Extracting the xFitter Likelihood

Ali Al Kadhim & Harrison B. Prosper

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Introduction

- Characterizing PDF uncertainties is important – they directly affect our inferences from data.
- This will become increasingly important as we move to Run 3 and the HL-LHC era.
- It is well-known that if a small number of datasets are used, one can safely apply standard statistical procedures to estimate confidence intervals ($\Delta\chi^2 = 1$).
- However, when the fit includes a large number of datasets, tolerance factors (T) are used to arrive at uncertainties that are deemed to be meaningful ($T = \sqrt{\Delta\chi^2}$).

Introduction

- Our goal is to extract the xFitter likelihood for increasing numbers of datasets and study the tolerance factors.
- Ideally, every experimental result would be published along with its statistical model $P(x|\theta)$, see Prosper et. al. [1], and PDF fits would be performed using the sum of the associated negative log-likelihoods.
- However, all PDF fits are performed by minimizing a χ^2 function.
- In our studies, we assume that the xFitter likelihood function, $L(\theta) \equiv P(D|\theta)$, is given by

$$-2 \log L(\theta) = \chi^2$$

[1] H. B. Prosper et. al. “Publishing statistical models: Getting the most out of particle physics experiments” https://scipost.org/SciPostPhys.12.1.037/pdf

Procedure

- We sample the PDF parameters θ from a prior $\pi(\theta)$, whose support, ideally, roughly matches that of the likelihood $L(\theta)$.
- In order to approximate the likelihood, we weight each point, k, by

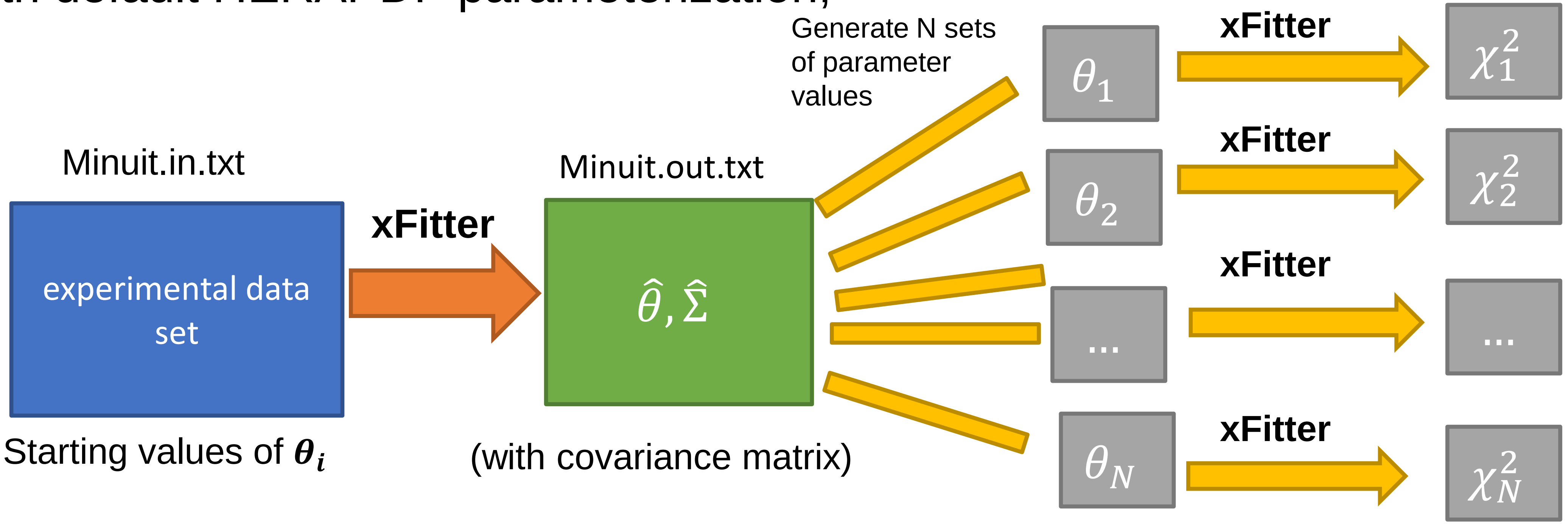
$$\mathrm{w_i} = \frac{L(\theta_i)}{\pi(\theta_i)}$$

