Cake Seminar
Jefferson Lab, April 4, 2018

PDF uncertainties.
What is the meaning of this?

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Jefferson Lab

Outline

- Why are PDF uncertainties important to know?

- Why the need for a new global QCD analysis paradigm?
  - $\longrightarrow$ Bayesian approach to fitting
  - $\longrightarrow$ single-fit (Hessian) vs. Monte Carlo approaches

- Incompatible data sets
  - $\longrightarrow$ "tolerance" factors

- Generalization to non-Gaussian likelihoods
  - $\longrightarrow$ disjoint probabilities, empirical Bayes, …

- Outlook

Why are PDF uncertainties important?

- In searches for new physics beyond the Standard Model a major source of uncertainty on limits/discoveries is from calculation of QCD backgrounds $\longrightarrow$ PDF errors!

"The PDF and α_S uncertainties were calculated using the PDF4LHC prescription [39] with the MSTW2008 68% CL NNLO [40, 41], CT10 NNLO [42, 43], and NNPDF2.3 5f FFN [44] PDF sets, and added in quadrature to the scale uncertainty."

Measurements of the charge asymmetry in top-quark pair production in the dilepton final state at $\sqrt{s}$ = 8 TeV with the ATLAS detector PRD **94**, 032006 (2016)

$\longrightarrow$ drives a large part of the global PDF community (esp. LHC)

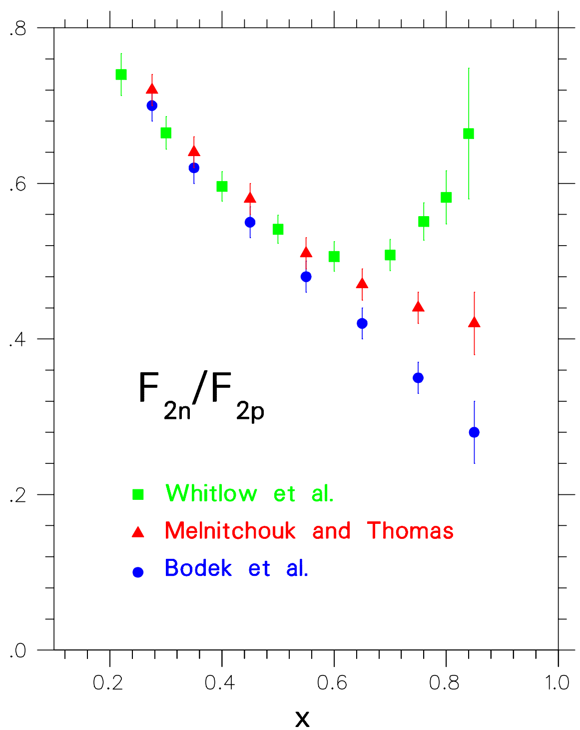
- Limits understanding of nucleon structure

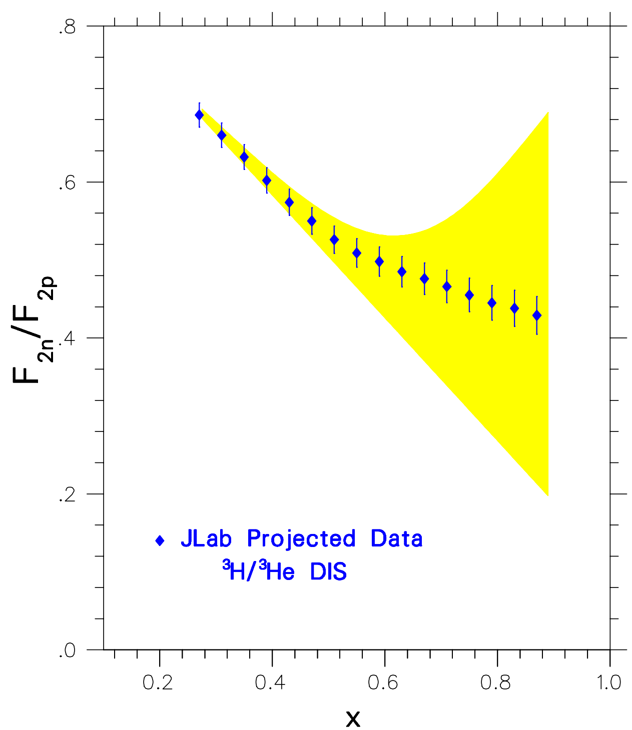
$\longrightarrow$ *e.g.* momentum and spin distributions of d quarks at large x

$\longrightarrow$ motivation for several JLab12 experiments (MARATHON, BONuS, SoLID, …)

d/u ratio at large x

- Traditionally extracted from neutron / proton structure function ratio (where "neutron" ~ deuteron − proton), but large nuclear uncertainties affect high-x region



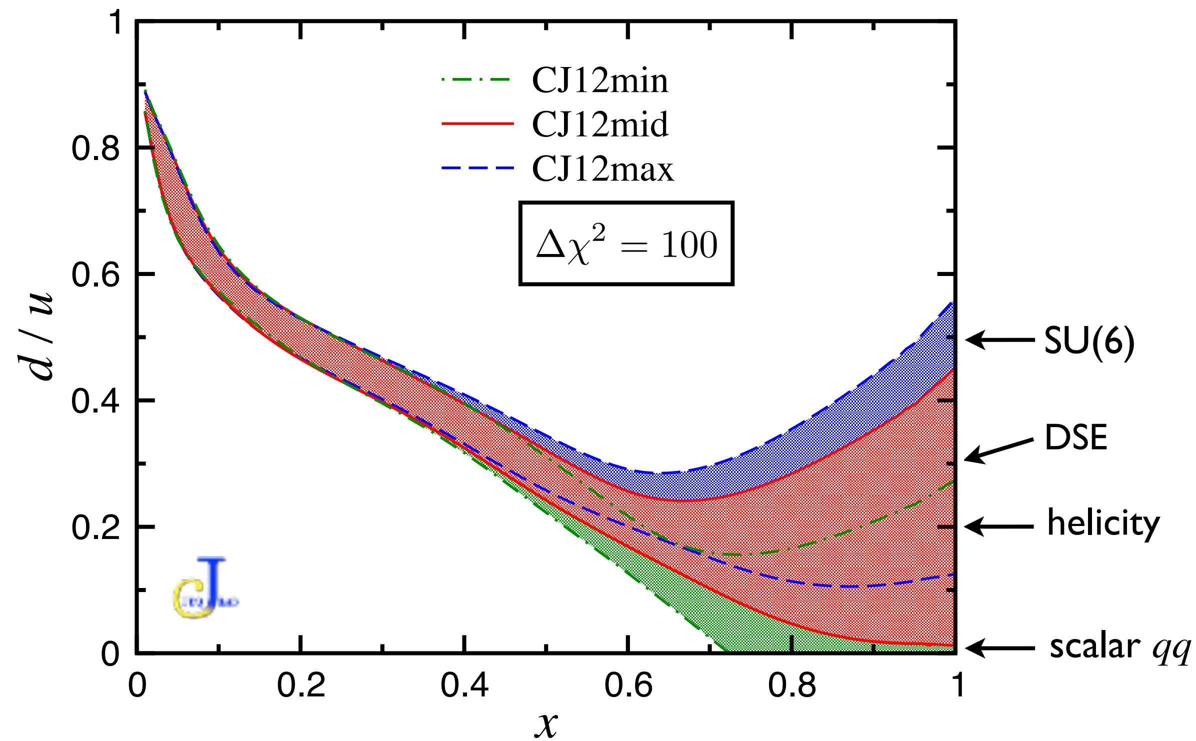


MARATHON Collaboration
Petratos, Katramatou, Gomez et al.

d/u ratio at large x

- Traditionally extracted from neutron / proton structure function ratio (where "neutron" ~ deuteron − proton), but large nuclear uncertainties affect high-x region

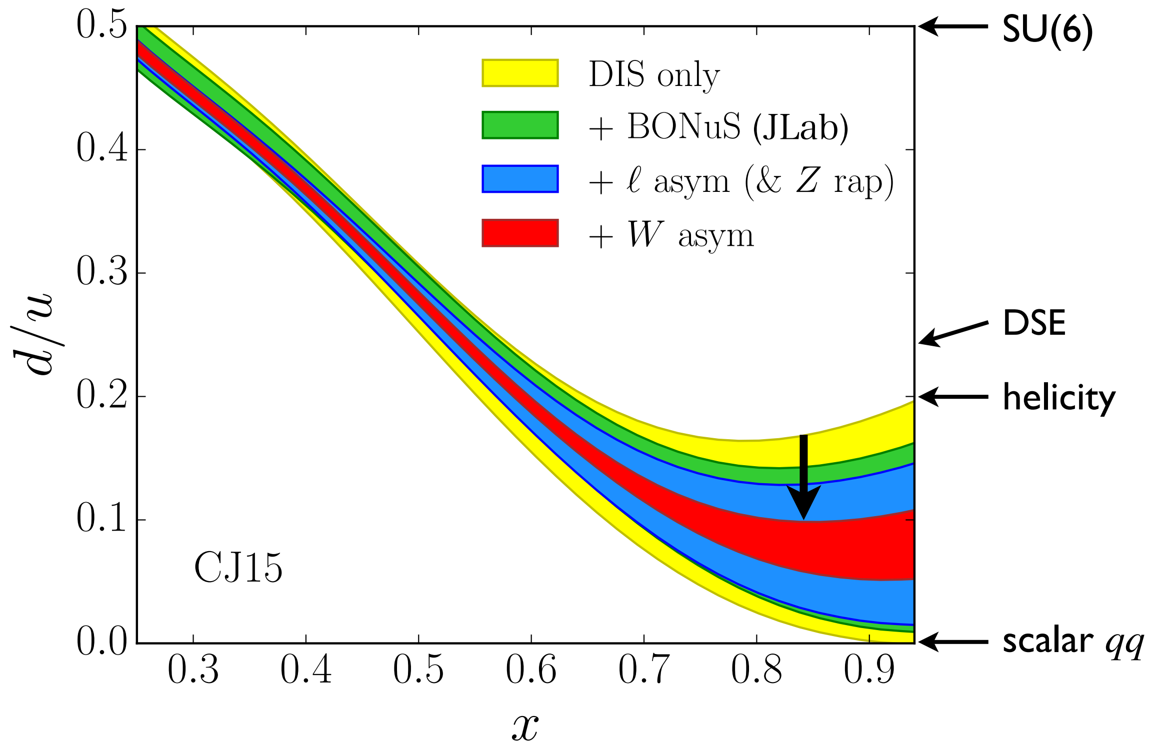
→ cannot discriminate between predictions for d/u at $x \sim 1$

