The Flavor Structure of the Nucleon Sea Institute for Nuclear Theory October 2, 2017

New approaches to global PDF analysis



with Nobuo Sato



Connecticut / JLab

Outline

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

- 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, χ^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

- Previous attempts sought to address tensions in data sets by introducing
 - → "tolerance" factors (artificially inflating PDF errors)
- However, to address the problem in a more statistically rigorous way, one requires going *beyond* the standard χ^2 minimization paradigm
 - \rightarrow utilize modern techniques based on Bayesian statistics!

- In the near future, standard χ^2 minimization techniques will be unsuitable even in the absence of tensions *e.g.* for
 - → simultaneous analysis of collinear distributions (unpolarized & polarized PDFs, fragmentation functions)

→ "JAM17": Jake Ethier (Tuesday)

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

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

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

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 χ^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"!

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

$$E[\mathcal{O}] = \int d^{n} a \,\mathcal{P}(\vec{a}|\text{data}) \,\mathcal{O}(\vec{a})$$
$$V[\mathcal{O}] = \int d^{n} a \,\mathcal{P}(\vec{a}|\text{data}) \left[\mathcal{O}(\vec{a}) - E[\mathcal{O}]\right]^{2}$$

"Bayesian master formulas"

■ Using Bayes' theorem, probability distribution \mathcal{P} given by $\mathcal{P}(\vec{a}|\text{data}) = \frac{1}{Z} \mathcal{L}(\text{data}|\vec{a}) \pi(\vec{a})$

in terms of the likelihood function \mathcal{L}

Likelihood function

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

is a Gaussian form in the data, with χ^2 function

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

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

$$Z = \int d^n a \, \mathcal{L}(\text{data}|\vec{a}) \, \pi(\vec{a})$$

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

Two methods generally used for computing Bayesian master formulas:

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

Monte Carlo

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

 \rightarrow maximize probability distribution \mathcal{P} by minimizing χ^2 for a set of best-fit parameters \vec{a}_0

 $E\left[\vec{a}\right] = \vec{a}_0$

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 $E\left[\,\vec{a}\,\right]=\vec{a}_0$

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

 $E\left[\mathcal{O}(\vec{a})\right] \approx \mathcal{O}(\vec{a}_0)$

Two methods generally used for computing Bayesian master formulas:

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

 \rightarrow variance computed by expanding $\mathcal{O}(\vec{a})$ about \vec{a}_0 e.g. in 1 dimension have "master formula"

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

where

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

Two methods generally used for computing Bayesian master formulas:

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

→ 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

$$H_{ij} = \frac{1}{2} \left. \frac{\partial^2 \chi^2(\vec{a})}{\partial a_i \partial a_j} \right|_{\vec{a} = \vec{a}_0}$$

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

Two methods generally used for computing Bayesian master formulas:

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

 \rightarrow basic assumption: \mathcal{P} factorizes along each eigendirection

$$\mathcal{P}(\Delta a) \approx \prod_k \mathcal{P}_k(t_k)$$

where

$$\mathcal{P}_k(t_k) = \mathcal{N}_k \exp\left[-\frac{1}{2}\chi^2 \left(a_0 + t_k \frac{\hat{e}_k}{\sqrt{v_k}}\right)\right]$$

<u>note</u>: in quadratic approximation for χ^2 , this becomes a normal distribution

Two methods generally used for computing Bayesian master formulas:

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

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

$$(\Delta \mathcal{O}_k)^2 \approx \frac{1}{4} \left[\mathcal{O}\left(a_0 + T_k \frac{\hat{e}_k}{\sqrt{v_k}}\right) - \mathcal{O}\left(a_0 - T_k \frac{\hat{e}_k}{\sqrt{v_k}}\right) \right]^2$$

where T_k is finite step size in t_k , with total variance

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

Two methods generally used for computing Bayesian master formulas:

Monte Carlo

- → 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

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

Two methods generally used for computing Bayesian master formulas:

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

- fast
- assumes Gaussianity
- no guarantee that global minimum has been found
- errors only characterize local geometry of χ^2 function

Monte Carlo

• slow

- does not rely on
 Gaussian assumptions
- includes all possible solutions
- accurate

- 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

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

 \rightarrow effectively modifies the likelihood function

Simple example: consider observable m, and two measurements $(m_1, \delta m_1), (m_2, \delta m_2)$

 \rightarrow compute exactly the χ^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

$$E[m] = \frac{m_1 \delta m_2^2 + m_2 \delta m_1^2}{\delta m_1^2 + \delta m_2^2}$$