- We anticipate that as more datasets are added and more discrepancies appear between them, the true width W_L of the 68% intervals computed using the posterior density, derived from the likelihood, will satisfy

$$\frac{\mathrm{W}_{L(\theta)}}{\mathrm{W}_{\Delta\chi^2=1}} \approx T$$

Procedure

- With default HERAPDF parameterization,



- We generate N sets of parameter values according to $\theta_i \sim \pi(\theta)$.

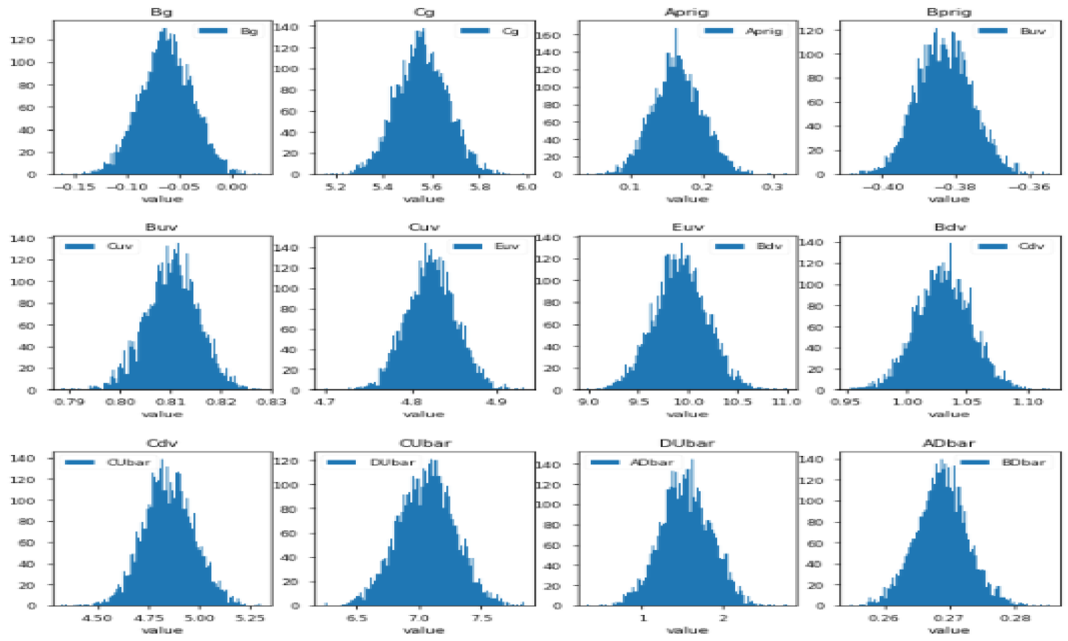
Procedure; Prior $\pi(\theta)$

- In our current studies we take $\pi(\theta) = \mathcal{N}\left(\mu = \hat{\theta}, \Sigma = \hat{\Sigma}\right)$.
- HERAPDF parameterization:

$$xf\left(x,\mu_0^2\right) = Ax^B(1-x)^C\left(1+Dx+Ex^2\right) - A'x^{B'}(1-x)^{C'}$$