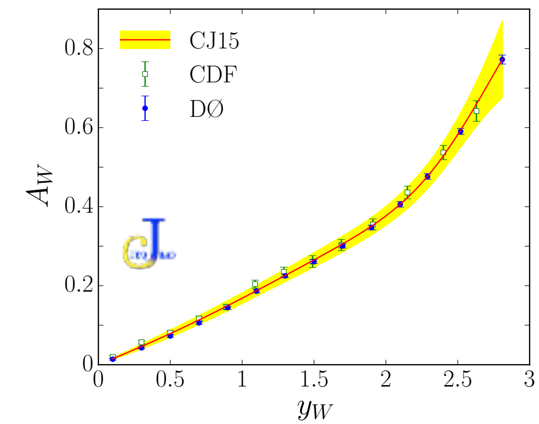


Owens, Accardi, WM (2013)

d/u ratio at large x

- More recently CJ15 analysis found significant reduction of PDF errors with inclusion of DØ W-asymmetry & BONuS data





Accardi, Brady, WM, Owens, Sato (2016)

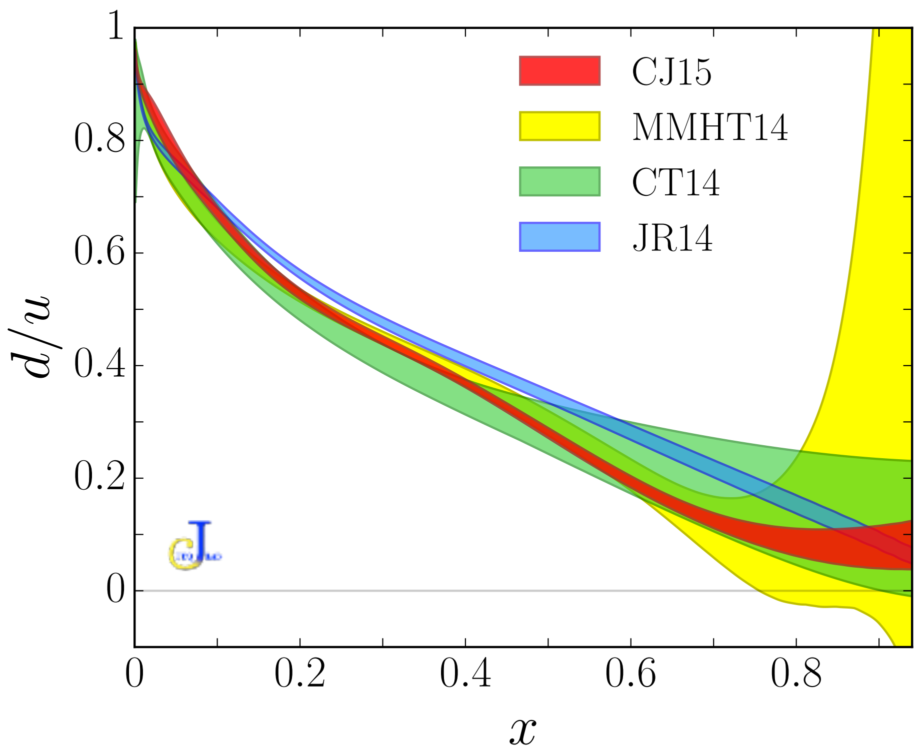
→ extrapolated ratio at $x = 1$: $d/u \rightarrow 0.09 \pm 0.03$

→ **note**: errors are 90% CL ($\Delta\chi^2 = 2.7$)

d/u ratio at large x

- Different groups use different definitions of PDF uncertainties to take into account *tensions* between data sets

$\longrightarrow$ multiply uncertainties by "tolerance" factor $T = \sqrt{\Delta\chi^2}$



$\longrightarrow$ CJ15: $\Delta\chi^2 = 2.7$

$\longrightarrow$ MMHT: $\Delta\chi^2 \approx 25 - 100$

$\longrightarrow$ CT14: $\Delta\chi^2 \approx 100$

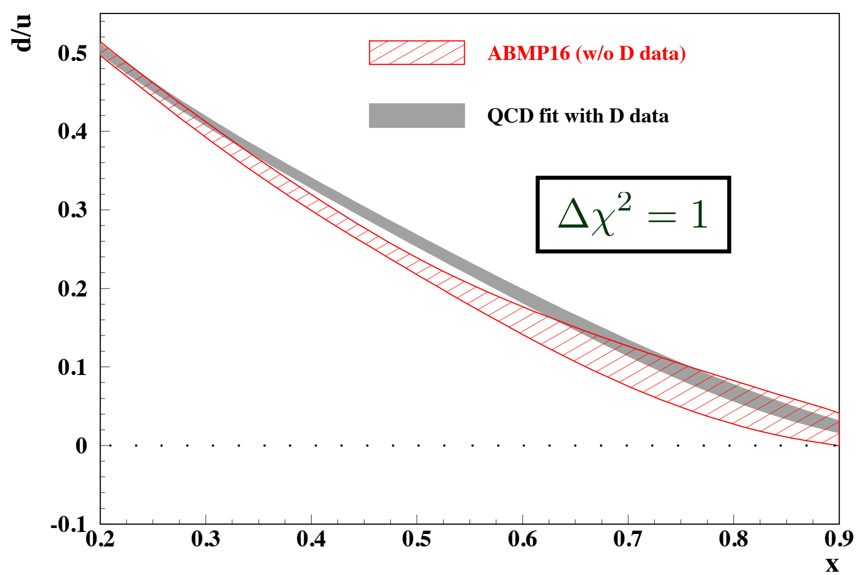
$\longrightarrow$ JR14: $\Delta\chi^2 = 1$

… is this a meaningful comparison?

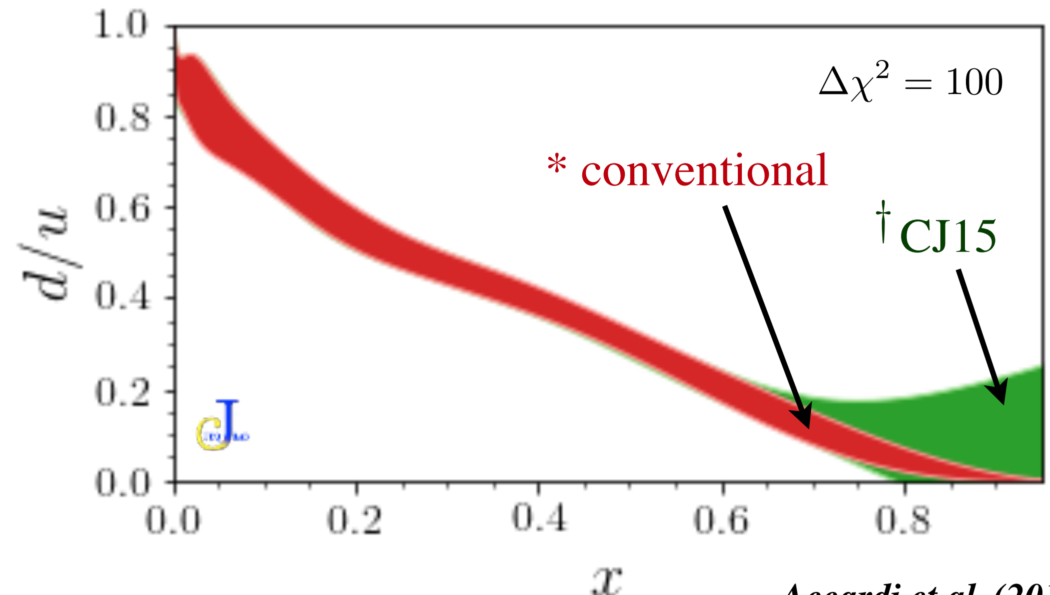
d/u ratio at large x

- Dependence on PDF parametrization

→ recent analysis by AKP has tiny uncertainties, and $d/u \to 0$, which we (CJ) believe is simply parametrization bias!



Alekhin, Kulagin, Petti (2017)



Accardi et al. (2017)

* same functional form for u & d $\sim (1-x)^\beta$

† more flexible form $d \to d + a\,x^b\,u$

… is there a more robust analysis?

Need for new technology

- 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)

  → "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 χ^2 minimization paradigm

  → utilize modern techniques based on Bayesian statistics!