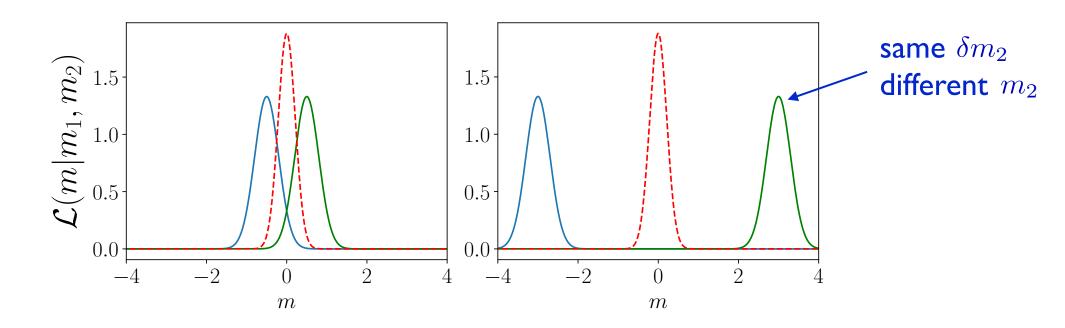
and variance

nce

$$V[m] = H^{-1} = \frac{\delta m_1^2 \, \delta m_2^2}{\delta m_1^2 + \delta m_2^2} \qquad \qquad \begin{array}{c} \text{does not} \\ \text{depend on} \\ m_1 - m_2 \, ! \end{array}$$

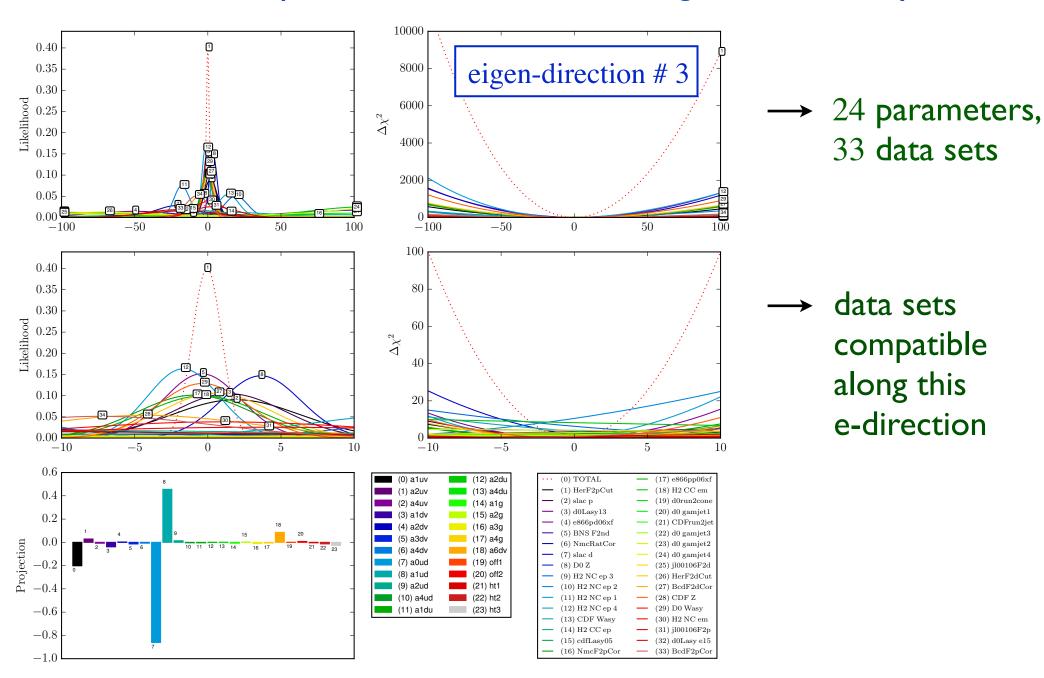
 \blacksquare Simple example: consider observable m , and two measurements