- Data: HERA I & II + ZEUS combined

Parameter	xFitter Name	Starting Value	Step Size	Best-Fit Value	Approximate Error
B_g	Bg	-0.061953	0.027133	-00.61856	0.25134E-01
C_g	Cg	5.562367	0.318464	5.5593	0.10838
A'_g	Aprig	0.166118	0.028009	0.16618	0.34574E-01
B'_g	Bprig	-0.383100	0.009784	-0.38300	0.76253E-02
B_{u_v}	Buv	0.810476	0.016017	0.81056	0.53604E-02
C_{u_v}	Cuv	4.823512	0.063844	4.8239	0.29342E-01
E_{u_v}	Euv	9.921366	0.835891	9.9226	0.27481
B_{d_v}	Bdv	1.029995	0.061123	1.0301	0.23240E-01
C_{d_v}	Cdv	4.846279	0.295439	4.8456	0.12584
$C_{\bar{U}}$	CUbar	7.059694	0.809144	7.0603	0.22306
$D_{\bar{U}}$	DUbar	1.548098	1.096540	1.5439	0.31340
$A_{\bar{D}}$	ADbar	0.268798	0.008020	0.26877	0.39536E-02
$B_{\bar{D}}$	BDbar	-0.127297	0.003628	-0.12732	0.17428E-02
$C_{\bar{D}}$	CDbar	9.586246	1.448861	9.5810	0.60834



Procedure: Reweighting

- As noted, to approximate the likelihood, we weight each point by

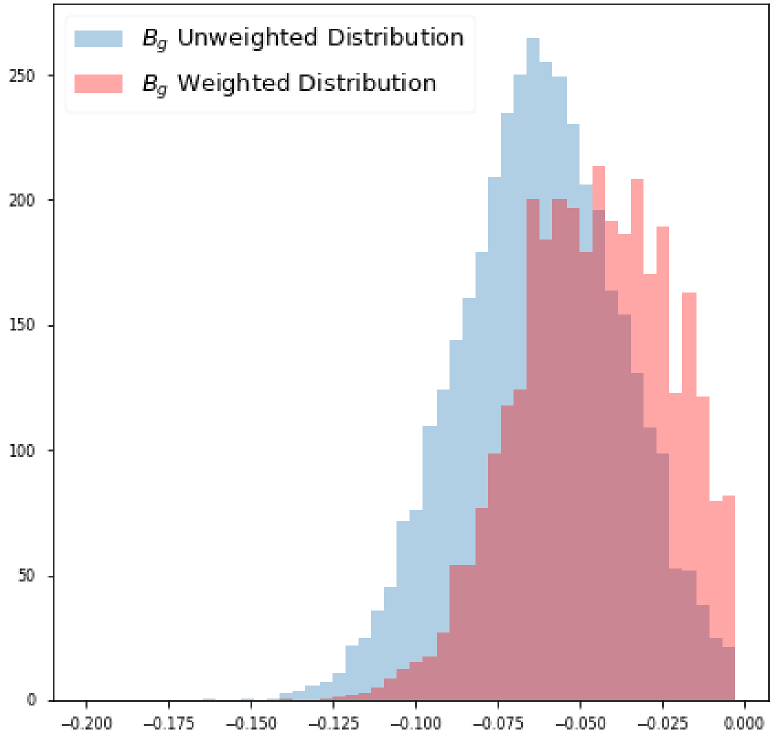
$$w_{\mathrm{i}} = \frac{L(\theta_i)}{\pi(\theta_i)}$$

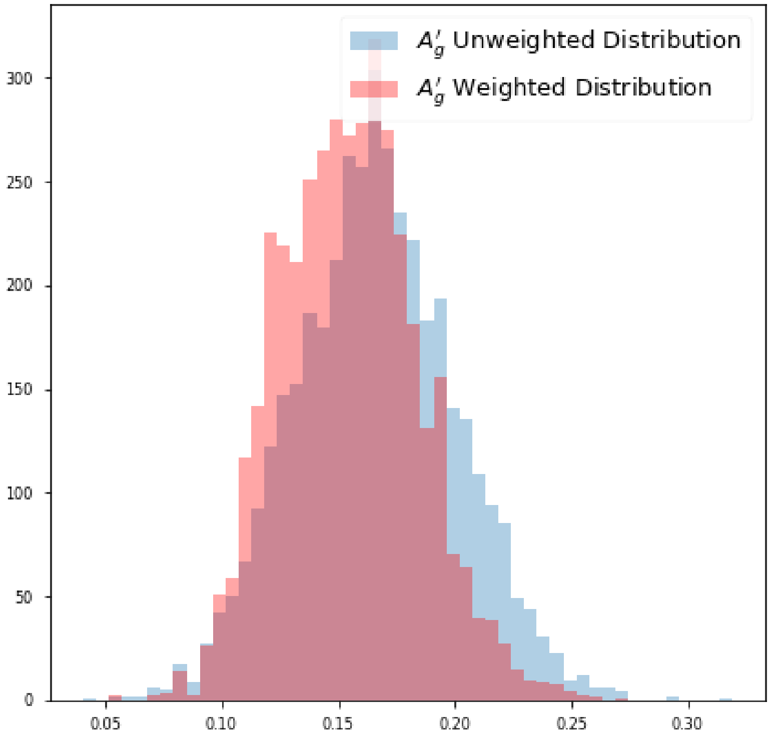
- In the limit of infinite number of sampled points, the weighted distribution will recover the true likelihood.