Need for new technology

- In the near future, standard χ^2 minimization techniques will be unsuitable — even in the absence of tensions — $e.g.$ for

  $\longrightarrow$ simultaneous analysis of collinear distributions (unpolarized $\&$ polarized PDFs, fragmentation functions)

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

Need for new technology

- 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, …

$\longrightarrow$ 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

Bayesian approach to fitting

Nobuo Sato

main instigator

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 $\vec{a}$

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

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

"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 $\mathcal{L}$

Bayesian approach to fitting

- 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

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

⟶ 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
(χ^2 minimization)

Monte Carlo

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood
(χ^2 minimization)

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

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

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

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

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood
(χ^2 minimization)

⟶ 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

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

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood

(χ^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

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

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

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood
(χ^2 minimization)

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

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

where

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

note: in quadratic approximation for χ^2, this becomes a normal distribution

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

<u>Maximum Likelihood</u>
(χ^2 minimization)

$\longrightarrow$ 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

$$V[\mathcal{O}] = \sum_k (\Delta\mathcal{O}_k)^2$$

Bayesian approach to fitting

- 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

→ Monte Carlo approach samples parameter space and assigns weights w_k to each set of parameters a_k

→ expectation value and variance are then weighted averages

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

Bayesian approach to fitting

- Two methods generally used for computing Bayesian master formulas:

Maximum Likelihood
(χ^2 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

N. Sato, M. Albright, WM, H. Prosper, M. White (2017)

A. Accardi, E. Nocera, N. Sato, WM (2018)

Incompatible data sets

- Incompatible data sets can arise because of errors in determining central values, or underestimation of systematic experimental uncertainties

  $\longrightarrow$ requires some sort of modification to standard statistics

- Modify the master formula by introducing a "tolerance" factor T

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

$e.g.$ for one dimension

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

$\longrightarrow$ effectively modifies the likelihood function

Incompatible data sets

- Simple example: consider observable m, and two measurements

$$(m_1, \delta m_1), \quad (m_2, \delta m_2)$$

$\longrightarrow$ 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

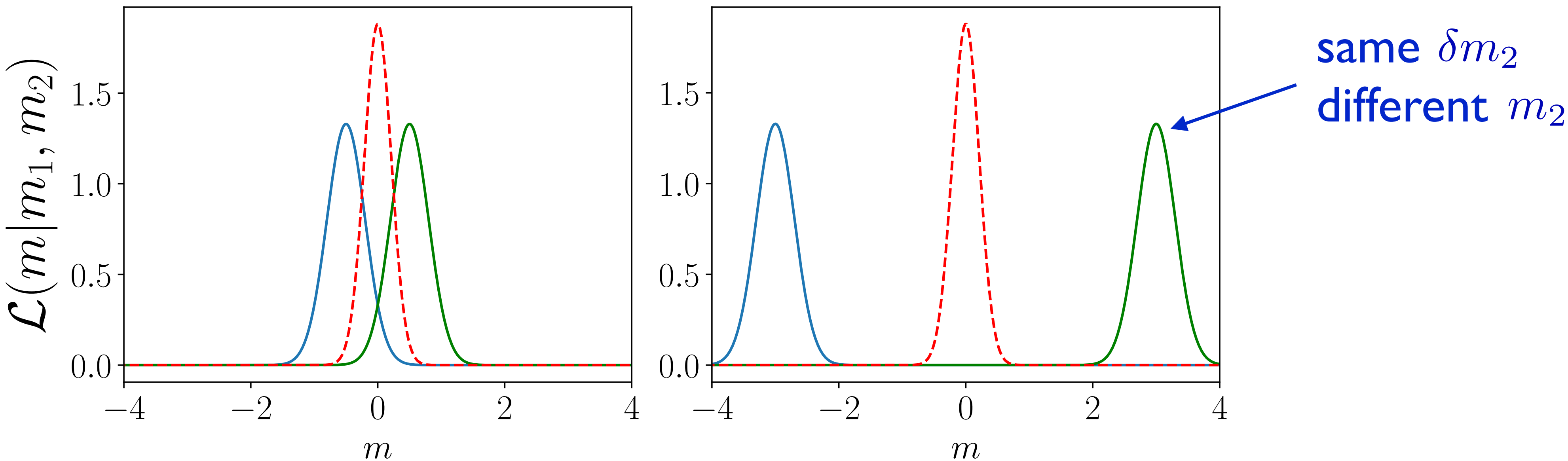
$$V[m] = H^{-1} = \frac{\delta m_1^2 \, \delta m_2^2}{\delta m_1^2 + \delta m_2^2}$$

does not depend on $m_1 - m_2$!

