}$	0.031	$0.024^{+0.020}_{-0.017}$
Δ_g^v	0.265	$0.239^{+0.043}_{-0.037}$	Δ_g^s	0.245	$0.241^{+0.047}_{-0.036}$

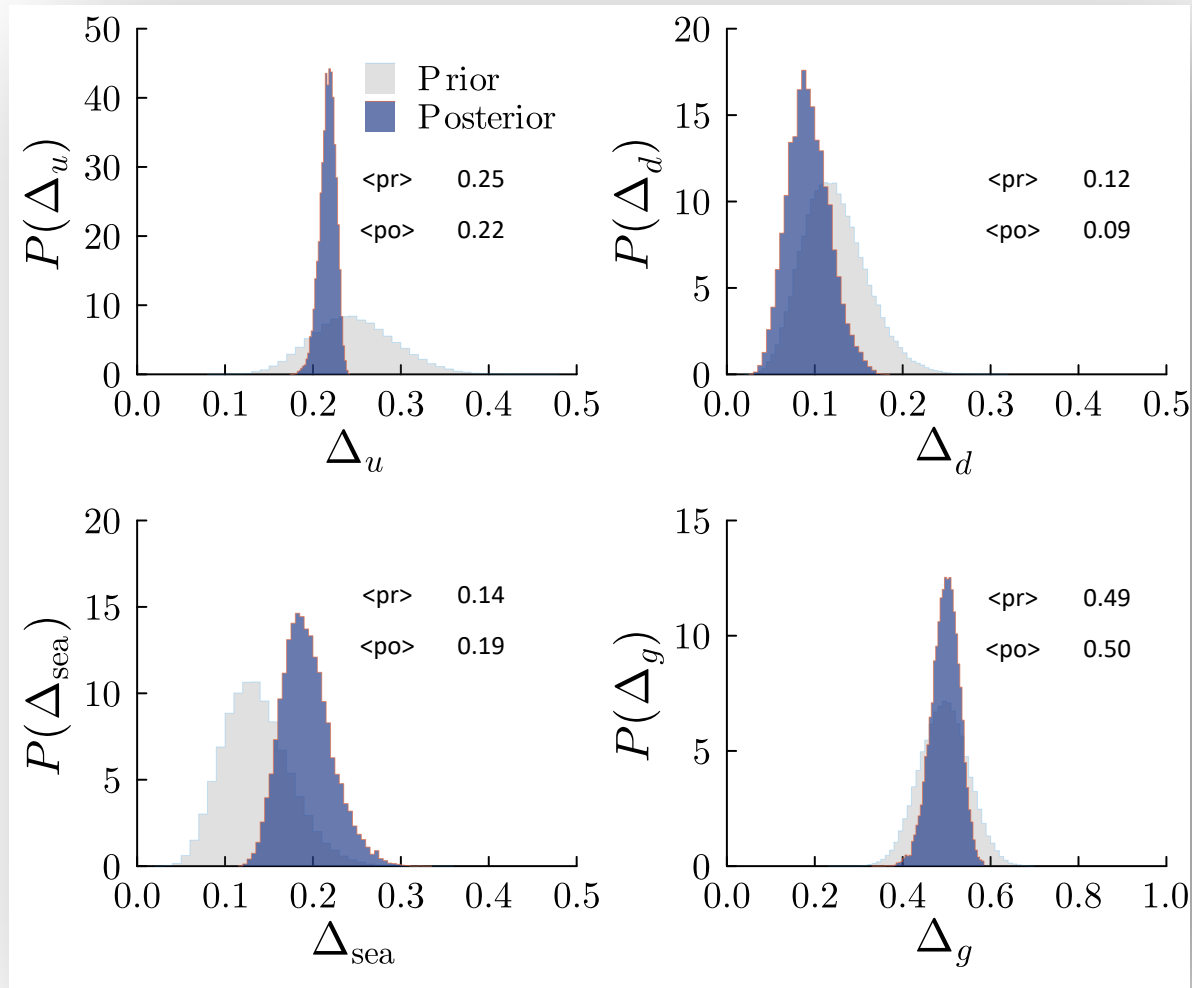
Fitted event counts versus data



- Compute event predictions from posterior mode parameters (bands) and compare to observed event counts (dots), plotted at the bin centers
- Pierson chi-squared gives $\chi^2/\text{pt} = 321/306$ with a p-value of 0.27

