Bayesian constraint curve fitting for lattice QCD

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INT Bayesian Methods in Nuclear Physics

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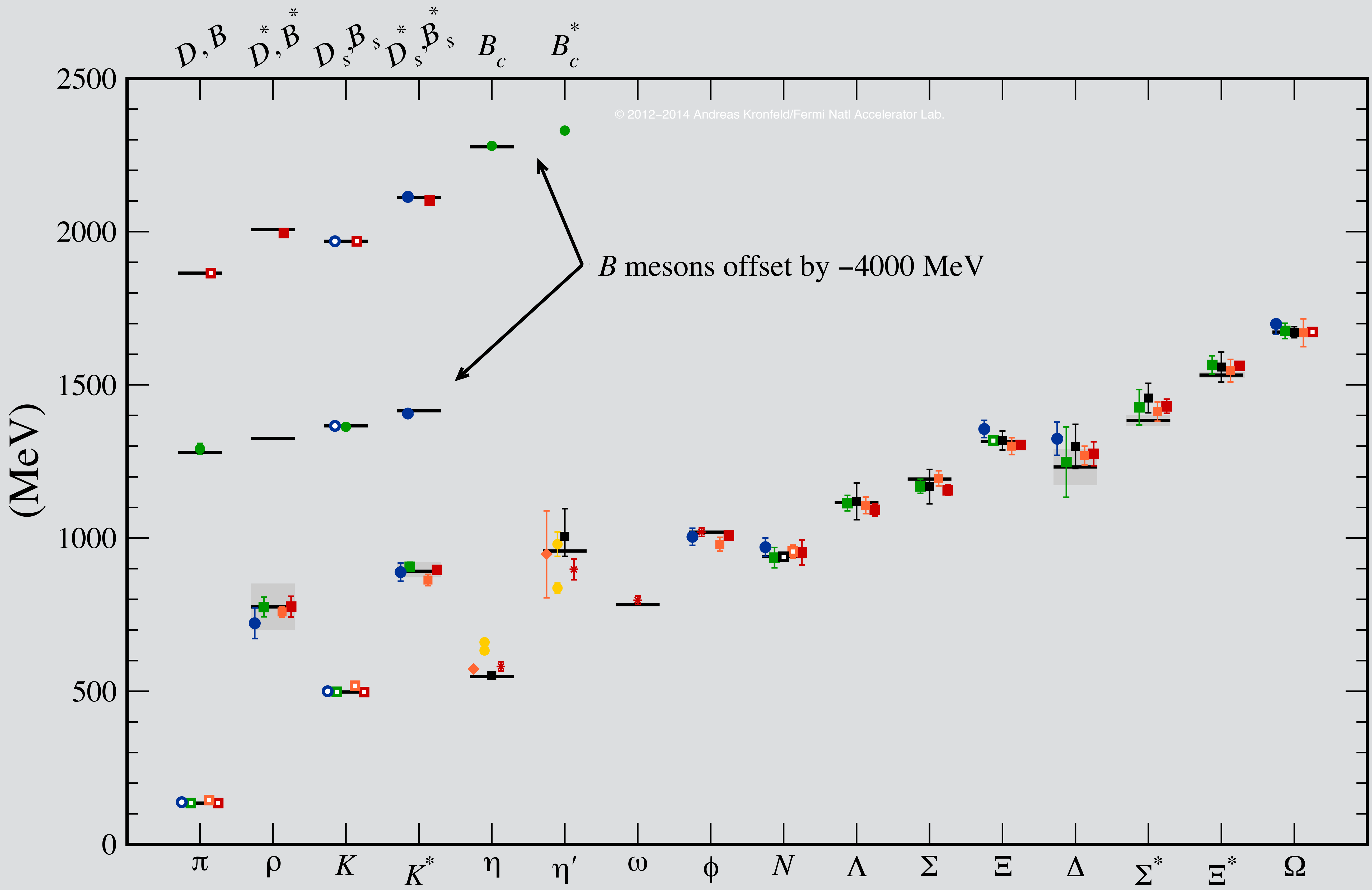
Outline

- What is Lattice QCD?
- Description of data and model
- Analysis strategy
- Examples

What is QCD?

Theory of quarks, gluons and their interactions

- Gives rise to rich emergent phenomena after fixing quark masses and strong coupling
- At low energies (~100 MeV) QCD is strongly interacting
- No small parameter @ strong coupling limit
- Need non-perturbative approach



updated version of the plot in [hep-lat/1203.1204]
very good summary of modern lattice QCD results

What is lattice QCD?

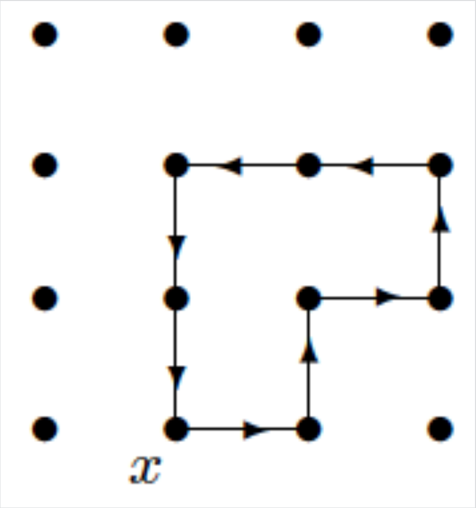
calculate observables from Feynman Path Integral

$$\langle\Omega|A|\Omega\rangle \propto \int dU\, A[U] e^{-S[U]}$$

reformulate as simple average

$$\langle\Omega|A|\Omega\rangle \simeq \frac{1}{N}\sum_{n=1}^{N} A(U_n) \quad \text{where} \quad U \sim e^{-S}$$