Incompatible data sets

- Simple example: consider observable m, and two measurements

$$(m_1, \delta m_1), \quad (m_2, \delta m_2)$$

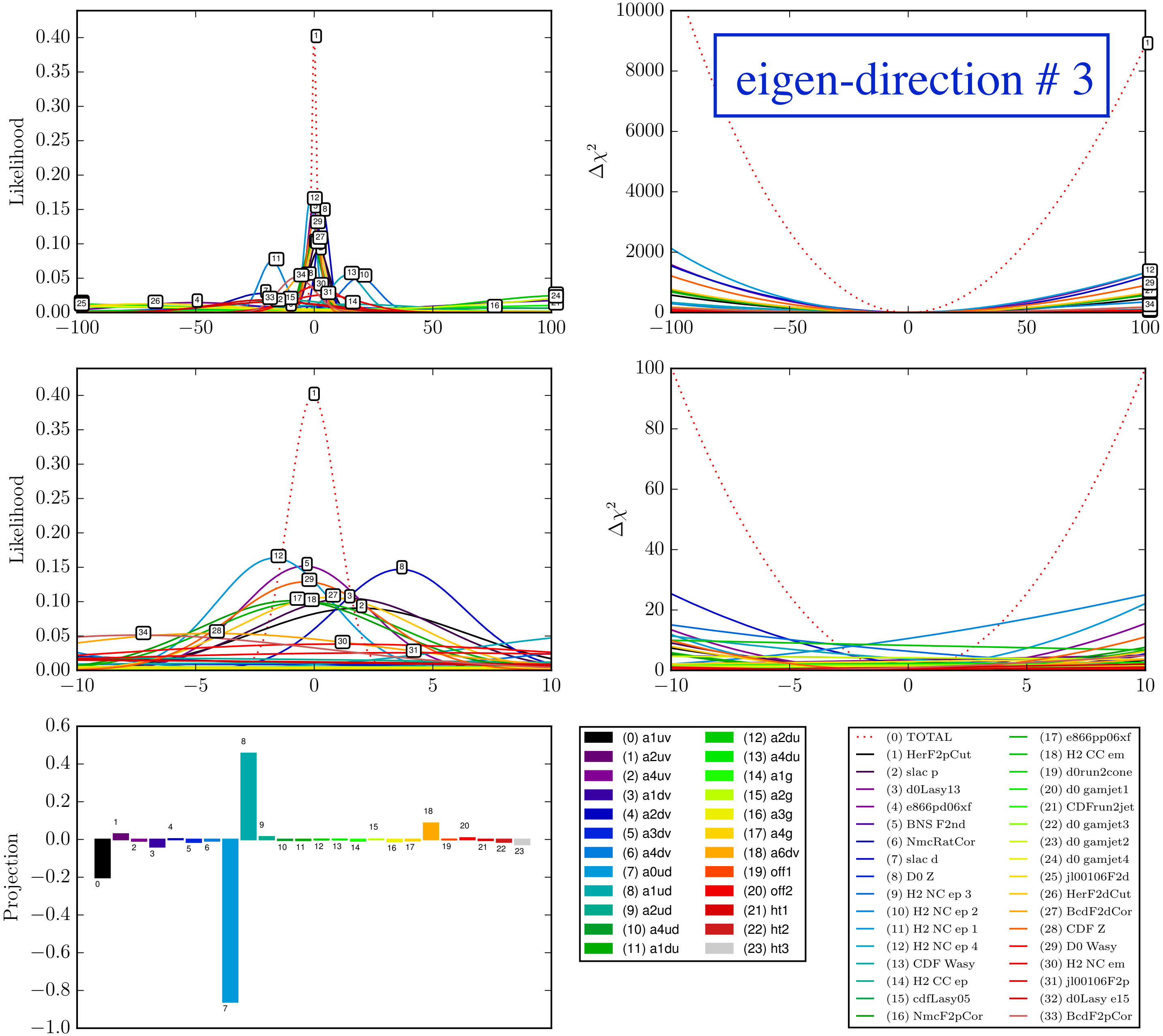


⟶ total uncertainty remains independent of degree of (in)compatibility of data

⟶ Gaussian likelihood gives unrealistic representation of true uncertainty

Incompatible data sets

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



→ 24 parameters, 33 data sets

→ data sets compatible along this e-direction

Incompatible data sets

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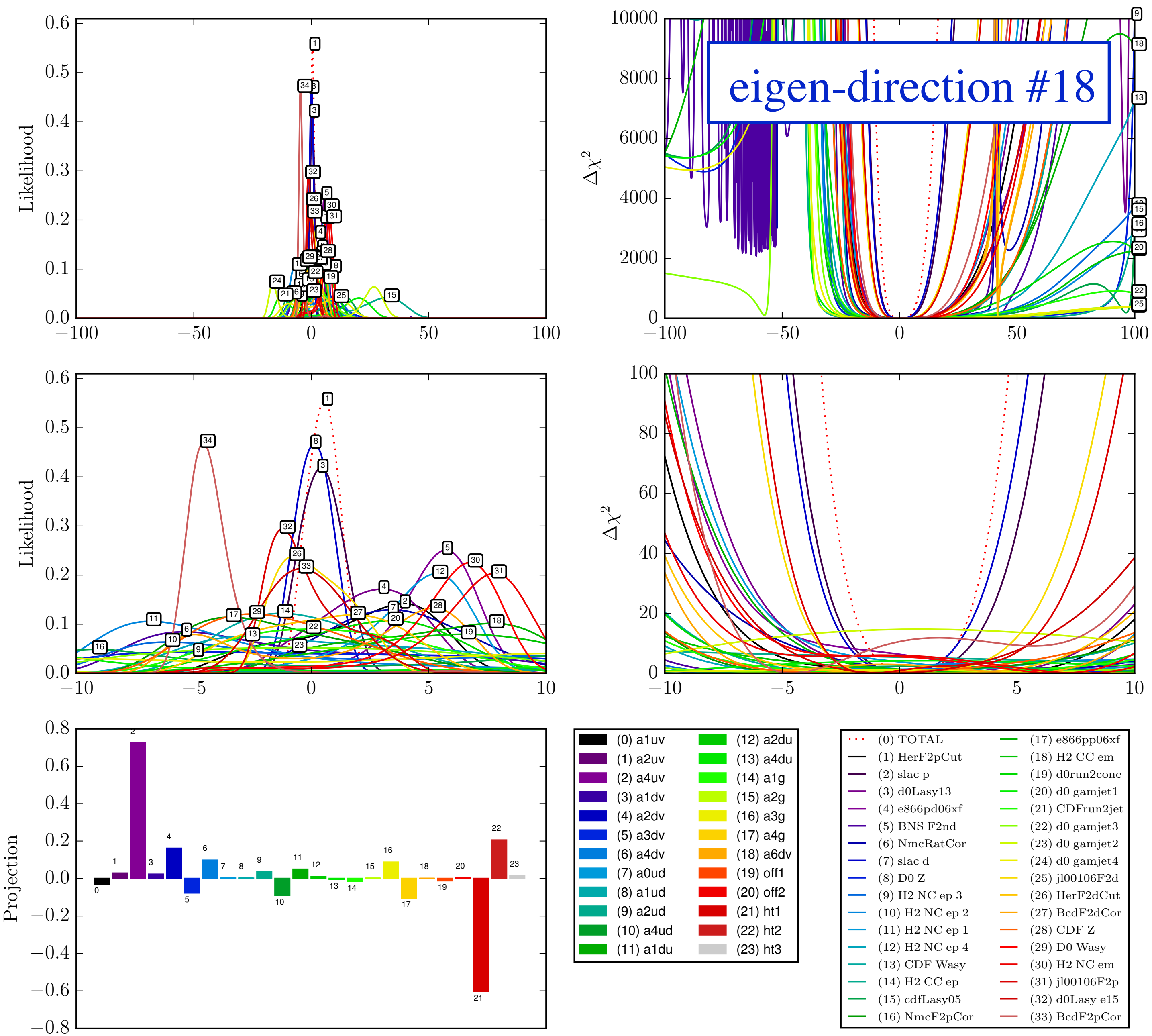

→ 24 parameters, 33 data sets

→ data sets not compatible along this e-direction

Incompatible data sets

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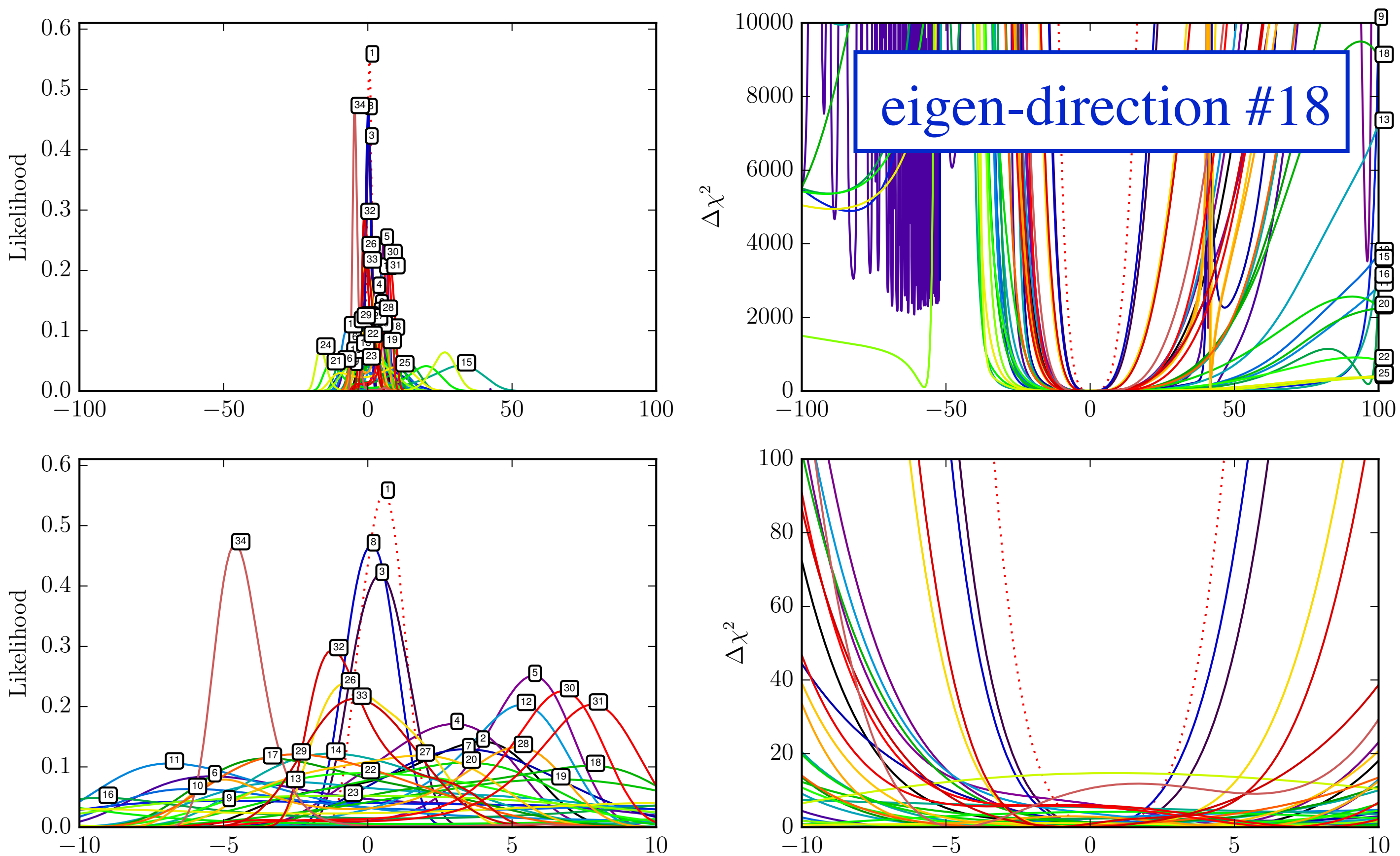