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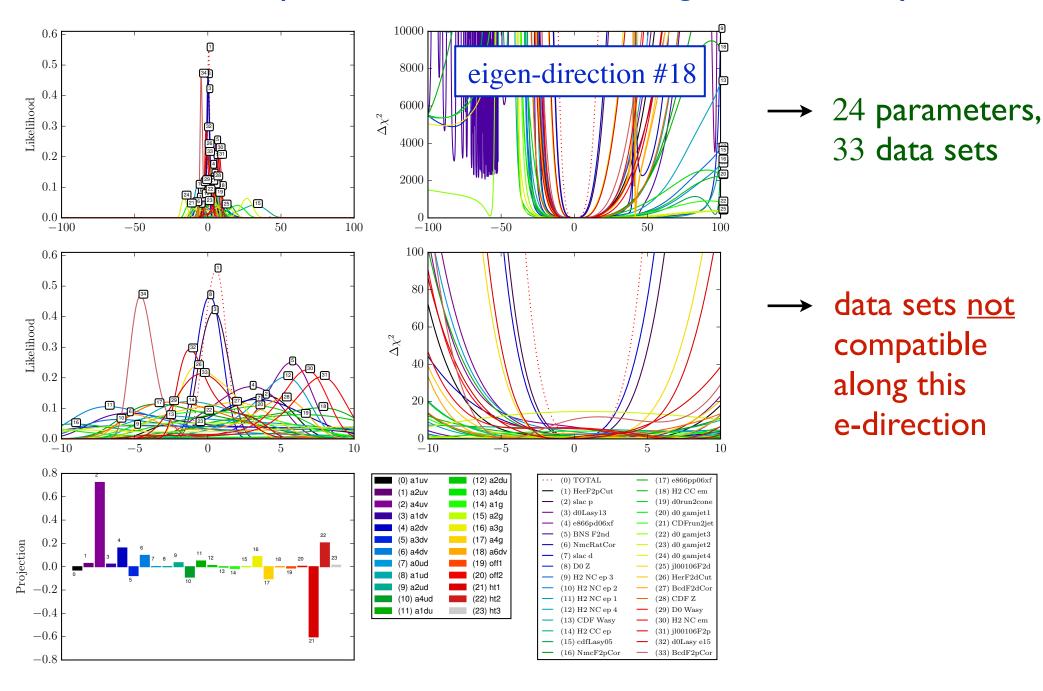


- → total uncertainty remains independent of degree of (in)compatibility of data
- → Gaussian likelihood gives unrealistic representation of true uncertainty

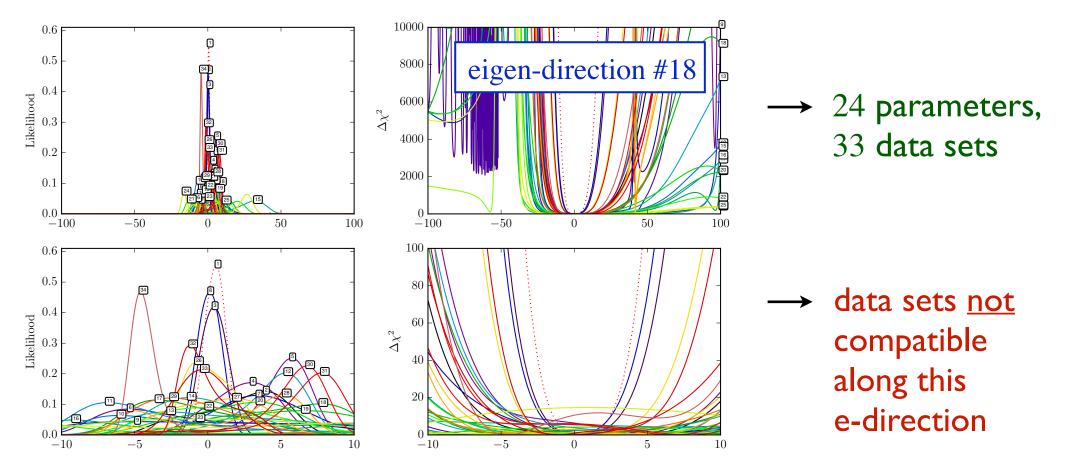
■ <u>Realistic example:</u> recent CJ (CTEQ-JLab) global PDF analysis



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 standard Gaussian likelihood incapable of accounting for underestimated individual errors (leading to incompatible data sets)
 — not designed for such scenarios!

Two ways in which tolerance factors usually implemented

→ CTEQ "tolerance criteria" (variations adopted by other groups, *e.g.*, MMHT, CJ)

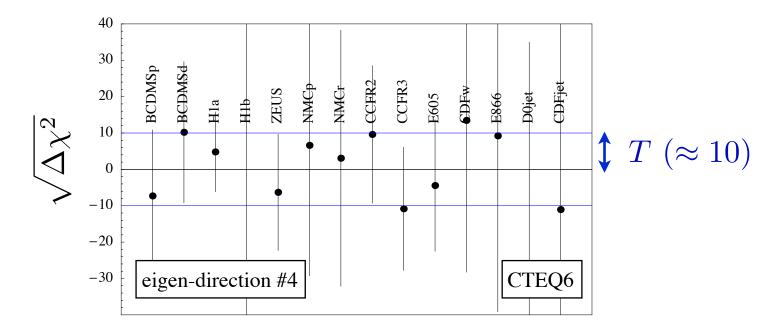
> Pumplin, Stump, Huston, Lai, Nadolsky, Tung JHEP 07 (2002) 012

