# New approaches to global PDF analysis 

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## Outline

- Motivation - why the need for a new paradigm?
- Bayesian approach to fitting
$\longrightarrow$ single-fit (Hessian) vs. Monte Carlo approaches
$\longrightarrow$ shortcomings of Hessian (Gaussian) approach
- Incompatible data sets
$\longrightarrow$ "tolerance" factors (uncertainties should not depend on \# of parameters!)
- Monte Carlo methods
$\longrightarrow$ iterative MC, nested sampling, ...
- Generalization to non-Gaussian likelihoods
$\longrightarrow$ disjoint probabilities, empirical Bayes, ...
■ Outlook


## Motivation

- With limited number of observables and finite statistics, need a robust analysis framework to extract meaningful parton information from experiment
- Over the first ~2-3 decades of global PDF analysis efforts, $\chi^{2}$ minimization (single-fit) analysis (with Hessian error propagation) has generally been sufficient to map out global characteristics of partonic structure
$\rightarrow e . g$. shapes of quark PDFs from DIS, where data are plentiful
- A major challenge has been to characterize PDF uncertainties - in a statistically meaningful way - in the presence of tensions among data sets


## Motivation

- Previous attempts sought to address tensions in data sets by introducing
$\longrightarrow$ "tolerance" factors (artificially inflating PDF errors)
$\longrightarrow$ "neural net" parametrization (instead of polynomial parametrization), together with MC techniques
- However, to address the problem in a more statistically rigorous way, one requires going beyond the standard $\chi^{2}$ minimization paradigm
$\rightarrow$ utilize modern techniques based on Bayesian statistics!


## Motivation

- In the near future, standard $\chi^{2}$ minimization techniques will be unsuitable - even in the absence of tensions e.g. for
$\rightarrow$ simultaneous analysis of collinear distributions (unpolarized \& polarized PDFs, fragmentation functions)

$$
\longrightarrow \text { "JAM17": Jake Ethier (Tuesday) }
$$

$\rightarrow$ new types of observables - TMDs or GPDs that will involve $>\mathcal{O}\left(10^{5}\right)$ data points, with $\mathcal{O}\left(10^{3}\right)$ parameters

## Motivation

- Typically PDF parametrizations are nonlinear functions of the PDF parameters, e.g.

$$
x f(x, \mu)=N x^{\alpha}(1-x)^{\beta} P(x)
$$

where $P$ is a polynomial e.g. $P(x)=1+\epsilon \sqrt{x}+\eta x$, or Chebyshev, neural net, ...
$\rightarrow$ have multiple local minima present in the $\chi^{2}$ function

- Robust parameter estimation that thoroughly scans over a realistic parameter space, including multiple local minima, is only possible using MC methods!
- Need more reliable algorithms - "PDFs beyond the LHC"!


## Bayesian approach to fitting

## Bayesian approach to fitting

- Analysis of data requires estimating expectation values $E$ and variances $V$ of "observables" $\mathcal{O}$ (= PDFs, FFs) which are functions of parameters $\vec{a}$

$$
\begin{aligned}
& E[\mathcal{O}]=\int d^{n} a \mathcal{P}(\vec{a} \mid \text { data }) \mathcal{O}(\vec{a}) \\
& V[\mathcal{O}]=\int d^{n} a \mathcal{P}(\vec{a} \mid \text { data })[\mathcal{O}(\vec{a})-E[\mathcal{O}]]^{2}
\end{aligned}
$$

"Bayesian master formulas"

