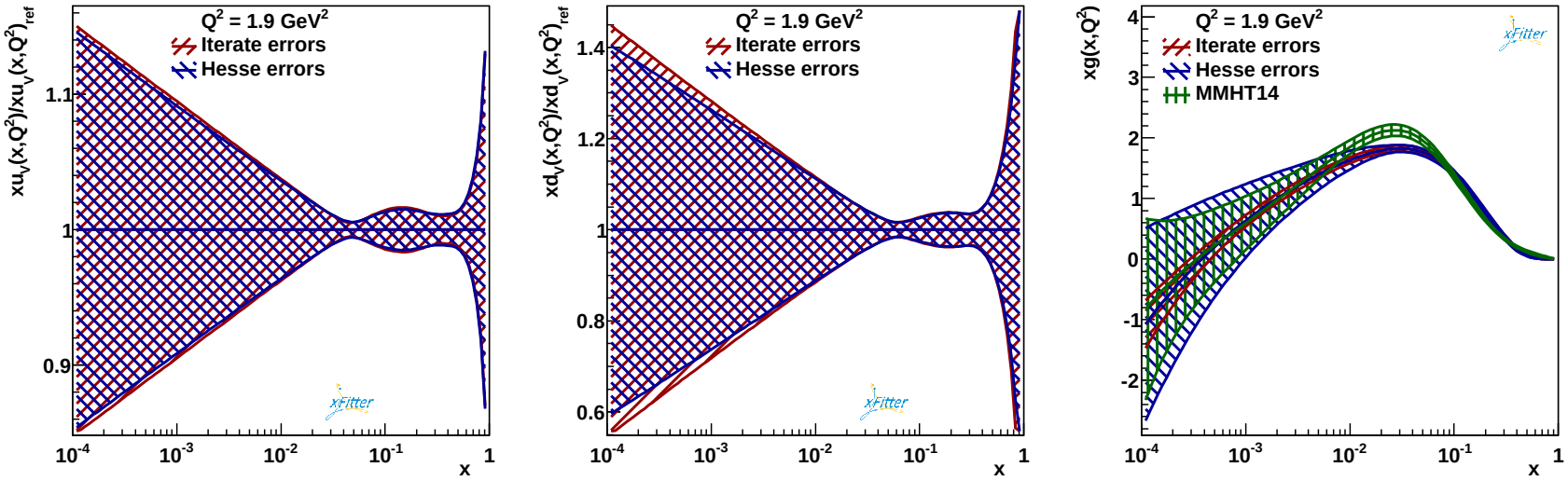
EXPERIMENTAL Symmetric Hessian errors in xFitter

- Two main methods for uncertainty bands present in xFitter – MC errors and asymmetric Hessian errors based on J. Pumplin "Iterate" procedure (Phys.Rev.D65:014011,2001).
- Symmetric Hessian errors provide more compact representation of the errors and can be sufficiently accurate for many applications.
- The code from "Iterate" is not absolutely stable and does not allow for parameter limits
- Use built in Minuit Hesse method instead, and diagonalize covariance matrix using the usual method: $C = V^T DV = \Gamma^T \Gamma$ where $\Gamma = \sqrt{D}V$
- Activated by "DoBandsSym" flag in Output namelist. Note that DoBandsSym and DoBands flags are mutually exclusive: the code stops if both are activated.
- Usual pdfs_q2val_s01s_0X.txt and LHAPDF6 symmetric grids are produced when the flag is activated: xfitter-draw and lhapdf6 tools work without any modifications.

Validation: HERA-II fit with ZMVFNS



- Use HERA-II default set, ZMVFNS (with $m_c = 1.8$ GeV) for fast tests.
- Use default 14 p parametersiation with negative gluon.
- Good agreement observed for all quark densitives (u_v and d_v are shown as example). Huge difference for the gluon uncertainty.

→ Hesse gluon uncertainty band is more similar to total HERA-II band or to MMHT14 error band, shown for comparison.