 \rightarrow scaling of $\Delta \chi^2$ with number of parameters (or number of degrees of freedom)

e.g. Brodsky, Gardner PRL (Comment) **116**, 019101 (2016)

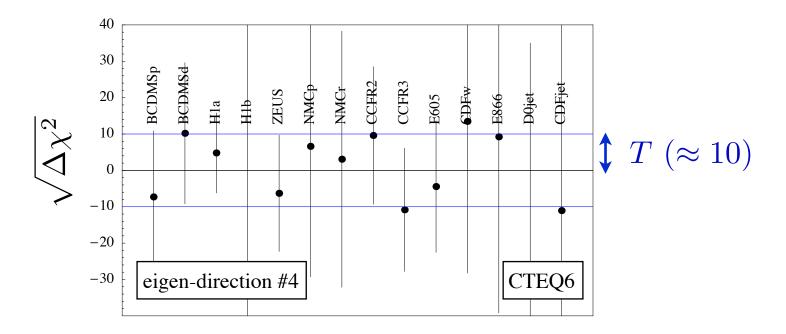
JDHLM assess their PDF errors using a tolerance criteria of $\Delta \chi^2 = 1$ at 1σ ; however, the actual value of $\Delta \chi^2$ to be employed depends on the number of parameters to be simultaneously determined in the fit. This is illustrated in Table 38.2 of Ref. [15] and is used broadly, noting, 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 1σ (68% 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.

□ CTEQ tolerance criteria



- for each experiment, find minimum χ^2 along given e-direction
- from χ^2 distribution determine 90% 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 $T \sim 5 10$)

■ CTEQ tolerance criteria



■ This approach is *not consistent* with Gaussian likelihood

→ no clear Bayesian interpretation of uncertainties (ultimately, a prescription...)

■ Scaling of $\Delta \chi^2$ with # of parameters: " $\Delta \chi^2$ paradox"

- Simple example: two parameters θ_i (i = 1, 2)with mean values μ_i and standard deviation σ_i
 - \rightarrow joint probability distribution

$$\mathcal{P}(\theta_1, \theta_2) = \prod_{i=1,2} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left[-\frac{1}{2} \left(\frac{\theta_i - \mu_i}{\sigma_i}\right)^2\right]$$

 \rightarrow change variables $\theta_i \rightarrow t_i = (\theta_i - \mu_i)/\sigma_i$ and use polar coordinates $r^2 = t_1^2 + t_2^2$, $\phi = \tan^{-1}(t_2/t_1)$

$$d\theta_1 d\theta_2 \mathcal{P}(\theta_1, \theta_2) = \frac{d\phi}{2\pi} r dr \exp\left[-\frac{1}{2}r^2\right]$$

Scaling of $\Delta \chi^2$ with # of parameters: " $\Delta \chi^2$ paradox"

 \rightarrow confidence volume

$$CV \equiv \int d\theta_1 d\theta_2 \,\mathcal{P}(\theta_1, \theta_2) = \int_0^R dr \,r \,\exp\left[-\frac{1}{2}r^2\right]$$
$$= 68\% \text{ for } R = 2.279$$

 t_2

R

 \rightarrow note that $R^2 = t_1^2 + t_2^2 \equiv \chi^2$, so that confidence region for parameters $\max[t_i] = R$

 \rightarrow 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

$$E[\theta_i] = \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\infty} dr \,\mathcal{P}(r,\phi) \,\theta_i$$
$$= \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\infty} dr \,r \,e^{-r^2/2} \left(\mu_i + t_i \,\sigma_i\right) = \mu_i \quad\checkmark$$

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$$V[\theta_i] = \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\infty} dr \, \mathcal{P}(r,\phi) \, (\theta_i - \mu_i)^2$$
$$= \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{\infty} dr \, r \, e^{-r^2/2} \, (t_i \, \sigma_i)^2 = \sigma_i^2 \quad \checkmark$$

Scaling of $\Delta \chi^2$ with # of parameters: " $\Delta \chi^2$ paradox"

→ no paradox if use $\Delta \chi^2 = 1$ for <u>any number</u> of parameters to characterize the 1σ CL

 \rightarrow 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
 - → for ~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 (χ^2 flat locally)
 - \rightarrow introduces <u>bias</u>, does not guarantee that flat χ^2 globally
- □ Cannot guarantee solution is <u>unique</u>
- Error propagation characterized by quadratic χ^2 near minimum \rightarrow no guarantee this is quadratic globally (*e.g.* Student *t*-distribution?)
- □ Introduction of <u>tolerance</u> modifies Gaussian statistics

Monte Carlo methods

Monte Carlo

- Designed to faithfully compute Bayesian master formulas
- Do not assume a <u>single minimum</u>, include all possible solutions (with appropriate weightings)
- **Do not assume likelihood is** <u>Gaussian</u> in parameters
- Allows likelihood analysis to be extended to <u>address tensions</u> among data sets via Bayesian inference
- More <u>computationally demanding</u> 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