- Using Bayes' theorem, probability distribution $\mathcal{P}$ given by

$$
\mathcal{P}(\vec{a} \mid \text { data })=\frac{1}{Z} \mathcal{L}(\text { data } \mid \vec{a}) \pi(\vec{a})
$$

in terms of the likelihood function $\mathcal{L}$

## Bayesian approach to fitting

- Likelihood function

$$
\mathcal{L}(\text { data } \mid \vec{a})=\exp \left(-\frac{1}{2} \chi^{2}(\vec{a})\right)
$$

is a Gaussian form in the data, with $\chi^{2}$ function

$$
\chi^{2}(\vec{a})=\sum_{i}\left(\frac{\operatorname{data}_{i}-\text { theory }_{i}(\vec{a})}{\delta(\text { data })}\right)^{2}
$$

with priors $\pi(\vec{a})$ and "evidence" $Z$

$$
Z=\int d^{n} a \mathcal{L}(\operatorname{data} \mid \vec{a}) \pi(\vec{a})
$$

$\rightarrow \quad Z$ tests if e.g. an $n$-parameter fit is statistically different from ( $n+1$ )-parameter fit

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood<br>Monte Carlo<br>( $\chi^{2}$ minimization)

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood ( $\chi^{2}$ minimization)

$\rightarrow$ maximize probability distribution $\mathcal{P}$ by minimizing $\chi^{2}$ for a set of best-fit parameters $\vec{a}_{0}$

$$
E[\vec{a}]=\vec{a}_{0}
$$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood

( $\chi^{2}$ minimization)
$\longrightarrow$ maximize probability distribution $\mathcal{P}$ by minimizing $\chi^{2}$ for a set of best-fit parameters $\vec{a}_{0}$

$$
E[\vec{a}]=\vec{a}_{0}
$$

$\longrightarrow$ if $\mathcal{O}$ is $\approx$ linear in the parameters, and if probability is symmetric in all parameters

$$
E[\mathcal{O}(\vec{a})] \approx \mathcal{O}\left(\vec{a}_{0}\right)
$$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood

$$
\left(\chi^{2} \text { minimization }\right)
$$

$\longrightarrow$ variance computed by expanding $\mathcal{O}(\vec{a})$ about $\vec{a}_{0}$ $e . g$. in 1 dimension have "master formula"

$$
V[\mathcal{O}] \approx \frac{1}{4}[\mathcal{O}(a+\delta a)-\mathcal{O}(a-\delta a)]^{2}
$$

where

$$
\delta a^{2}=V[a]
$$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood

( $\chi^{2}$ minimization)
$\longrightarrow$ generalization to multiple dimensions via Hessian approach: find set of (orthogonal) contours in parameter space around $\vec{a}_{0}$ such that $\mathcal{L}$ along each contour is parametrized by statistically independent parameters - directions of contours given by eigenvectors $\hat{e}_{k}$ of Hessian matrix $H$, with elements

$$
H_{i j}=\left.\frac{1}{2} \frac{\partial^{2} \chi^{2}(\vec{a})}{\partial a_{i} \partial a_{j}}\right|_{\vec{a}=\vec{a}_{0}}
$$

and contours parametrized as $\Delta a^{(k)}=a^{(k)}-a_{0}=t_{k} \frac{\hat{e}_{k}}{\sqrt{v_{k}}}$,
with $v_{k}$ eigenvectors of $H$ with $v_{k}$ eigenvectors of $H$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood

( $\chi^{2}$ minimization)
$\longrightarrow$ basic assumption: $\mathcal{P}$ factorizes along each eigendirection

$$
\mathcal{P}(\Delta a) \approx \prod_{k} \mathcal{P}_{k}\left(t_{k}\right)
$$

where

$$
\mathcal{P}_{k}\left(t_{k}\right)=\mathcal{N}_{k} \exp \left[-\frac{1}{2} \chi^{2}\left(a_{0}+t_{k} \frac{\hat{e}_{k}}{\sqrt{v_{k}}}\right)\right]
$$

note: in quadratic approximation for $\chi^{2}$, this becomes a normal distribution