Differences between Hesse and Iterate

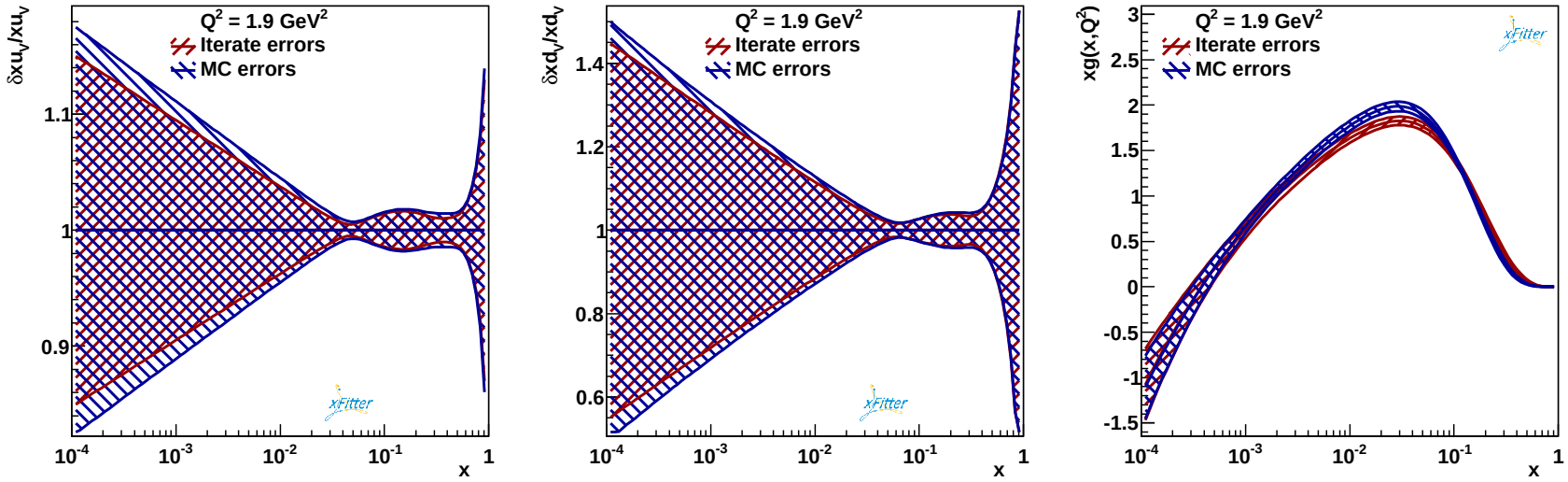
Both Hesse and Iterate methods are used to numerically estimate second derivative of the χ^2 function with respect to the fit parameters which close to the minumum takes the form:

$$\begin{aligned} \chi^2(a) &= \chi^2_{\text{min}} + \tfrac{1}{2} \sum_{i,j} V_{ij} a_i a_j \\ V_{ij} &= \frac{\partial^2 \chi^2}{\partial a_i \partial a_j} \end{aligned}$$

The methods differ in the way it is done:

- Hesse uses small variation of a_j to get better approximation of the local derivative. In order to speedup calculations, the χ^2 function is evaluated only in a minimally required set of points.
- Iterate attempts to approximate the derivative by finite variations of the parameters, corresponding to $\delta\chi^2 = N$ where for xFitter $N = 1$. The directions for these variations are determined in iterative procedure, starting from initial approximation of the matrix V_{ij} by varying parameters a_j. For the next iterations eigenvectors of V_{ij} from the previous iteration are used. To improve accuracy and effectively take into account higher orders, the χ^2 function is evaluated for all up and down variations of the parameters ($\times 4$ amount of variations in Hesse).