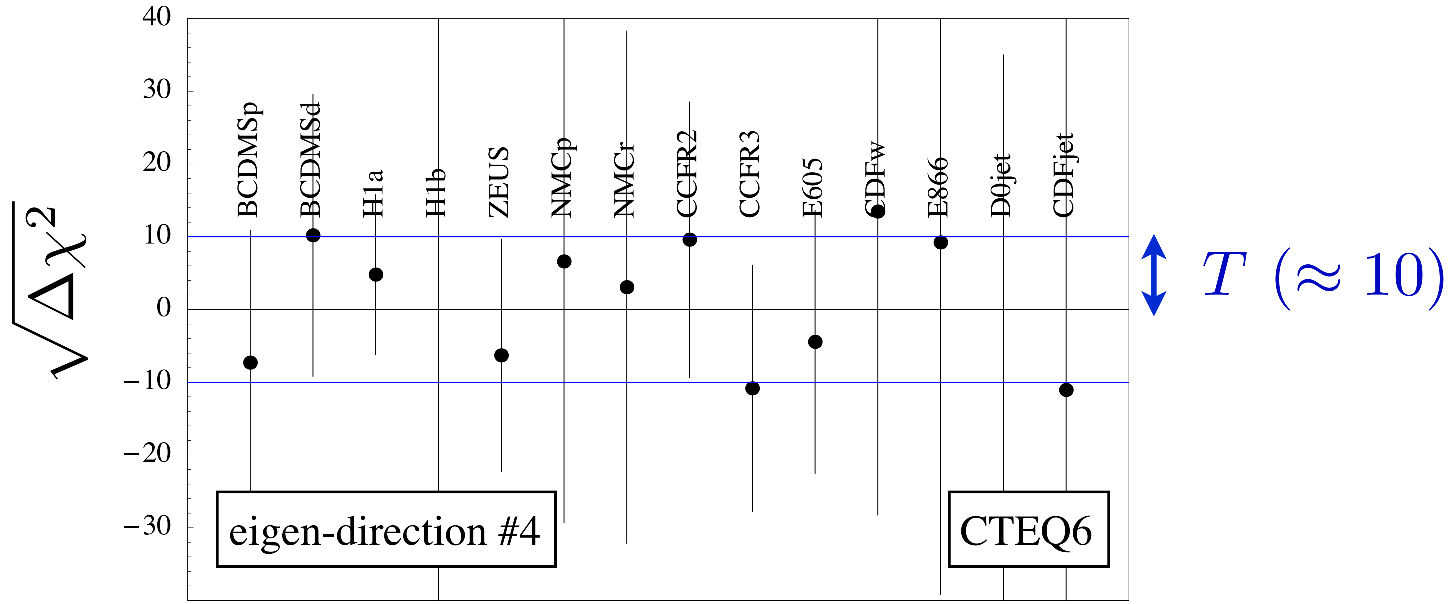
→ 24 parameters, 33 data sets

→ data sets <u>not</u> compatible along this e-direction

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

Incompatible data sets

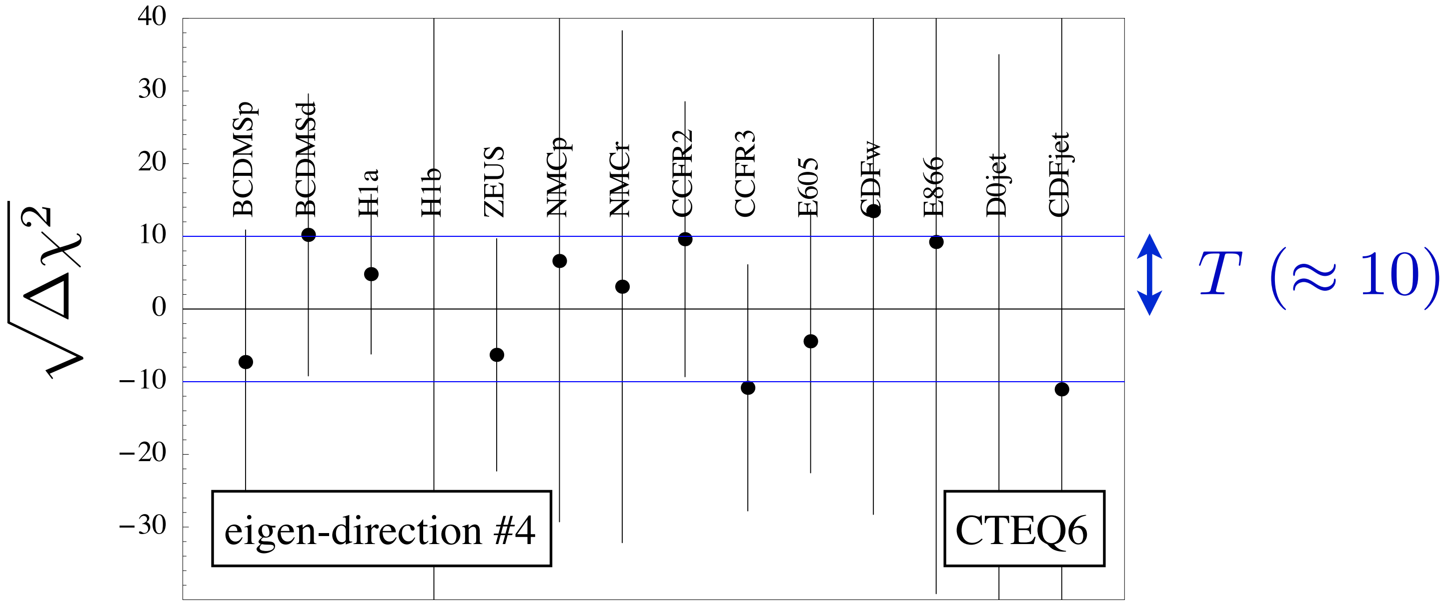
CTEQ tolerance criteria



- 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 $T \sim 5 - 10$)

Incompatible data sets

- CTEQ tolerance criteria



- This approach is *not consistent* with Gaussian likelihood

  $\longrightarrow$ no clear Bayesian interpretation of uncertainties (ultimately, a prescription…)

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)

  ⟶ introduces bias, does not guarantee that flat χ^2 globally

- Cannot guarantee solution is unique

- Error propagation characterized by quadratic χ^2 near minimum

  ⟶ no guarantee this is quadratic globally ($e.g.$ Student t-distribution?)

- Introduction of tolerance modifies Gaussian statistics

Monte Carlo methods

Monte Carlo

- Designed to faithfully compute Bayesian master formulas

- Do not assume a single minimum, include all possible solutions (with appropriate weightings)

- Do not assume likelihood is Gaussian in parameters

- Allows likelihood analysis to be extended to address tensions among data sets via Bayesian inference

- 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

Forte et al. (2002)

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

— α, β are fitted "preprocessing coefficients"

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

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

Gbedo, Mangin-Brinet (2017)

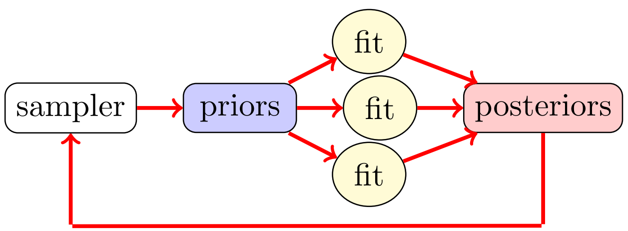
- Nested sampling (NS) — computes integrals in Bayesian master formulas (for $E,\ V,\ Z$) explicitly

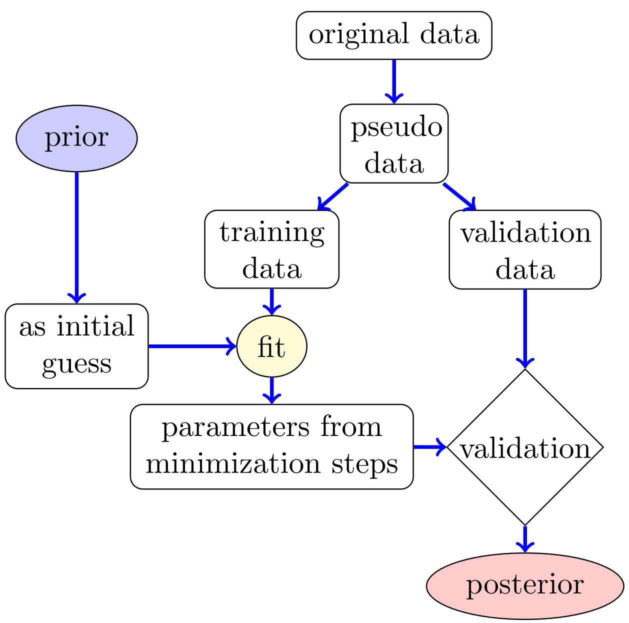
Skilling (2004)

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)





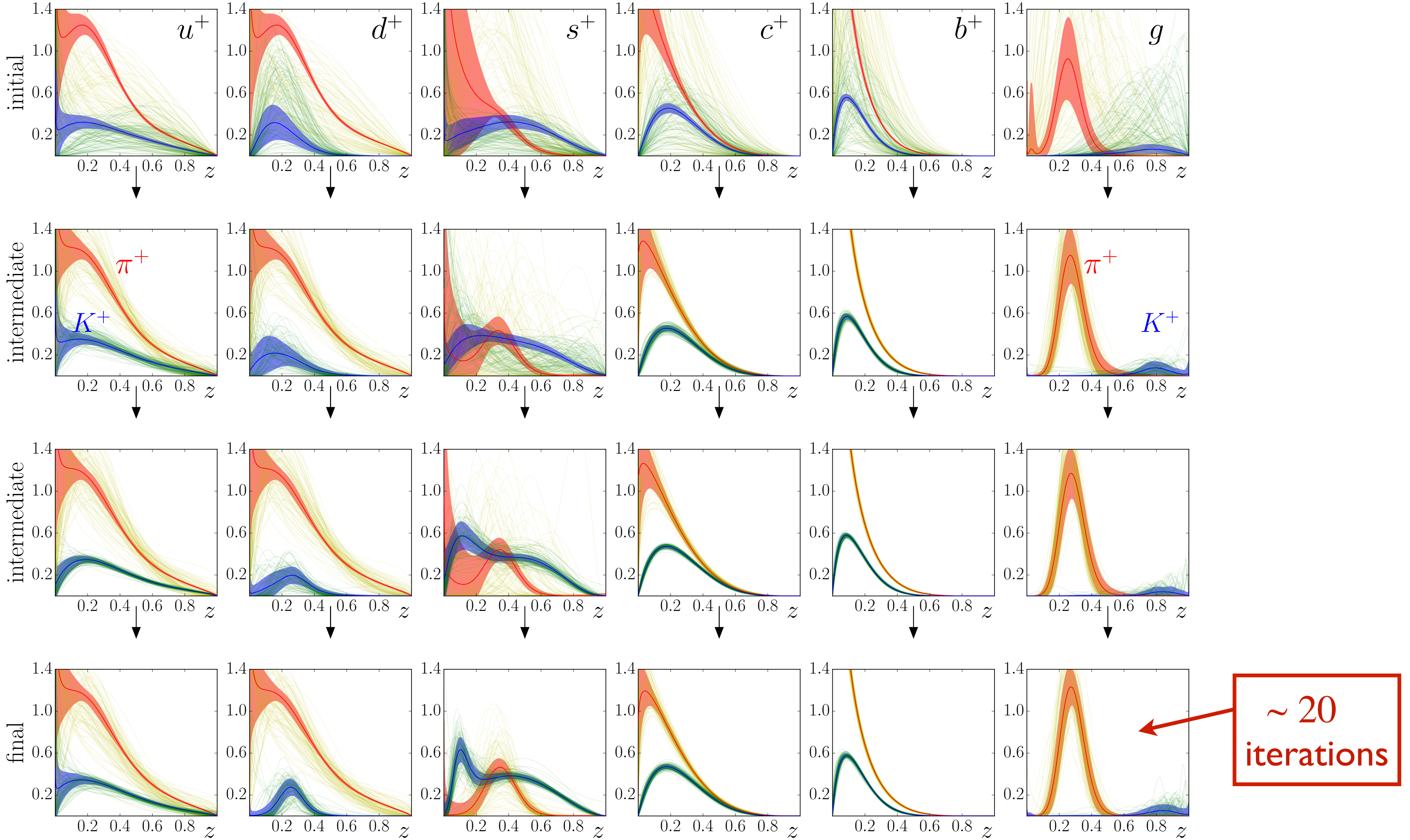
→ no assumptions for exponents

→ cross-validation to avoid overfitting

→ iterate until convergence criteria satisfied

Iterative Monte Carlo (IMC)