Our parameterisation yields an excellent description of the data

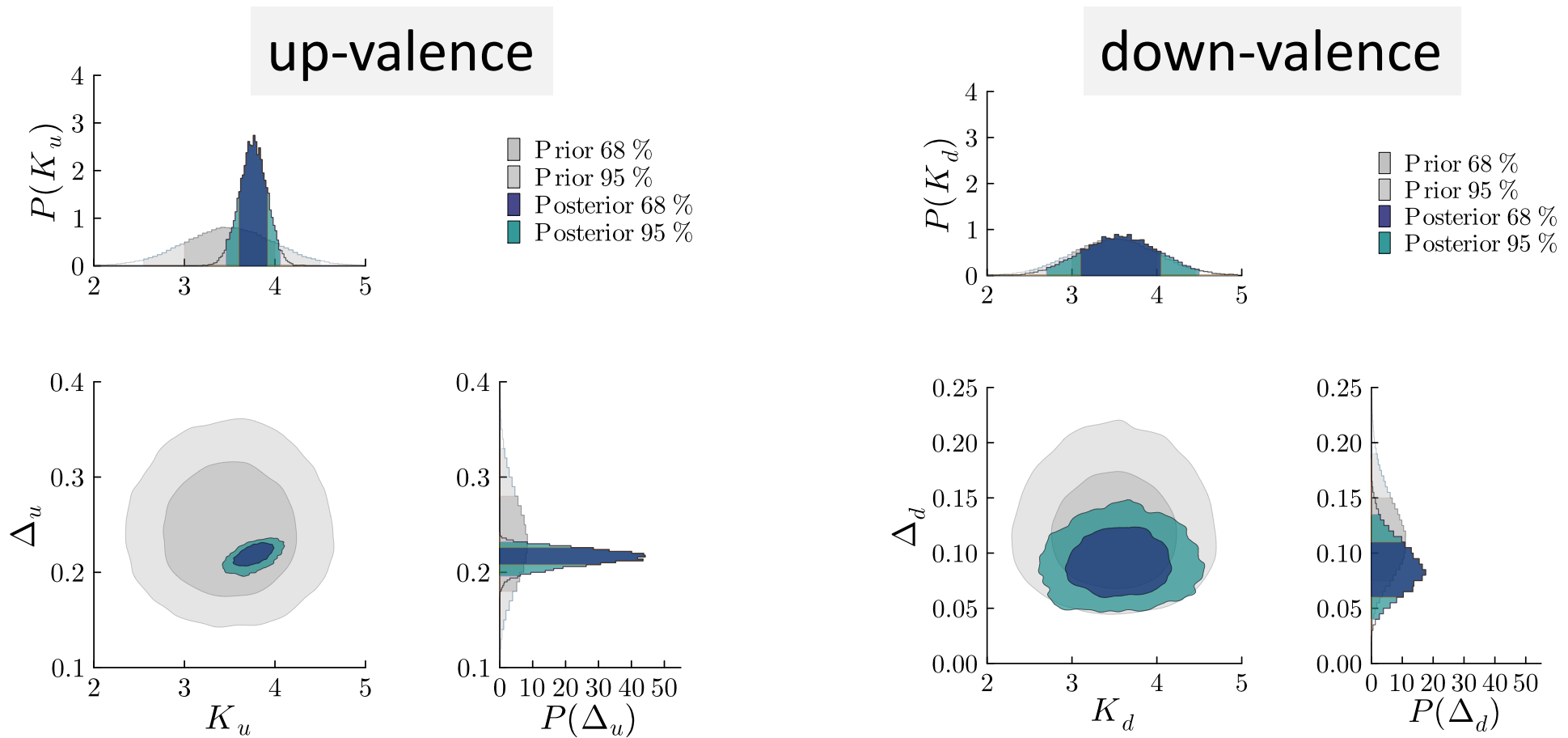
Momentum fraction priors and posteriors



- The data very much constrain the momentum carried by the up-valence
- Weaker constraints on the down-valence, sea and gluon
- From global mode we find