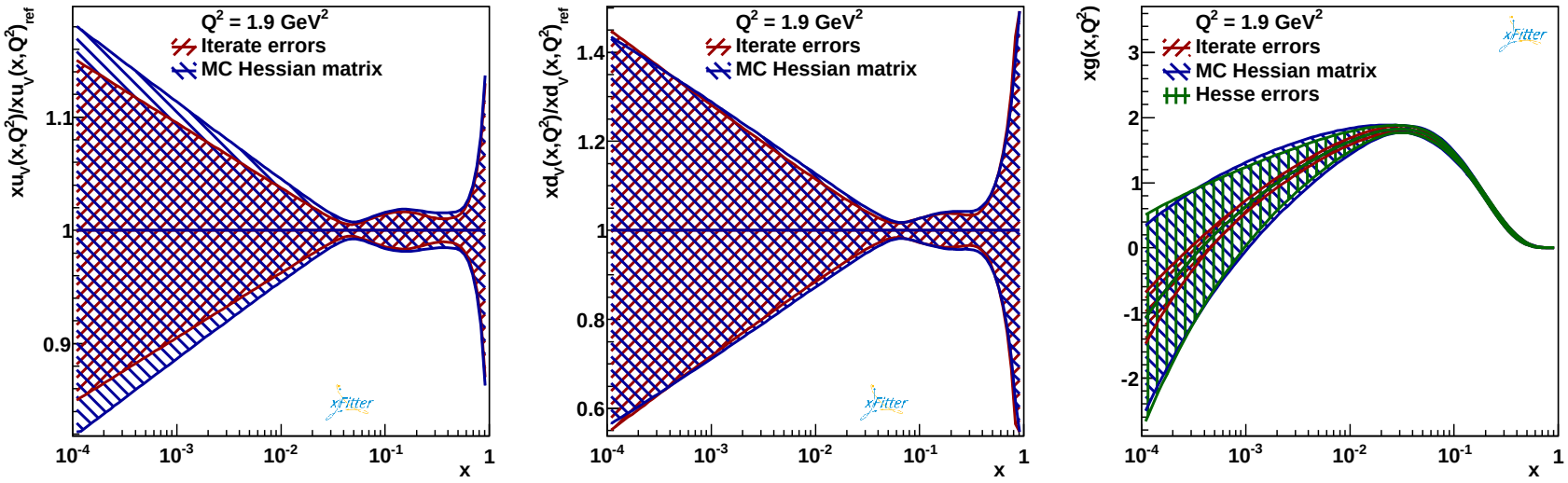
Check: use MC error bands



- Check bands using MC method (2000, 1950 converged, new file OUTPUT/STATUS.OUT file with one string "OK" or "Failed" to simplify convergence check)
- MC bands are slightly bigger for u_v and d_v and in reasonable agreement with Iterate for the gluon.

→ Pumplin's Iterate errors seem to be correct.

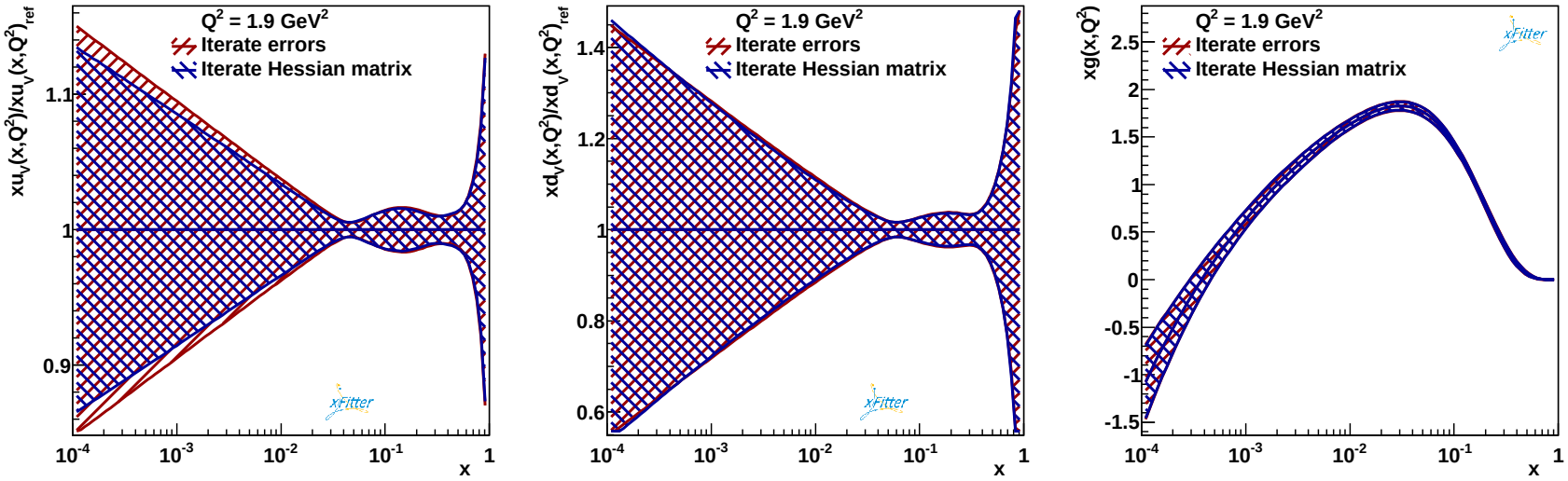
Check II: use MC covariance matrix for PDF pars