- *e.g.* of convergence (for fragmentation functions) in IMC



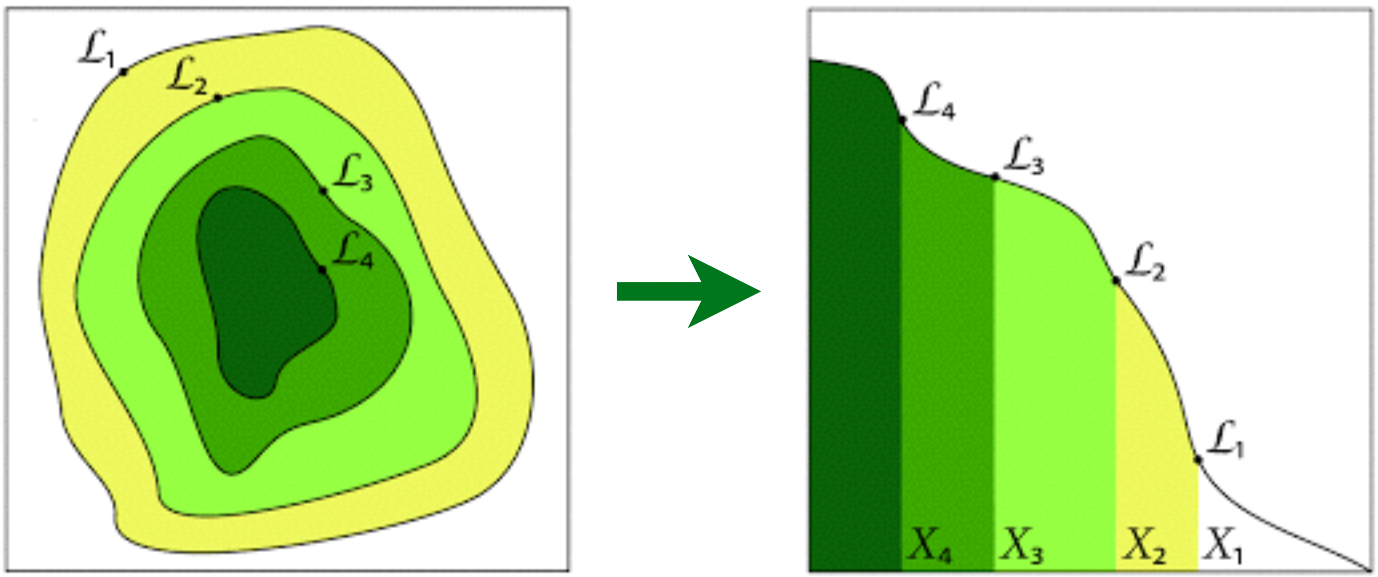
Sato, Ethier, WM, Hirai, Kumano, Accardi (2016)

Nested Sampling

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

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

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

$$Z \approx \sum_i \mathcal{L}_i \, w_i \qquad \text{with weights} \quad w_i = \frac{1}{2}(X_{i-1} - X_{i+1})$$

- Algorithm:

  → randomly select samples from full prior s.t. initial volume $X_0 = 1$

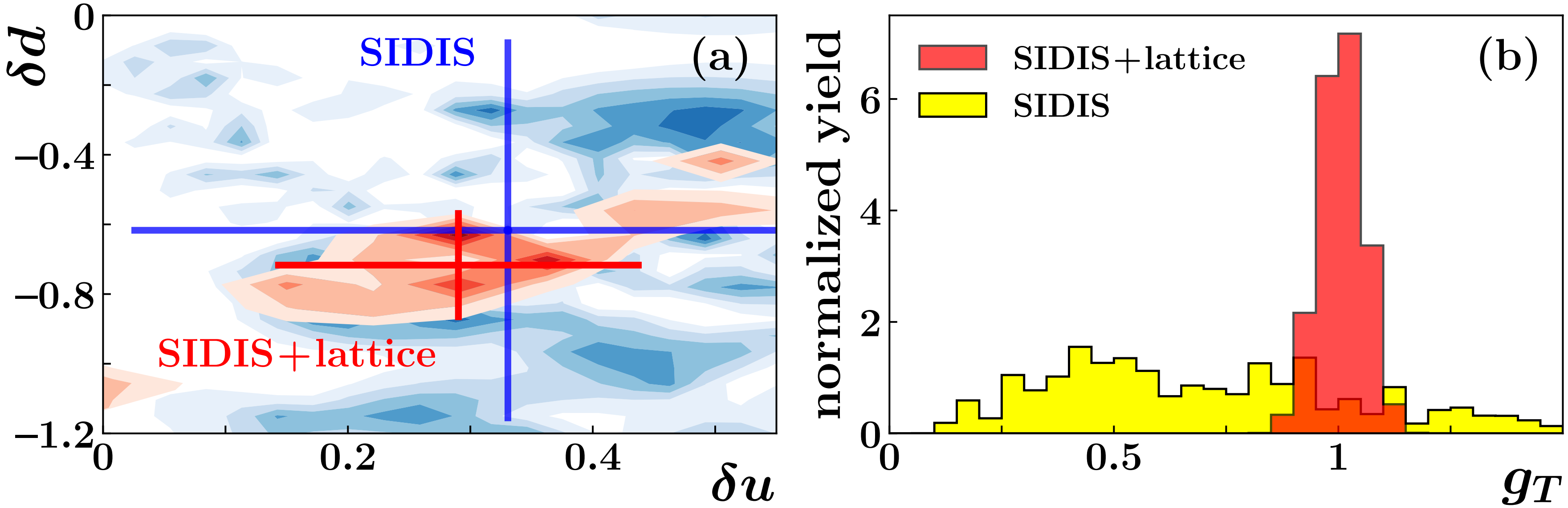
  → for each iteration, remove point with lowest $\mathcal{L}_i$, replacing it with point from prior with constraint that its $\mathcal{L} > \mathcal{L}_i$

  → 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
  (SIDIS data + lattice QCD constraint on isovector moment)



Lin, WM, Prokudin, Sato, Shows (PRL, 2018)

→ distributions do not look very Gaussian!

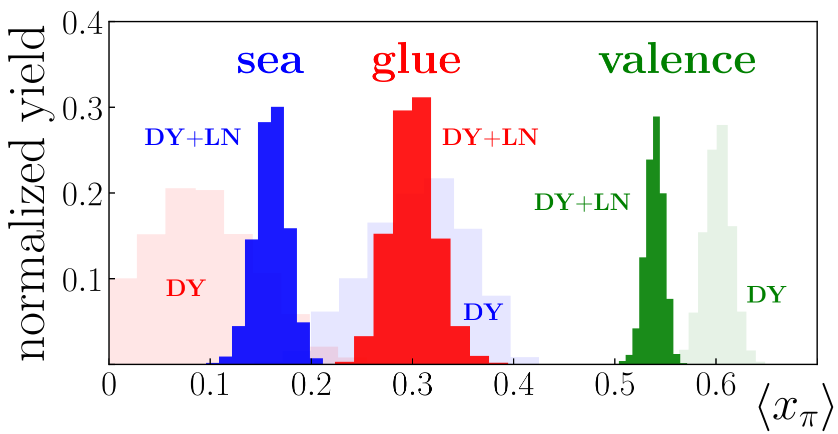
→ MC analysis gives $\delta u = 0.3 \pm 0.2,\ \delta d = -0.7 \pm 0.2$ → $g_T = 1.0 \pm 0.1$

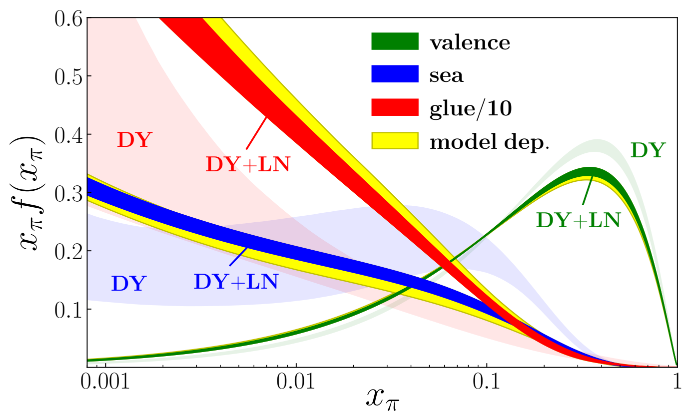
→ maximum likelihood analysis would have given $g_T \approx 0.5$

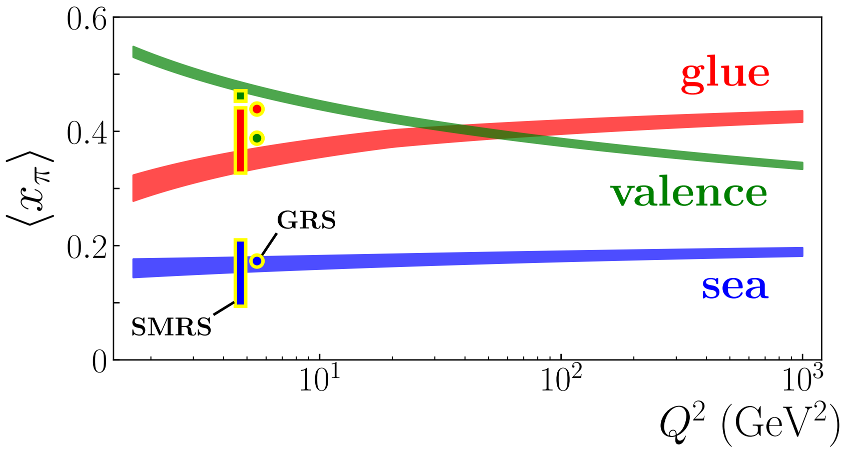
Nested Sampling

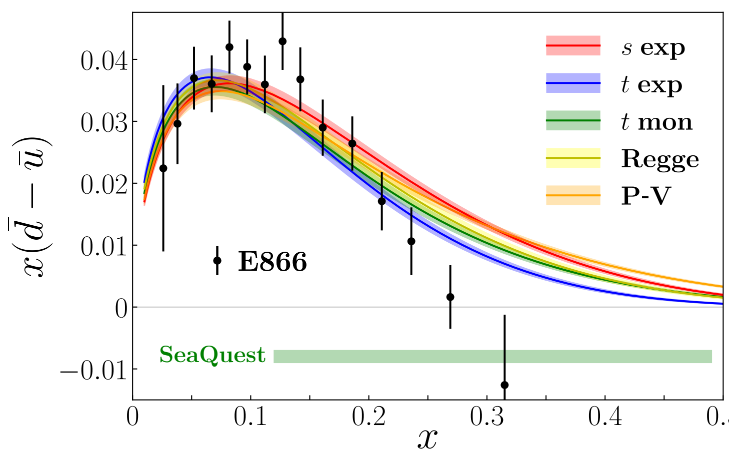
- **Most recently applied to global analysis of pion PDFs**