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood

$$
\left(\chi^{2} \text { minimization }\right)
$$

$\longrightarrow$ uncertainties on $\mathcal{O}$ along each eigendirection (assuming linear approximation)

$$
\left(\Delta \mathcal{O}_{k}\right)^{2} \approx \frac{1}{4}\left[\mathcal{O}\left(a_{0}+T_{k} \frac{\hat{e}_{k}}{\sqrt{v_{k}}}\right)-\mathcal{O}\left(a_{0}-T_{k} \frac{\hat{e}_{k}}{\sqrt{v_{k}}}\right)\right]^{2}
$$

where $T_{k}$ is finite step size in $t_{k}$, with total variance

$$
V[\mathcal{O}]=\sum_{k}\left(\Delta \mathcal{O}_{k}\right)^{2}
$$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Monte Carlo

$\rightarrow$ in practice, generally one has $E[\mathcal{O}(\vec{a})] \neq \mathcal{O}(E[\vec{a}])$ so the maximal likelihood method will sometimes fail
$\rightarrow$ Monte Carlo approach samples parameter space and assigns weights $w_{k}$ to each set of parameters $a_{k}$
$\rightarrow$ expectation value and variance are then weighted averages

$$
E[\mathcal{O}(\vec{a})]=\sum_{k} w_{k} \mathcal{O}\left(\vec{a}_{k}\right), \quad V[\mathcal{O}(\vec{a})]=\sum_{k} w_{k}\left(\mathcal{O}\left(\vec{a}_{k}\right)-E[\mathcal{O}]\right)^{2}
$$

## Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:


## Maximum Likelihood <br> ( $\chi^{2}$ minimization)

O fast

- assumes Gaussianity

O no guarantee that global minimum has been found

O errors only characterize local geometry of $\chi^{2}$ function

## Monte Carlo

O slow
O does not rely on
Gaussian assumptions
o includes all possible solutions

O accurate

## Incompatible data sets

## Incompatible data sets

- Incompatible data sets can arise because of errors in determining central values, or underestimation of systematic experimental uncertainties
$\rightarrow$ requires some sort of modification to standard statistics
- Often one modifies the master formula by introducing a "tolerance" factor $T$

$$
V[\mathcal{O}] \rightarrow T^{2} V[\mathcal{O}]
$$

e.g. for one dimension

$$
V[\mathcal{O}]=\frac{T^{2}}{4}[\mathcal{O}(a+\delta a)-\mathcal{O}(a-\delta a)]^{2}
$$

$\rightarrow$ effectively modifies the likelihood function

## Incompatible data sets

■ Simple example: consider observable $m$, and two measurements

$$
\left(m_{1}, \delta m_{1}\right), \quad\left(m_{2}, \delta m_{2}\right)
$$

$\rightarrow$ compute exactly the $\chi^{2}$ function

$$
\chi^{2}=\left(\frac{m-m_{1}}{\delta m_{1}}\right)^{2}+\left(\frac{m-m_{2}}{\delta m_{2}}\right)^{2}
$$

and, from Bayesian master formula, the mean value

$$
E[m]=\frac{m_{1} \delta m_{2}^{2}+m_{2} \delta m_{1}^{2}}{\delta m_{1}^{2}+\delta m_{2}^{2}}
$$

and variance

$$
V[m]=H^{-1}=\frac{\delta m_{1}^{2} \delta m_{2}^{2}}{\delta m_{1}^{2}+\delta m_{2}^{2}} \leadsto \begin{array}{r}
\text { does not } \\
\text { depend on } \\
m_{1}-m_{2}!
\end{array}
$$

## Incompatible data sets

■ Simple example: consider observable $m$, and two measurements

$$
\left(m_{1}, \delta m_{1}\right), \quad\left(m_{2}, \delta m_{2}\right)
$$



$\longrightarrow$ total uncertainty remains independent of degree of (in)compatibility of data
$\rightarrow$ Gaussian likelihood gives unrealistic representation of true uncertainty

## Incompatible data sets

## $\square$ Realistic example: recent CJ (CTEQ-JLab) global PDF analysis






$\longrightarrow$ data sets compatible along this e-direction
$\longrightarrow 24$ parameters, 33 data sets

## Incompatible data sets

- Realistic example: recent CJ (CTEQ-JLab) global PDF analysis


$\longrightarrow 24$ parameters, 33 data sets
$\longrightarrow$ data sets not compatible along this e-direction


## Incompatible data sets

$\square$ Realistic example: recent CJ (CTEQ-JLab) global PDF analysis


$\rightarrow 24$ parameters,
33 data sets
$\longrightarrow$ data sets not compatible along this e-direction
$\longrightarrow$ standard Gaussian likelihood incapable of accounting for underestimated individual errors (leading to incompatible data sets) - not designed for such scenarios!