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

— α, β are fitted "preprocessing coefficients"

Iterative Monte Carlo (IMC), developed by JAM Collaboration, variant of NNPDF, tailored to non-neutral net parametrizations

→ J. Ethier

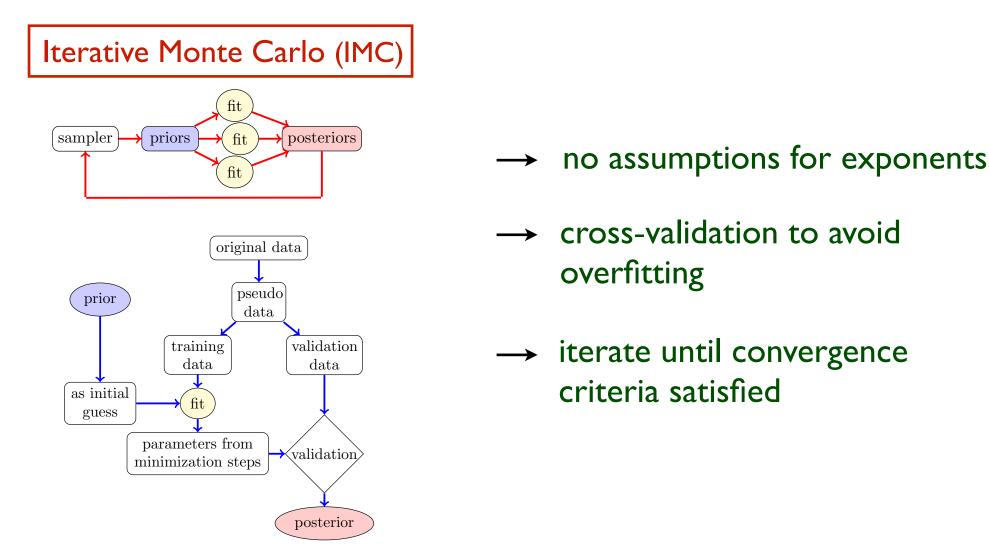
Markov Chain MC (MCMC) / Hybid MC (HMC)
 — recent "proof of principle" analysis, ideas from lattice QCD

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

Nested sampling (NS) — computes integrals in Bayesian master formulas (for E, V, Z) explicitly
Skilling (2004)

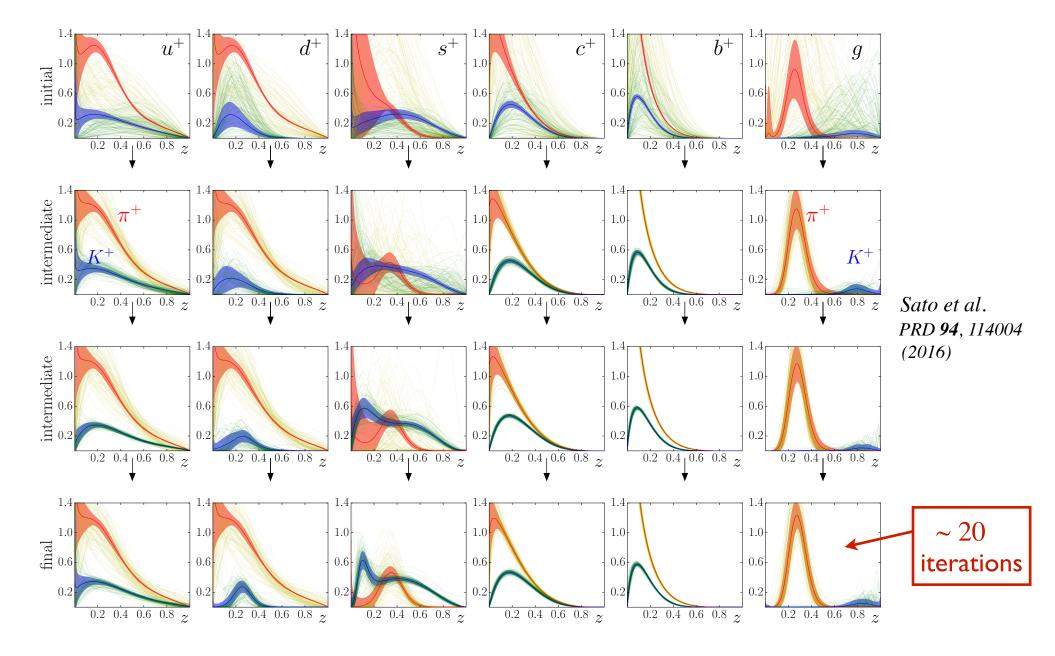
Iterative Monte Carlo (IMC)