- Extend the method for symmetric error bands by allowing external covarnace matrix of parameters (OUTPUT namelist variables READPARSFROMFILE, PARSFILENAME, and COVFILENAME.
- Use the covariance matrix of fit parameters a_j determined based on converged MC-method fits
- The error bands are again very large for the gluon density, in agreement wit Hesse-based evaluation.

→ Hesse Hessian matrix of parameters is not incorrect.

Check III: use Iterate covariance matrix



- "Iterate" returns hessian matrix as one of the outputs.
- Plugin this matrix as external into new symmetric code: all error bands in reasonable agreement with the direct asymmetric Pumplin's bands.

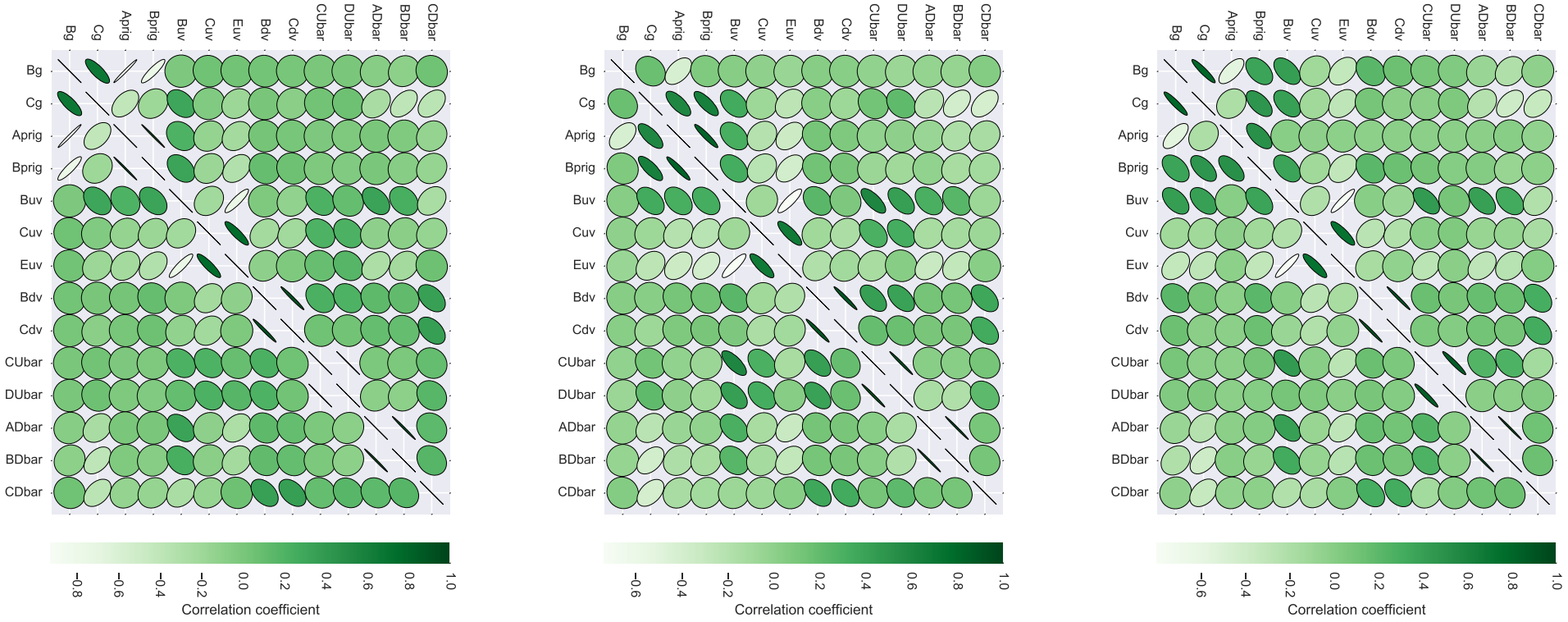
→ Implementation of the Hessian matrix eigenvector representation is correct.