## Incompatible data sets

## - Two ways in which tolerance factors usually implemented

$\rightarrow$ CTEQ "tolerance criteria" (variations adopted by other groups, e.g., MMHT, CJ)

Pumplin, Stump, Huston, Lai, Nadolsky, Tung
JHEP 07 (2002) 012

## $\longrightarrow$ scaling of $\Delta \chi^{2}$ with number of parameters (or number of degrees of freedom)

e.g. Brodsky, Gardner

PRL (Comment) 116, 019101 (2016)

> JDHLM assess their PDF errors using a tolerance criteria of $\Delta \chi^{2}=1$ at $1 \sigma$; however, the actual value of $\Delta \chi^{2}$ to be employed depends on the number of parameters to be simultaneously determined in the fit. This is illustrated in Table 38.2 of Ref. [15] and is used broadly, noting, e.g., Refs. [16-19]. Ref. [7] employs the CT10 PDF analysis [20], so that it contains 25 parameters, plus one for intrinsic charm. Figure 38.2 of Ref. [15] then shows that $\Delta \chi^{2} \approx 29$ at $1 \sigma\left(68 \%\right.$ CL), whereas $\Delta \chi^{2} \approx 36$ at $90 \%$ CL. Ref. [7] uses the criterion $\Delta \chi^{2}>100$, determined on empirical grounds, to indicate a poor fit. JDHLM employs the framework of Ref. [21] which contains 25 parameters for the PDFs and 12 for the higher-twist contributions, so that a much larger tolerance than $\Delta \chi^{2}=1$ is warranted.

## Incompatible data sets

- CTEQ tolerance criteria

- for each experiment, find minimum $\chi^{2}$ along given e-direction
- from $\chi^{2}$ distribution determine $90 \% \mathrm{CL}$ for each experiment
- along each side of e-direction, determine maximum range $d_{k}^{ \pm}$ allowed by the most constraining experiment
- $T$ computed by averaging over all $d_{k}^{ \pm}$(typically $T \sim 5-10$ )


## Incompatible data sets

- CTEQ tolerance criteria

$\square$ This approach is not consistent with Gaussian likelihood
$\longrightarrow$ no clear Bayesian interpretation of uncertainties (ultimately, a prescription...)


## Incompatible data sets

- Scaling of $\Delta \chi^{2}$ with \# of parameters: " $\Delta \chi^{2}$ paradox"
- Simple example: two parameters $\theta_{i} \quad(i=1,2)$ with mean values $\mu_{i}$ and standard deviation $\sigma_{i}$
$\rightarrow$ joint probability distribution

$$
\mathcal{P}\left(\theta_{1}, \theta_{2}\right)=\prod_{i=1,2} \frac{1}{\sqrt{2 \pi \sigma_{i}^{2}}} \exp \left[-\frac{1}{2}\left(\frac{\theta_{i}-\mu_{i}}{\sigma_{i}}\right)^{2}\right]
$$

$\rightarrow$ change variables $\theta_{i} \rightarrow t_{i}=\left(\theta_{i}-\mu_{i}\right) / \sigma_{i}$ and use polar coordinates $r^{2}=t_{1}^{2}+t_{2}^{2}, \quad \phi=\tan ^{-1}\left(t_{2} / t_{1}\right)$

$$
d \theta_{1} d \theta_{2} \mathcal{P}\left(\theta_{1}, \theta_{2}\right)=\frac{d \phi}{2 \pi} r d r \exp \left[-\frac{1}{2} r^{2}\right]
$$