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



Iterative Monte Carlo (IMC)

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

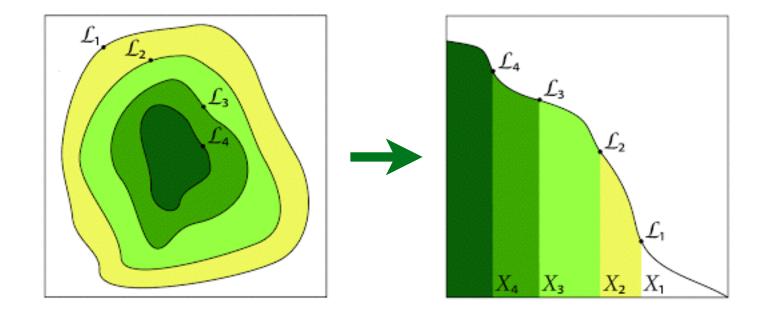


Nested Sampling

 \square Basic idea: transform *n*-dimensional integral to 1-D integral

$$Z = \int d^n a \,\mathcal{L}(\text{data}|\vec{a}) \,\pi(\vec{a}) = \int_0^1 dX \,\mathcal{L}(X)$$

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



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

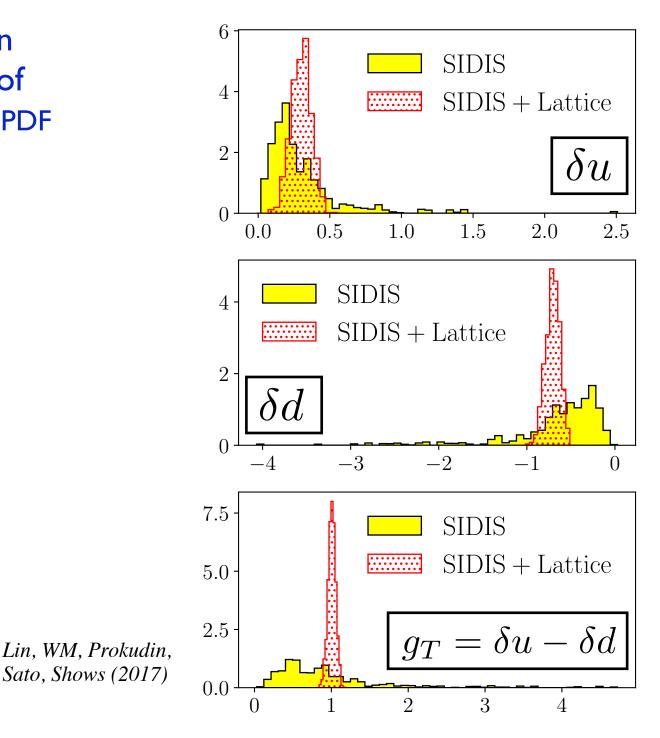
$$Z \approx \sum_{i} \mathcal{L}_{i} w_{i}$$
 with weights $w_{i} = \frac{1}{2}(X_{i-1} - X_{i+1})$

- 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
 - increasingly used in fields outside of (nuclear) analysis

Nested Sampling

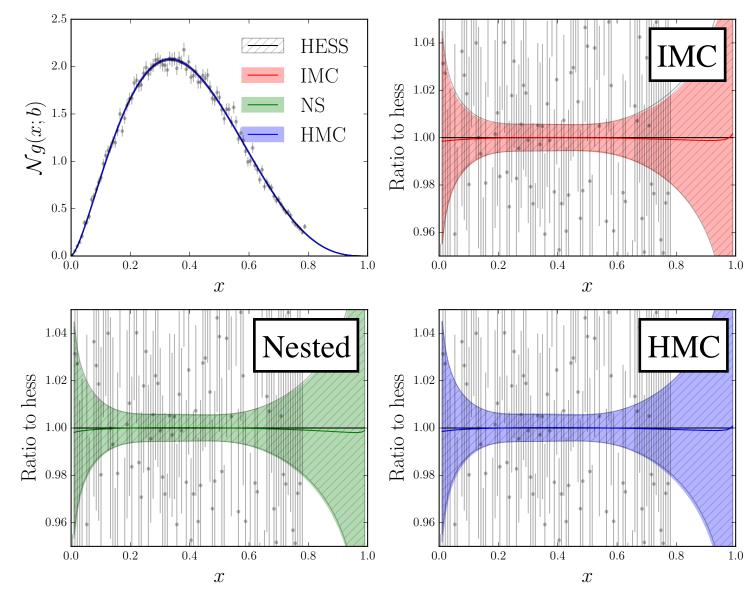
Recent application in global analysis of transversity TMD PDF