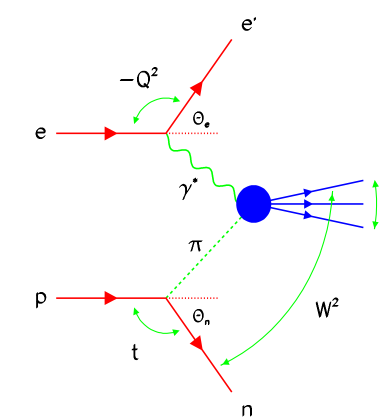
  (πA Drell-Yan data + leading neutron production at HERA)











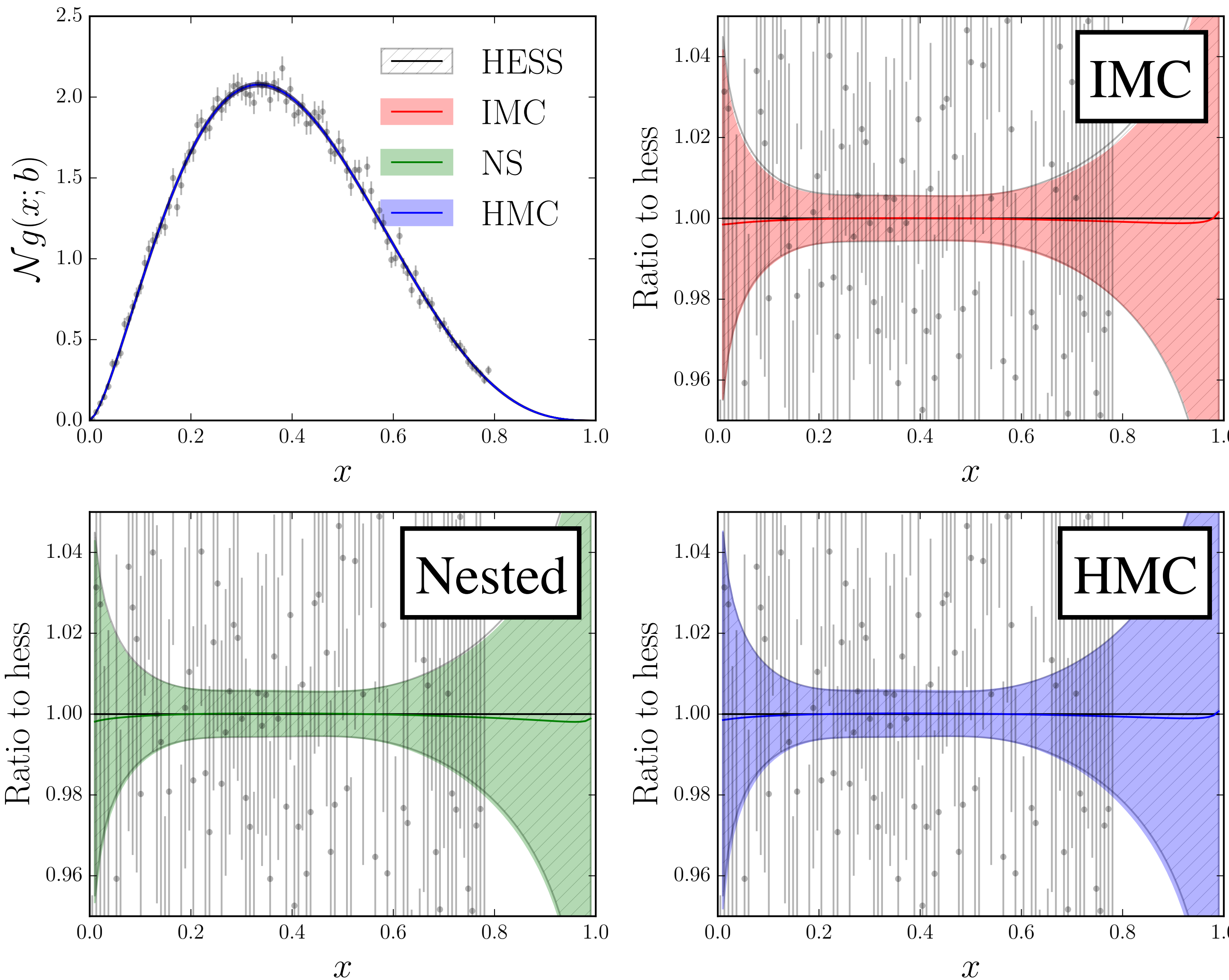
P. Barry, N. Sato, WM, C.-R. Ji (2018)

⟶ first constraints on sea quark PDFs in the pion

MC Error Analysis

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

→ analysis of pseudodata, generated using Gaussian distribution

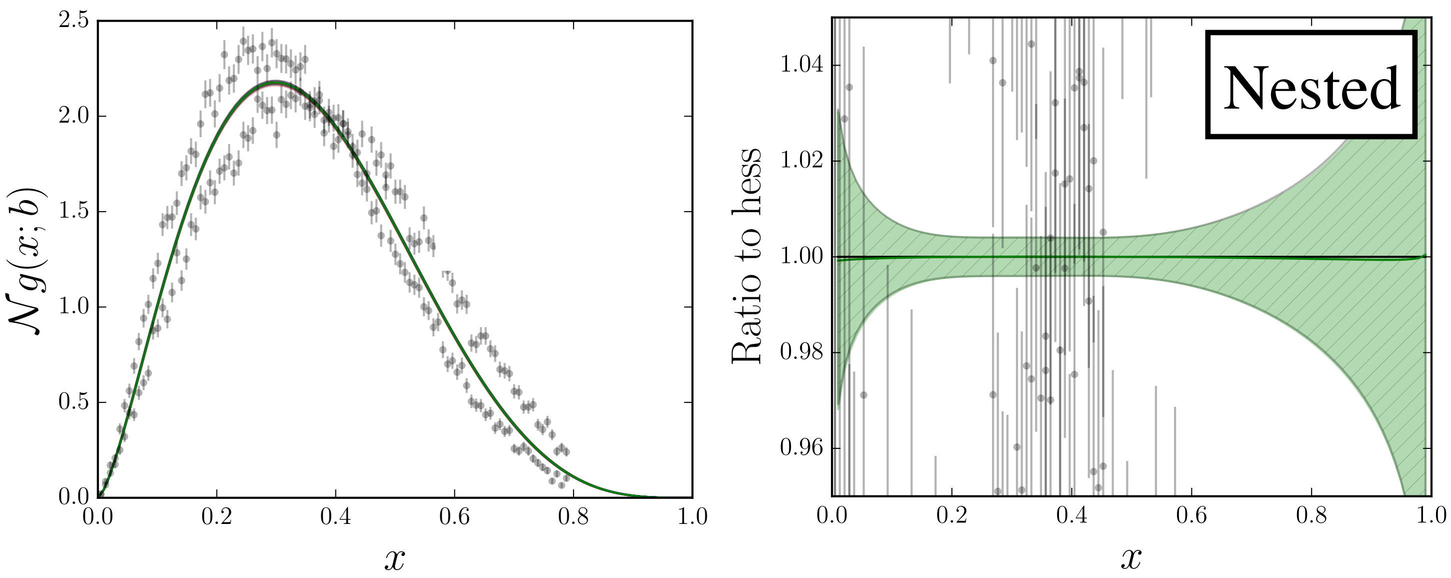


Sato et al. (2017)

MC Error Analysis

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

→ also for discrepant data



→ almost identical uncertainty bands for Hessian and for MC!

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

  $\longrightarrow$ how can this be? *E. Nocera, A. Accardi, N. Sato, WM, work in progress*

- 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 <u>product</u> ("and") of individual likelihoods, $e.g.$ for simple example of two measurements