## Incompatible data sets

- Scaling of $\Delta \chi^{2}$ with \# of parameters: " $\Delta \chi^{2}$ paradox"
$\rightarrow$ confidence volume

$$
\begin{aligned}
\mathrm{CV} & \equiv \int d \theta_{1} d \theta_{2} \mathcal{P}\left(\theta_{1}, \theta_{2}\right)=\int_{0}^{R} d r r \exp \left[-\frac{1}{2} r^{2}\right] \\
& =68 \% \text { for } R=2.279
\end{aligned}
$$

$\longrightarrow$ note that $R^{2}=t_{1}^{2}+t_{2}^{2} \equiv \chi^{2}$, so that confidence region for parameters max $\left[t_{i}\right]=R$
$\longrightarrow$ implies that $\theta_{i}=\mu_{i} \pm \sigma_{i} R$, which contradicts
 original premise that $\theta_{i}=\mu_{i} \pm \sigma_{i}$ !

- Scaling of $\Delta \chi^{2}$ with \# of parameters: " $\Delta \chi^{2}$ paradox"
$\rightarrow$ to resolve paradox, use Bayesian master formulas

$$
\begin{aligned}
E\left[\theta_{i}\right] & =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r \mathcal{P}(r, \phi) \theta_{i} \\
& =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r r e^{-r^{2} / 2}\left(\mu_{i}+t_{i} \sigma_{i}\right)=\mu_{i}
\end{aligned}
$$

## Incompatible data sets

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$\rightarrow$ to resolve paradox, use Bayesian master formulas

$$
\begin{aligned}
E\left[\theta_{i}\right] & =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r \mathcal{P}(r, \phi) \theta_{i} \\
& =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r r e^{-r^{2} / 2}\left(\mu_{i}+t_{i} \sigma_{i}\right)=\mu_{i} \\
V\left[\theta_{i}\right] & =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r \mathcal{P}(r, \phi)\left(\theta_{i}-\mu_{i}\right)^{2} \\
& =\int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \int_{0}^{\infty} d r r e^{-r^{2} / 2}\left(t_{i} \sigma_{i}\right)^{2}=\sigma_{i}^{2} \sqrt{ }
\end{aligned}
$$

## Incompatible data sets

- Scaling of $\Delta \chi^{2}$ with \# of parameters: " $\Delta \chi^{2}$ paradox"
$\rightarrow$ no paradox if use $\Delta \chi^{2}=1$ for any number of parameters to characterize the $1 \sigma \mathrm{CL}$
$\longrightarrow$ only consistent tolerance for Gaussian likelihood is $T=1$

To summarize standard maximum likelihood method...

- Gradient search (in parameter space) depends how "good" the starting point is
$\rightarrow$ for $\sim 30$ parameters trying different starting points is impractical, if do not have some information about shape
- Common to free parameters initially, then freeze those not sensitive to data ( $\chi^{2}$ flat locally)
$\rightarrow$ introduces bias, does not guarantee that flat $\chi^{2}$ globally
- Cannot guarantee solution is unique
- Error propagation characterized by quadratic $\chi^{2}$ near minimum $\longrightarrow$ no guarantee this is quadratic globally (e.g. Student $t$-distribution?)
- Introduction of tolerance modifies Gaussian statistics


## Monte Carlo methods

## Monte Carlo

ㅁ Designed to faithfully compute Bayesian master formulas
$\square$ Do not assume a single minimum, include all possible solutions (with appropriate weightings)
$\square$ Do not assume likelihood is Gaussian in parameters
$\square$ Allows likelihood analysis to be extended to address tensions among data sets via Bayesian inference
$\square$ More computationally demanding compared with Hessian method

## Monte Carlo

- First group to use MC for global PDF analysis was NNPDF, using neural network to parametrize $P(x)$ in

$$
f(x)=N x^{\alpha}(1-x)^{\beta} P(x)
$$

$-\alpha, \beta$ are fitted "preprocessing coefficients"