\rightarrow HW. Lin



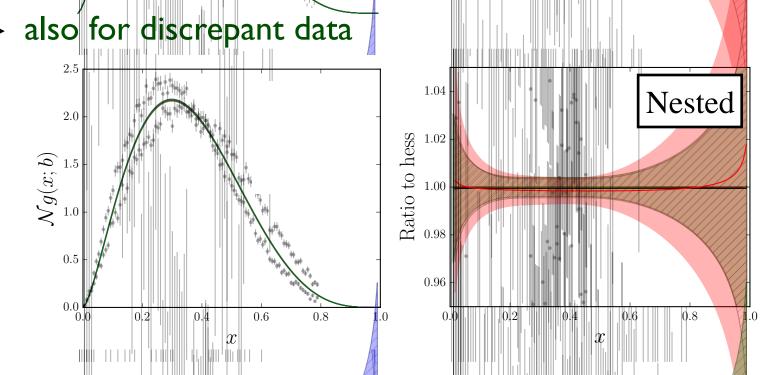
MC Error Analysis

- 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



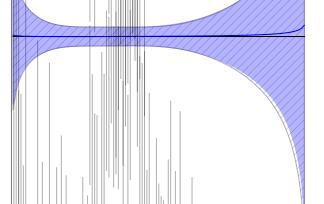
MC Error Analysis

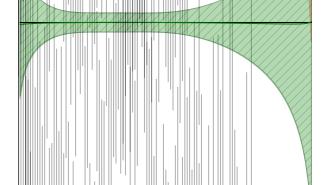
Assuming a single minimum, a Hessian or MC analysis must give same results, if using same likelihood function



almost identical uncertainty bands for Hessian and for MC!

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MC Error Analysis

- Assuming a single minimum, a Hessian or MC analysis *must* give same results, if using same likelihood function
- Approaches that use Hessian + tolerance factor not consistent with Gaussian likelihood function
- 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
 → how can this be?
- Assuming sufficient observables to determine PDFs, then PDF uncertainties cannot depend on parametrization!

Non-Gaussian likelihood

Incompatible data sets

- Rigorous (Bayesian) way to address incompatible data sets is to use generalization of Gaussian likelihood
 - joint vs. disjoint distributions
 - empirical Bayes
 - hierarchical Bayes
 - 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

 $\mathcal{L}(m_1m_2|m;\delta m_1\delta m_2) = \mathcal{L}(m_1|m;\delta m_1) \times \mathcal{L}(m_2|m;\delta m_2)$

use instead sum ("or") of individual likelihoods

$$\mathcal{L}(m_1m_2|m;\delta m_1\delta m_2) = \frac{1}{2} \Big[\mathcal{L}(m_1|m;\delta m_1) + \mathcal{L}(m_2|m;\delta m_2) \Big]$$

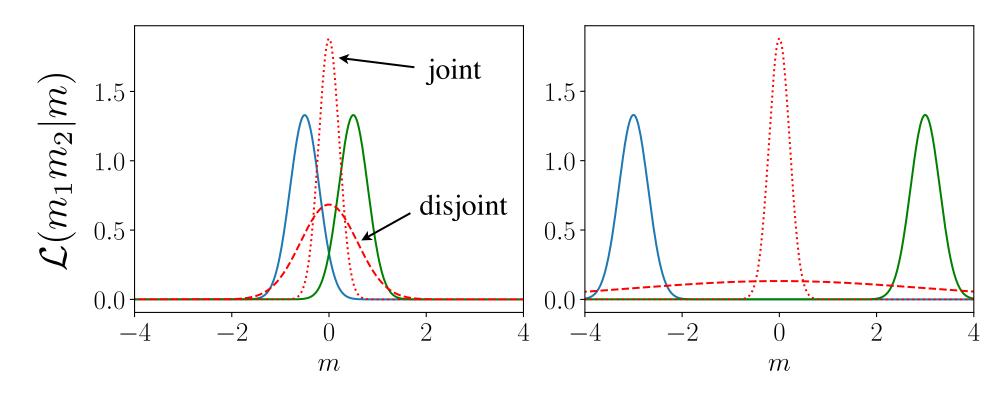
 \rightarrow gives rather different expectation value and variance

$$E[m] = \frac{1}{2}(m_1 + m_2)$$

$$V[m] = \frac{1}{2}(\delta m_1^2 + \delta m_2^2) + \left(\frac{m_1 - m_2}{2}\right)^2$$
depends on separation!