- The weighted distributions are what we expect to arrive at if we could do a Markov chain sampling of $L(\theta)$.

Results - 1

- Data: HERA I, II & ZEUS

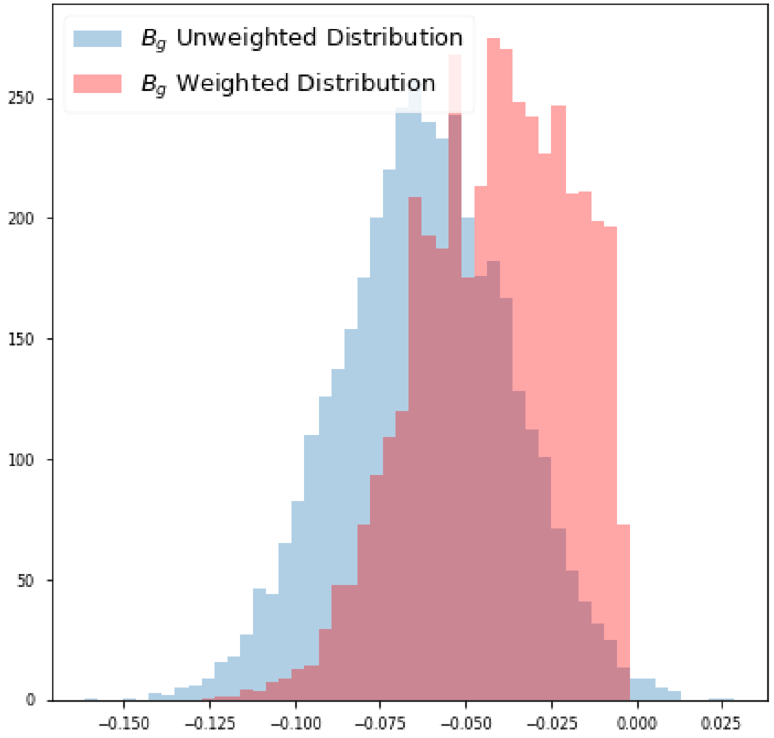


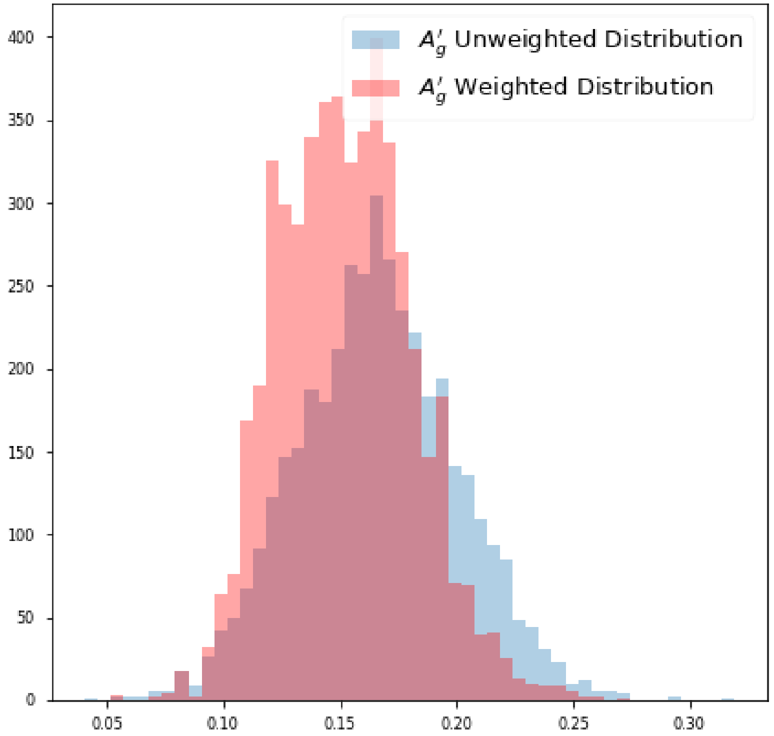


4,000 parameter sets
HERAPDF parameterization

Results - 2

- Data: HERA I+II & ZEUS + CDF W asymmetry + D0 Run II cone jets





4,000 data points (parameter sets)
HERAPDF parameterization

Available Code

- We have done many studies with xFitter (focusing on master version). All our code is available at:

  https://github.com/AliAlkadhim/PDF_Uncertainty/

- We also made a docker image with full xfitter-master and its dependencies and all datasets and our code installed

  docker run -it alialkadhim/pdf_uncertainty:v0

- Most recent studies with xFitter-master can be found in

  https://github.com/AliAlkadhim/PDF_Uncertainty/master_version/local

xFitter Wishlist

- Initialize all the datasets only once.
- Once the initialization is done, be able to feed xFitter a sequence of parameter points.
- For each parameter point, xFitter computes and returns a χ^2 value.
- In the future, xFitter would return $-2\log L(\theta)$.

Summary

- The weighting procedure for recovering the true likelihood seems to work, although it would be good to try different priors.
- However, in this study, we rerun xFitter for every parameter set, which is inefficient.
- We found xFitter to be an excellent tool for performing such studies, and with the changes we propose, it would make studies easier.
- We would like to thank the members of the xFitter team and Stefano for inviting us to make this presentation.