- Iterative Monte Carlo (IMC), developed by JAM Collaboration, variant of NNPDF, tailored to non-neutral net parametrizations
$\rightarrow$ J.Ethier
- Markov Chain MC (MCMC) / Hybid MC (HMC)
- recent "proof of principle" analysis, ideas from lattice QCD

Gbedo, Mangin-Brinet,
PRD 96, 014015 (2017)

- Nested sampling (NS) - computes integrals in Bayesian master formulas (for $E, V, Z$ ) explicitly


## Iterative Monte Carlo (IMC)

ㅁ Use traditional functional form for input distribution shape, but sample significantly larger parameter space than possible in single-fit analyses

```
Iterative Monte Carlo (IMC)
```


$\rightarrow$ no assumptions for exponents

$\rightarrow$ cross-validation to avoid overfitting
$\rightarrow$ iterate until convergence criteria satisfied

## Iterative Monte Carlo (IMC)

$\square e . g$. of convergence (for fragmentation functions) in IMC













Sato et al.
PRD 94, 114004













## Nested Sampling

ㅁ Basic idea: transform $n$-dimensional integral to 1-D integral

$$
Z=\int d^{n} a \mathcal{L}(\text { data } \mid \vec{a}) \pi(\vec{a})=\int_{0}^{1} d X \mathcal{L}(X)
$$

where prior volume $d X=\pi(\vec{a}) d^{n} a$

such that $0<\cdots<X_{2}<X_{1}<X_{0}=1$

Feroz et al.
arXiv:1306.2144 [astro-ph]

## Nested Sampling

- Approximate evidence by a weighted sum

$$
Z \approx \sum_{i} \mathcal{L}_{i} w_{i} \quad \text { with weights } w_{i}=\frac{1}{2}\left(X_{i-1}-X_{i+1}\right)
$$

- Algorithm:
$\rightarrow$ randomly select samples from full prior s.t. initial volume $X_{0}=1$
$\rightarrow$ for each iteration, remove point with lowest $\mathcal{L}_{i}$, replacing it with point from prior with constraint that its $\mathcal{L}>\mathcal{L}_{i}$
$\rightarrow$ repeat until entire prior volume has been traversed
- can be parallelized
- performs better than VEGAS for large dimensions

O increasingly used in fields outside of (nuclear) analysis

## Nested Sampling

## - Recent application

 in global analysis of transversity TMD PDF$$
\longrightarrow \text { H.-W.Lin }
$$




Lin, WM, Prokudin,
Sato, Shows (2017)

## MC Error Analysis

$\square$ Assuming a single minimum, a Hessian or MC analysis must give same results, if using same likelihood function
$\rightarrow$ analysis of pseudodata, generated using Gaussian distribution





## MC Error Analysis

$\square$ Assuming a single minimum, a Hessian or MC analysis must give same results, if using same likelihood function
$\rightarrow$ also for discrepant data


$\rightarrow$ almost identical uncertainty bands for Hessian and for MC!

## MC Error Analysis

ㅁ Assuming a single minimum, a Hessian or MC analysis must give same results, if using same likelihood function

ㅁ Approaches that use Hessian + tolerance factor not consistent with Gaussian likelihood function
$\square$ NNPDF group claim that within their neural net MC methodology, no need for a tolerance factor, since uncertainties similar to other groups who use Hessian + tolerance
$\rightarrow$ how can this be?
$\square$ Assuming sufficient observables to determine PDFs, then PDF uncertainties cannot depend on parametrization!