→ all seems to be technically OK.

Parameter uncertainties

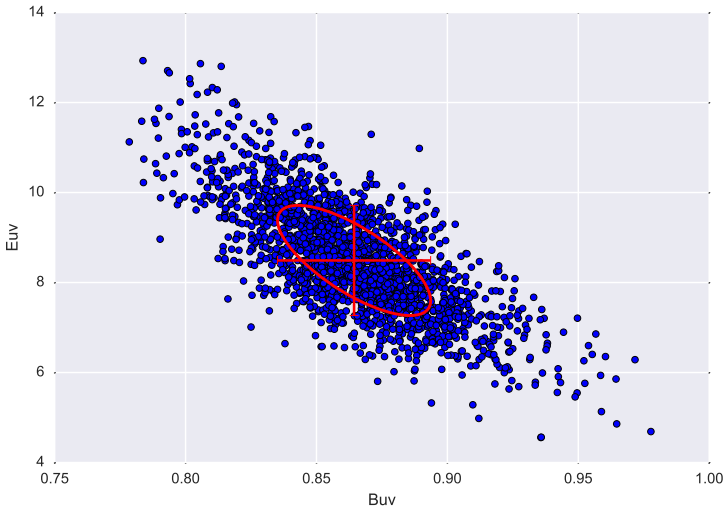
Parameter	Iterate errors	MC Hessian matrix	Hesse errors
'Bg'	0.03 ± 0.052	0.014 ± 0.031	0.029 ± 0.113
'Cg'	5.43 ± 0.510	6.726 ± 0.503	5.43 ± 0.591
'Aprig'	0.21 ± 0.062	0.418 ± 0.179	0.21 ± 0.266
'Bprig'	−0.300 ± 0.033	−0.254 ± 0.041	−0.300 ± 0.093
'Cprig'	25.00	25.00	25.00
'Buv'	0.854 ± 0.023	0.864 ± 0.029	0.854 ± 0.023
'Cuv'	4.747 ± 0.081	4.784 ± 0.090	4.747 ± 0.084
'Euv'	7.9 ± 1.04	8.49 ± 1.22	7.9 ± 1.1
'Bdv'	1.121 ± 0.069	1.123 ± 0.079	1.121 ± 0.071
'Cdv'	5.23 ± 0.34	5.21 ± 0.35	5.23 ± 0.342
'CUbar'	6.6 ± 1.29	7.97 ± 1.6	6.6 ± 3.57
'DUbar'	0.1 ± 1.19	4.31 ± 2.5	0.1 ± 3.94
'ADbar'	0.2631 ± 0.0071	0.2642 ± 0.0069	0.2631 ± 0.0071
'BDbar'	−0.1652 ± 0.0032	−0.1682 ± 0.0031	−0.1652 ± 0.0032
'CDbar'	11.7 ± 1.7	11.57 ± 1.86	11.6 ± 2.05
'alphas'	0.1180	0.1180	0.1180
'fs'	0.4000	0.4000	0.4000

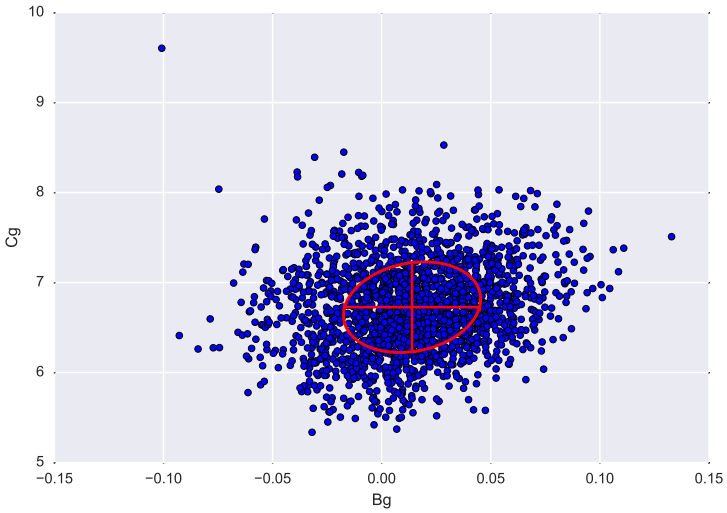
Correlation matrices



- Correlaton matrices of the fit parameters determined using Hessian (left) MC (middle) and Iterate (right) method show similar pattern for the quark-distributions but rather different for the gluon parameters.