Backup

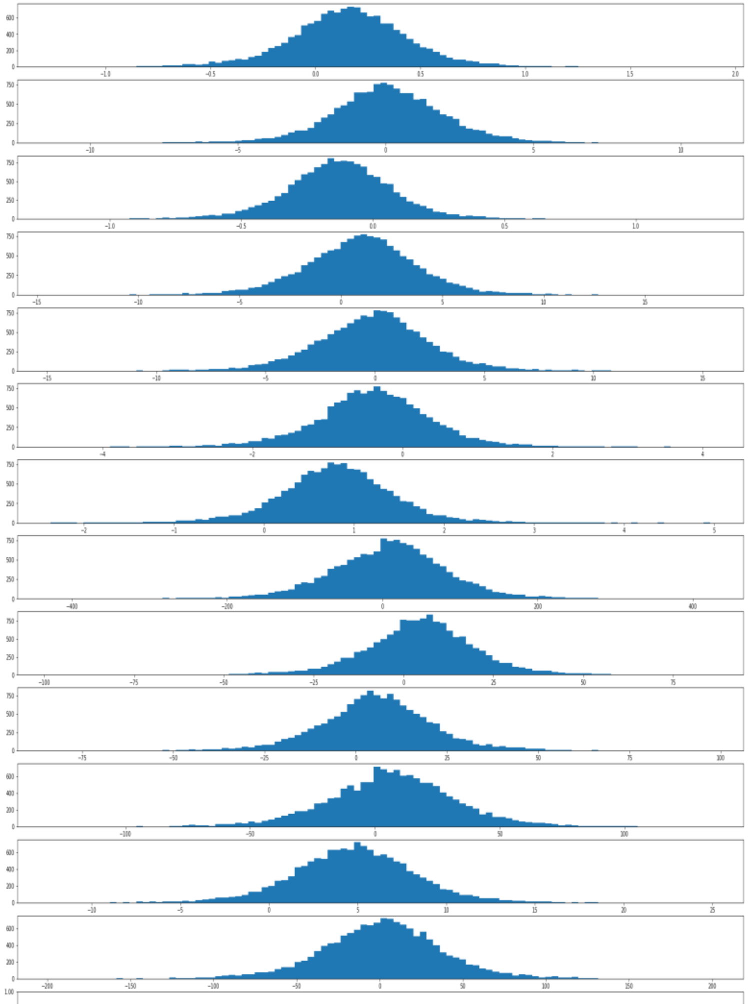
Technical Aspects & Suggestions

The more datasets used, the more programs that have to be initialized ⇒ More overhead time! e.g. a parameters.yml could look like:

- Decompositions: Proton
  - DefaultEvolution: proton-QCDNUM
- Evolutions:
  - proton-APFELff; include evolutions/APFEL.yaml
  - proton-QCDNUM; include evolutions/QCDNUM.yaml
  - …
- Decomposition:
  - Proton
  - Antiproton; class: FlipCharge
  - Neutron; class: FlipUD
  - proton-LHAPDF; class: LHAPDF ; set: \"NNPDF30_nlo_as_0118

xFitter-master Datasets used (all available but 1)
HERA I+II combined inclusive DIS
CDF Jets, W, Z production
D0 Jets, W, Z production
CMS W, Z production
CMS Jets
ATLAS W, Z production
ATLAS Drell-Yann