## Non-Gaussian likelihood

## Incompatible data sets

$\square$ Rigorous (Bayesian) way to address incompatible data sets is to use generalization of Gaussian likelihood

- joint vs. disjoint distributions
- empirical Bayes
- hierarchical Bayes
o others, used in different fields


## Disjoint distributions

- Instead of using total likelihood that is a product ("and") of individual likelihoods, e.g. for simple example of two measurements

$$
\mathcal{L}\left(m_{1} m_{2} \mid m ; \delta m_{1} \delta m_{2}\right)=\mathcal{L}\left(m_{1} \mid m ; \delta m_{1}\right) \times \mathcal{L}\left(m_{2} \mid m ; \delta m_{2}\right)
$$

use instead sum ("or") of individual likelihoods

$$
\mathcal{L}\left(m_{1} m_{2} \mid m ; \delta m_{1} \delta m_{2}\right)=\frac{1}{2}\left[\mathcal{L}\left(m_{1} \mid m ; \delta m_{1}\right)+\mathcal{L}\left(m_{2} \mid m ; \delta m_{2}\right)\right]
$$

$\rightarrow$ gives rather different expectation value and variance

$$
\begin{aligned}
E[m] & =\frac{1}{2}\left(m_{1}+m_{2}\right) \\
V[m] & =\frac{1}{2}\left(\delta m_{1}^{2}+\delta m_{2}^{2}\right)+\left(\frac{m_{1}-m_{2}}{2}\right)^{2}
\end{aligned}
$$

## Disjoint distributions

$\square$ Symmetric uncertainties $\delta m_{1}=\delta m_{2}$

disjoint: $\quad V[m]=\frac{1}{2}\left(\delta m_{1}^{2}+\delta m_{2}^{2}\right)+\left(\frac{m_{1}-m_{2}}{2}\right)^{2}$
joint: $\quad V[m]=\frac{\delta m_{1}^{2} \delta m_{2}^{2}}{\delta m_{1}^{2}+\delta m_{2}^{2}}$

## Disjoint distributions

- Asymmetric uncertainties $\delta m_{1} \neq \delta m_{2}$

$\rightarrow$ disjoint likelihood gives broader overall uncertainty, overlapping individual (discrepant) data


## Empirical Bayes

- Shortcoming of conventional Bayesian — still assume prior distribution follows specific form (e.g. Gaussian)
- Extend approach to more fully represent prior uncertainties, with final uncertainties that do not depend on initial choices
- In generalized approach, data uncertainties modified by distortion parameters, whose probability distributions given in terms of "hyperparameters" (or "nuisance parameters")
$\square$ Hyperparameters determined from data
$\rightarrow$ give posteriors for both PDF and hyperparameters


## Empirical Bayes

- Standard mean and variance that characterize data

$$
\theta=\mu+\sigma \longrightarrow f(\mu)+g(\sigma)
$$

where $f(\mu), g(\sigma)$ are unknown functions that account for faulty measurements

- Simple choice is

$$
(\mu, \sigma) \rightarrow\left(\zeta_{1} \mu+\zeta_{2}, \zeta_{3} \sigma\right)
$$

where $\zeta_{1,2,3}$ are distortion parameters, with prob. dists. described by hyperparameters $\phi_{1,2,3}$

- Likelihood function is then

$$
\mathcal{L}\left(\text { data } \mid \vec{a}, \zeta_{1,2,3}\right) \sim \exp \left[-\frac{1}{2} \sum_{i}\left(\frac{d_{1}-f\left(\mu_{i}\left(\vec{a}, \zeta_{1,2}\right)\right)}{g\left(\sigma, \zeta_{3}\right)}\right)^{2}\right] \pi_{1}\left(\zeta_{1} \mid \phi_{1}\right) \pi_{2}\left(\zeta_{1} \mid \phi_{2}\right) \pi_{3}\left(\zeta_{1} \mid \phi_{3}\right)
$$

## Empirical Bayes

## - Simple example of EB for symmetric \& asymmetric errors








## Outlook

- New paradigm needed in global QCD analysis
- simultaneous determination of collinear distributions (also TMDs) using Monte Carlo sampling of parameter space
- Treatment of discrepant data sets needs serious attention - Bayesian perspective has clear merits
- Necessary to benchmark MC extractions (not just NNPDF)
- Near-term future: "universal" QCD analysis of all observables sensitive to collinear (unpolarized \& polarized) PDFs and FFs
- Longer-term: apply MC technology to global QCD analysis of transverse momentum dependent (TMD) PDFs and FFs