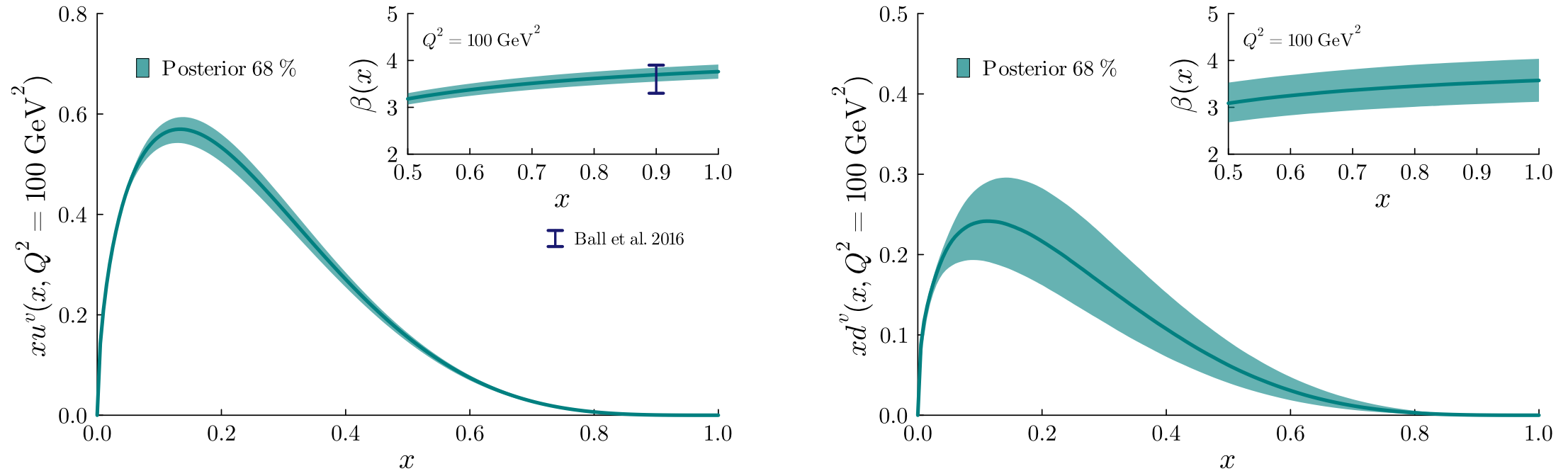
u_v	d_v	sea	gluon
0.22	0.10	0.17	0.51

Momentum Δ versus $1-x$ power K



Very strong constraint on the up-valence parameters

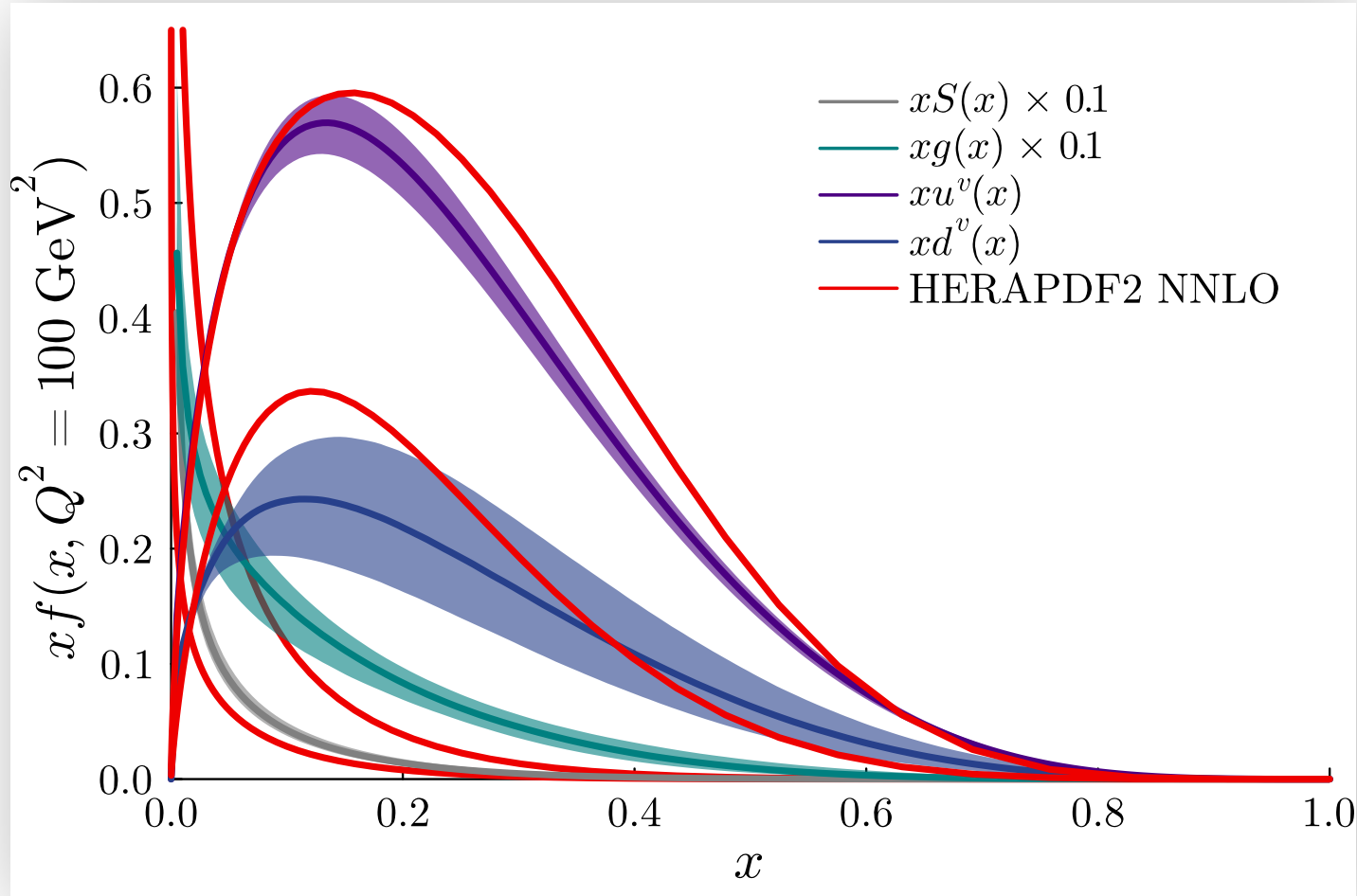
Up and down valence distributions



- The insets show the effective 1- x power $\beta(x) = d \ln x f / d \ln (1 - x)$
- The β slope of u_v agrees well with a recent summary from Ball *et al.*

R. Ball, E. Nocera and J. Rojo, Eur. Phys. J. C **76** (2016), 383, hep-ph:1604.00024

Compare to HERAPDF



- Analytic parameterisations strongly couple regions of small and large x
- HERAPDF parameterisation is similar to ours but fitted at much lower x (not using the ZEUS high- x data)
- This may explain at least part of the observed differences

Summary

- The Bayesian analysis of ZEUS high- x data shows that these data carry a lot of information on the up-valence distribution
- Given our parameterisation we obtain accurate results on the momentum Δ carried by the up-valence quark and its $(1-x)$ power K (marginal mode and 68% credible interval)

$$\Delta = 0.22^{+0.01}_{-0.01} \quad K = 3.8^{+0.1}_{-0.2}$$

What is next ...

- Paper with detailed description of our analysis is in preparation
- Extend the analysis to investigate parameterisations with Bayesian model-selection techniques
- Exploit in the extended analysis the many opportunities for parallel computing

Bayesian pdf fitting is a viable, challenging, and very interesting undertaking!