ATLAS Jets
ATLAS Dec 2016 W,Z
LHCb charm and beauty
CMS W+c
CMS 8 TeV jets

MCMC using all sets, Different $L'(\theta)$



MCMC is not efficient since it cannot be parallelized and computationally expensive.

However, it should return the true shape of the likelihoods.

Using 14336 points (many weeks of running), MCMC (Metropolis-Hastings) still yields Gaussian parameter likelihoods using the xFitter χ^2 values.

Reason: Not enough differing (discrepant) datasets (and not enough statistics, i.e. data points).

More Backup

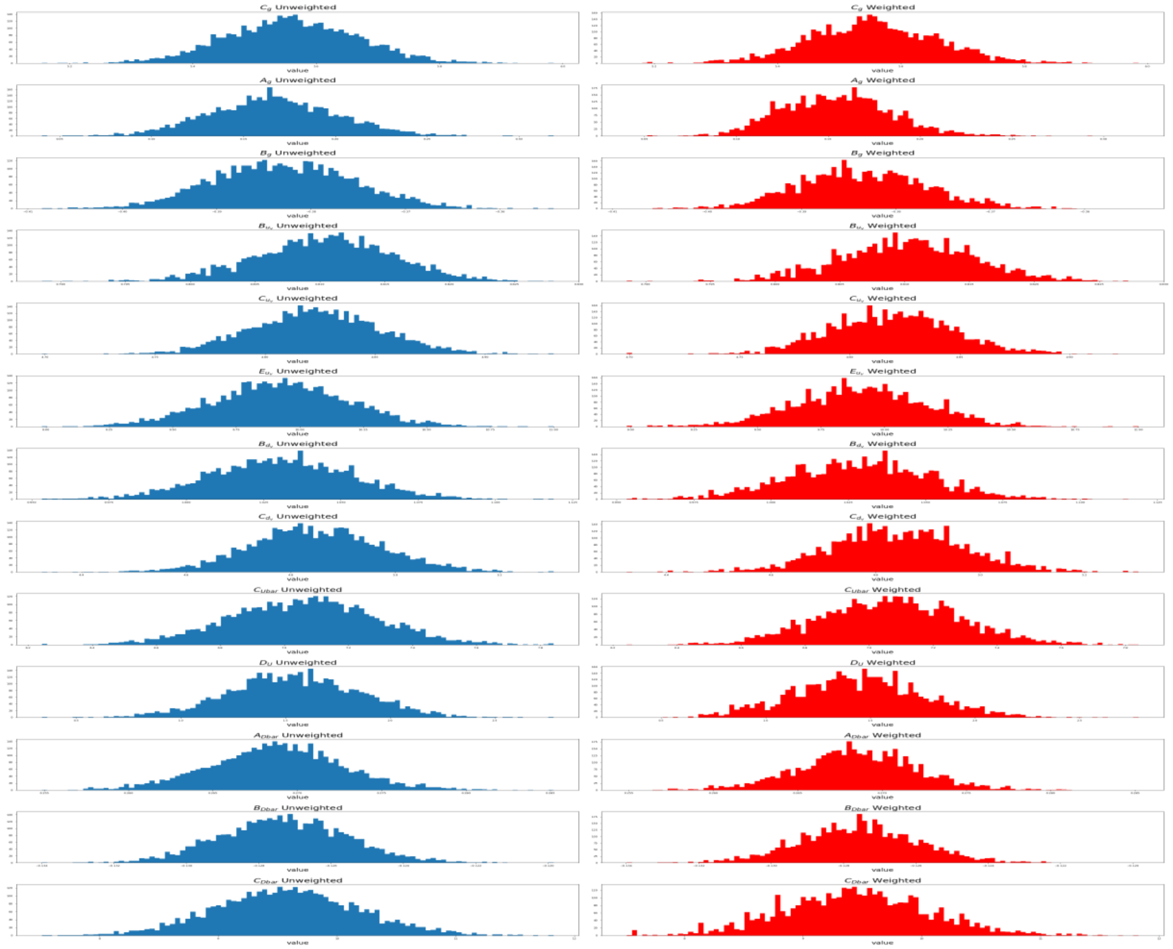
- If we approximate $\pi(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{D}|\widehat{\boldsymbol{\theta}}_{\boldsymbol{i}}, \widehat{\boldsymbol{\Sigma}}_{\boldsymbol{i}})$, then