Disjoint distributions

Symmetric uncertainties $\delta m_1 = \delta m_2$

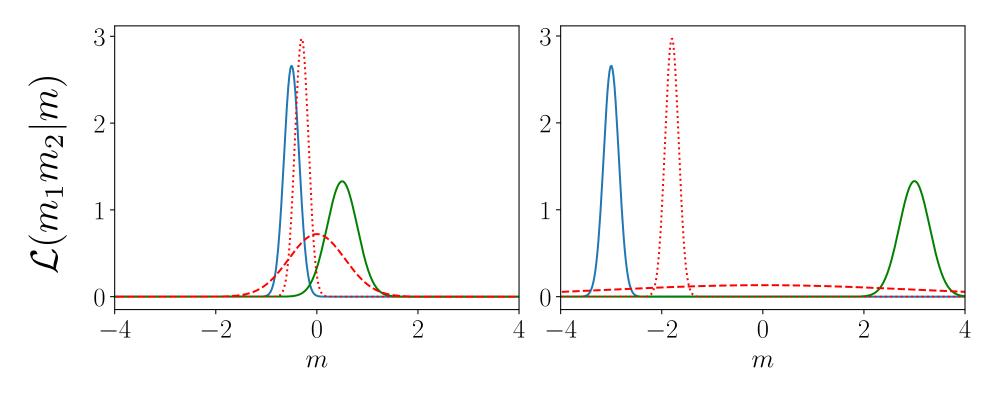


disjoint:
$$V[m] = \frac{1}{2}(\delta m_1^2 + \delta m_2^2) + \left(\frac{m_1 - m_2}{2}\right)^2$$

joint: $V[m] = \frac{\delta m_1^2 \ \delta m_2^2}{\delta m_1^2 + \delta m_2^2}$

Disjoint distributions

Asymmetric uncertainties $\delta m_1 \neq \delta m_2$



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

Empirical Bayes

- Shortcoming of conventional Bayesian still <u>assume</u> 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 <u>distortion parameters</u>, whose probability distributions given in terms of "hyperparameters" (or "nuisance parameters")
- Hyperparameters determined from data
 \rightarrow give posteriors for both PDF and hyperparameters

Empirical Bayes

■ Standard mean and variance that characterize data

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

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

Simple choice is

 $(\mu, \sigma) \rightarrow (\zeta_1 \,\mu + \zeta_2, \,\zeta_3 \,\sigma)$

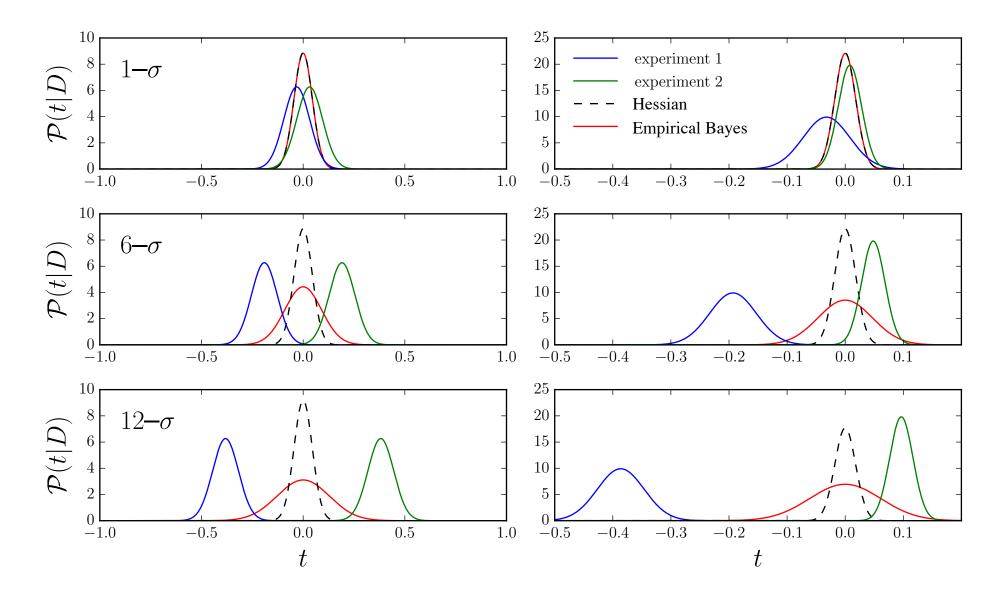
where $\zeta_{1,2,3}$ are distortion parameters, with prob. dists. described by hyperparameters $\phi_{1,2,3}$

Likelihood function is then

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

Empirical Bayes

■ Simple example of EB for symmetric & asymmetric errors



Outlook

New paradigm needed in global QCD analysis

- <u>simultaneous</u> determination of collinear distributions
 (also TMDs) using <u>Monte Carlo</u> sampling of parameter space
- Treatment of <u>discrepant data sets</u> 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