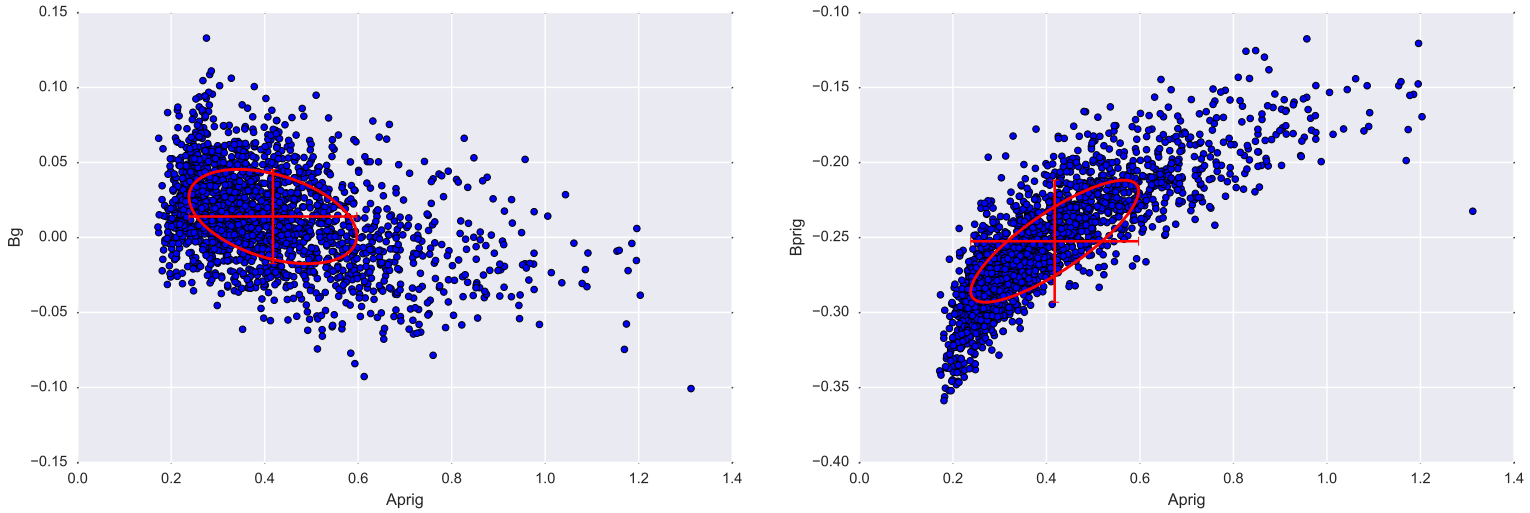
Correlation studies





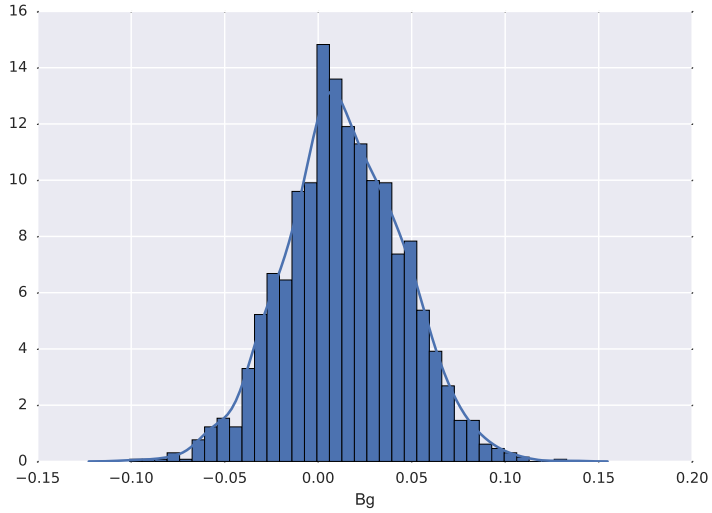
- Non-linear correlations can be studied using MC fits.
- For some parameters correlation patterns are not far from Gaussian.