$$w_k = \frac{L(\boldsymbol{\theta})}{\pi(\boldsymbol{\theta})} = \frac{N_{samples}}{\sum_{k=1}^{N_{samples}} w_k} \frac{e^{-\frac{1}{2}\chi_k^2}}{\mathcal{N}(\boldsymbol{D}|\widehat{\boldsymbol{\theta}_{\boldsymbol{k}}}, \widehat{\boldsymbol{\Sigma}_{\boldsymbol{k}}}),} = \begin{cases} \mathbf{1}, \text{Gauss. Approx. holds for } \mathrm{L}(\boldsymbol{\theta}) \\ \textbf{else}, \qquad \mathrm{L}(\boldsymbol{\theta}) \text{ is non} - \text{Gauss.} \end{cases}$$

- If the likelihood for θ is multivariate normal, the likelihood of a single observation is of the form
- $L(\boldsymbol{\theta}|\boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}[\mathbf{x} - g(\boldsymbol{\theta})]^T \boldsymbol{\Sigma}^{-\mathbf{1}}[\boldsymbol{x} - \mathrm{g}(\boldsymbol{\theta})]\right\} = \frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}\chi^2\right\} \longrightarrow \log L(\boldsymbol{\theta}) = -\frac{\mathbf{1}}{\mathbf{2}}\boldsymbol{\chi}^{\mathbf{2}}$
- 68% confidence intervals are obtained by finding points where $\Delta\chi^2 = 1$, i.e.
- $-2\Delta \log[\mathrm{L}] = -2[\log\left[L(\boldsymbol{\theta}_{\pm}|\boldsymbol{x})\right] - \log\left[L(\widehat{\boldsymbol{\theta}}|\boldsymbol{x})\right] = 1 \longrightarrow (\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}_{-}, \widehat{\boldsymbol{\theta}} + \boldsymbol{\theta}_{+})$ but this assumes normal sampling of data.
- The tolerance $T = \sqrt{\Delta\chi^2_{global}}$, ideally $T = 1$, but this assumes ideal gaussian errors & well-defined theory.
  - In global fits, $T > 1$ to account for discrepant data sets (e.g. see arxiv: 1410.8849).

All parameter Distributions

One Dataset



Multiple Datasets