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

use instead <u>sum</u> ("or") of individual likelihoods

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

→ gives rather different expectation value and variance

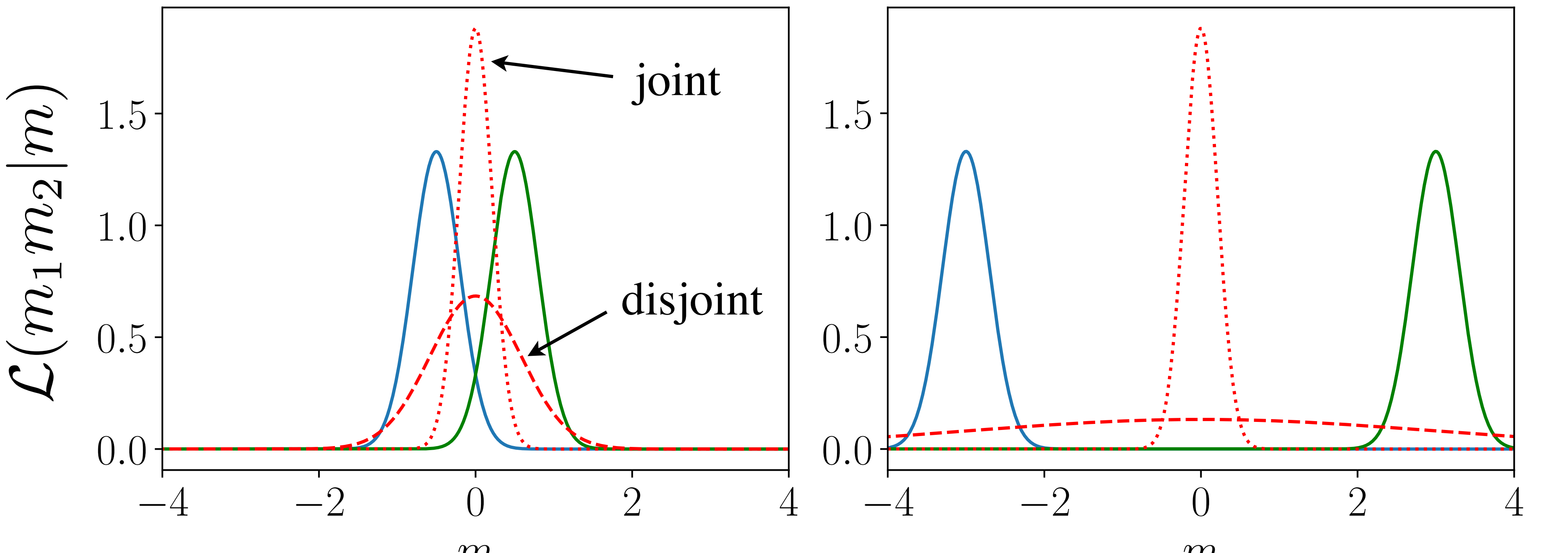
$$E[m] = \frac{1}{2}(m_1 + m_2)$$

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

depends on separation!

Disjoint distributions

- Symmetric uncertainties $\delta m_1 = \delta m_2$



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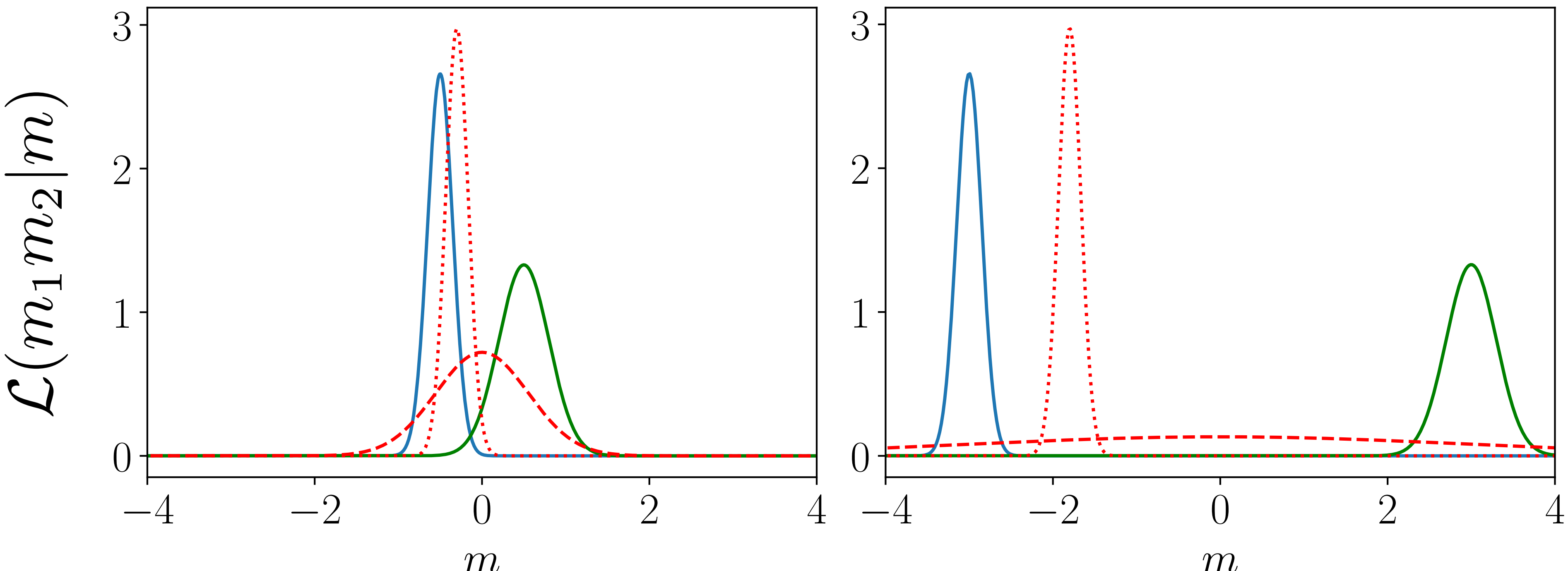
disjoint: $$V[m] = \frac{1}{2}(\delta m_1^2 + \delta m_2^2) + \left(\frac{m_1 - m_2}{2}\right)^2$$

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

Disjoint distributions

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



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→ 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")

- Hyperparameters determined from data
  $\longrightarrow$ 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

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

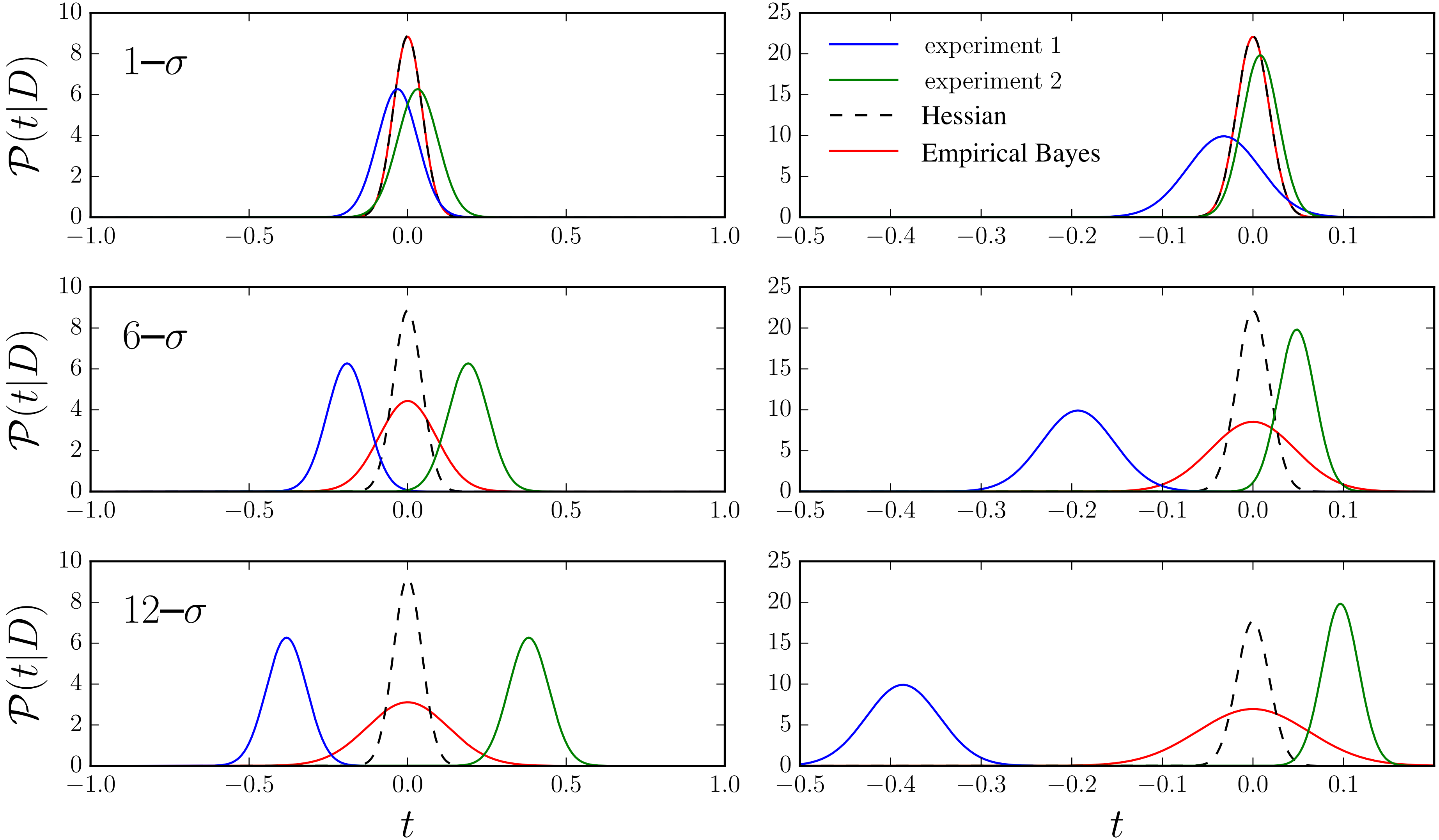
where $\zeta_{1,2,3}$ are distortion parameters, with prob. dists. described by hyperparameters $\phi_{1,2,3}$

- Likelihood function is then

$$\mathcal{L}(\mathrm{data}|\vec{a}, \zeta_{1,2,3}) \ \sim\ \exp\left[-\frac{1}{2}\sum_i \left(\frac{d_1 - f(\mu_i(\vec{a}, \zeta_{1,2}))}{g(\sigma, \zeta_3)}\right)^2\right] \pi_1(\zeta_1|\phi_1)\pi_2(\zeta_1|\phi_2)\pi_3(\zeta_1|\phi_3)$$

Empirical Bayes

- Simple example of EB for symmetric & asymmetric errors



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Outlook

- New approaches being developed for global QCD analysis
  — <u>simultaneous</u> determination of parton distributions using <u>Monte Carlo</u> sampling of parameter space

- Treatment of <u>discrepant data sets</u> needs serious attention
  — Bayesian perspective has clear merits

- 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


Nobuo


Jake


Alberto


Carlota

. . .


E = mc²