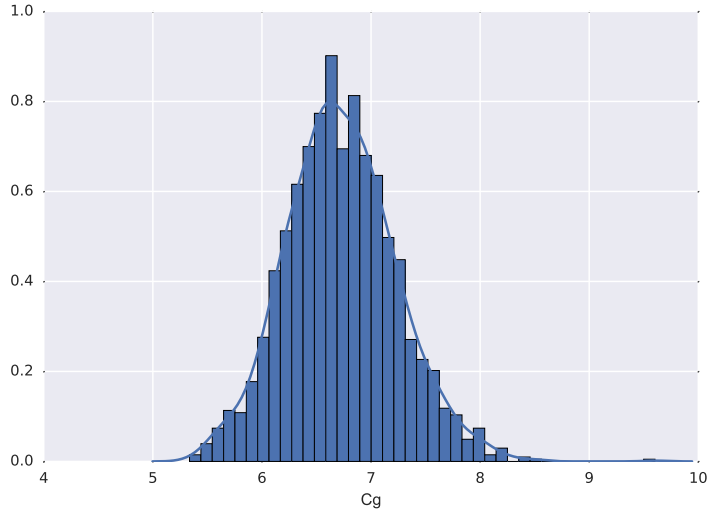
Correlation studies II

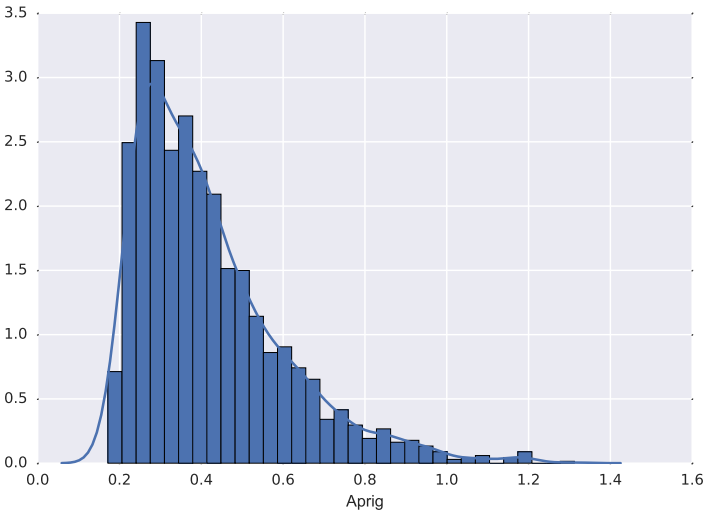


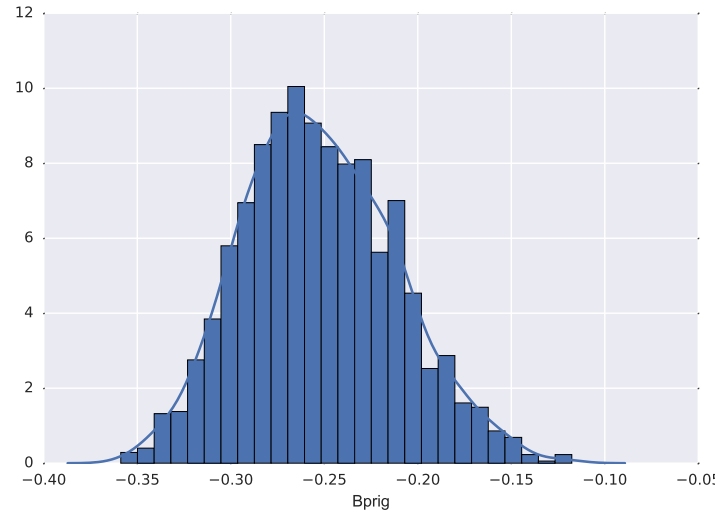
- For gluon parameters B_g, A'_g and B'_g the correlation pattern is highly non-linear, this probably explains the differen
- While Hesse uses small variations of the parameters around the minimum to determine the Hessian matrix, the Iterate method determines effective covariance using much larger parameter variations (along χ^2 eigenvectors, from the previous iteration) corresponding to $\Delta\chi^2 = 1$. This aparently allows to reproduce better the correlation patterns of PDFs.

Distribution of gluon PDF parameters









Cluster map for correlation matrix (MC method)