generate realizations of U_n from Monte Carlo

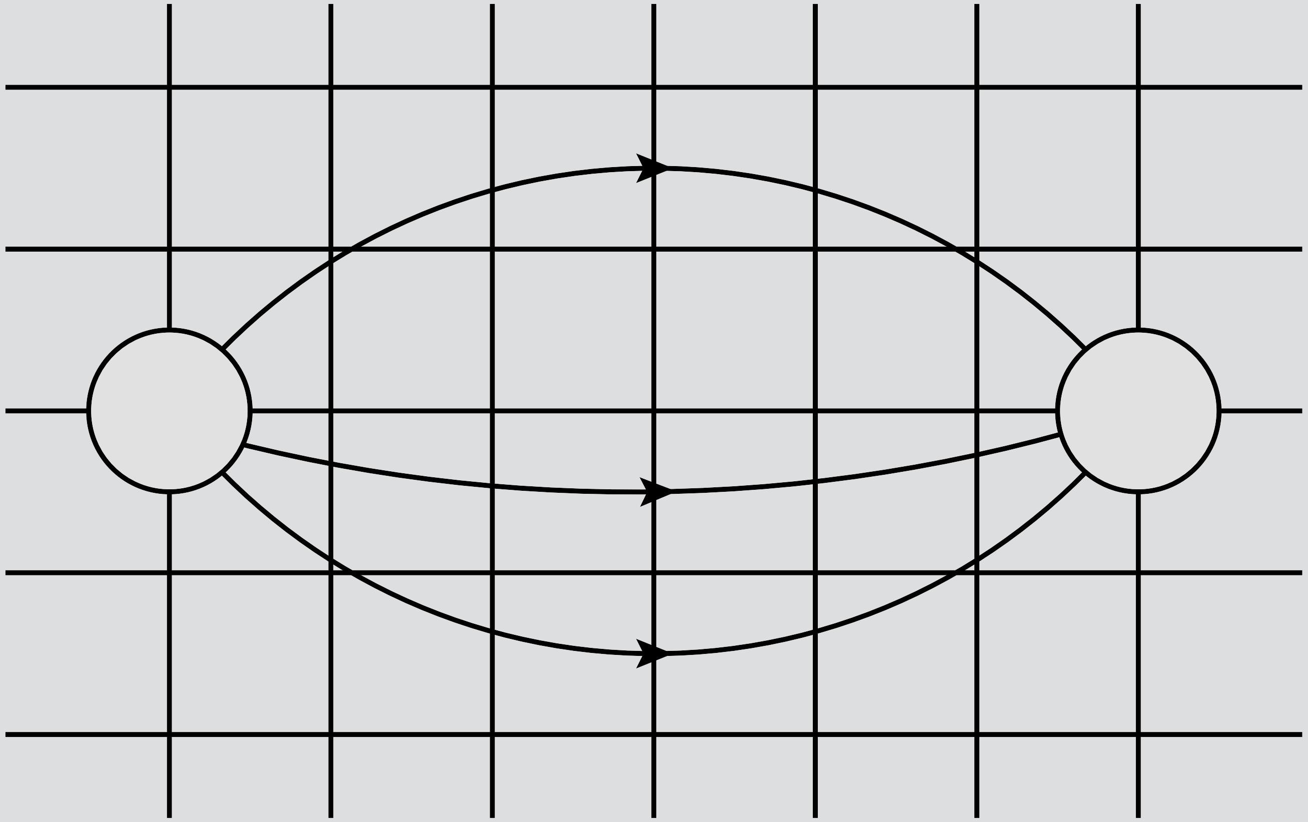


- valence quarks live on lattice sites
- sites are connected by links (gauge fields, parallel transport operators)
- observables are closed loops (gauge invar.)

[hep-lat/0506036] (very good introductory paper to lattice QCD)

data

Example of a proton propagating in time



t = 0
(source)

$$C_t = \langle \Omega | \bar{N}_t N_0 | \Omega \rangle$$

Dimensions of the data is N x T

N indep. realizations (MC time)
T correlated sink loc.

model

$$y_t = \sum_{n=0}^{\infty} Z_n^2 e^{-E_n t}$$

$$Z_n \equiv \langle n | N | \Omega \rangle$$

data distribution

We want the distribution of the **mean**

central limit theorem promises multivariate normal

$$P(C_t|Z,E) = \frac{1}{\sqrt{(2\pi)^\nu |\Sigma|}} e^{-\frac{1}{2}(y-\mu)_{t_1}\Sigma^{-1}_{t_1,t_2}(y-\mu)_{t_2}}$$

$$\propto e^{-\chi^2_{\rm data}/2}$$

where Σ is the standard error of the mean squared

$$\Sigma_{t_1,t_2} = \frac{1}{N}\left[\frac{1}{N}\sum_{i,j}^{N}(C_i-\mu)_{t_1}(C_j-\mu)_{t_2}\right]$$

constraint curve fit

sum of exponentials is ill-conditioned
motivate constraint via Bayes theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

mean distribution of fit parameters are normal also

$$P(Z, E) \propto e^{-\chi^2_{\mathrm{prior}}/2}$$

- we have conjugate priors
- normalization factor is trivial

we do not need MC to obtain the posterior distribution

$$P(Z, E|C_t) \propto e^{-(\chi^2_{\mathrm{data}}+\chi^2_{\mathrm{prior}})/2}$$

examples

- introduce standard Lattice QCD analysis tools
- Bayesian mainly as constraints
- Bayesian for systematic error propagation

proton example

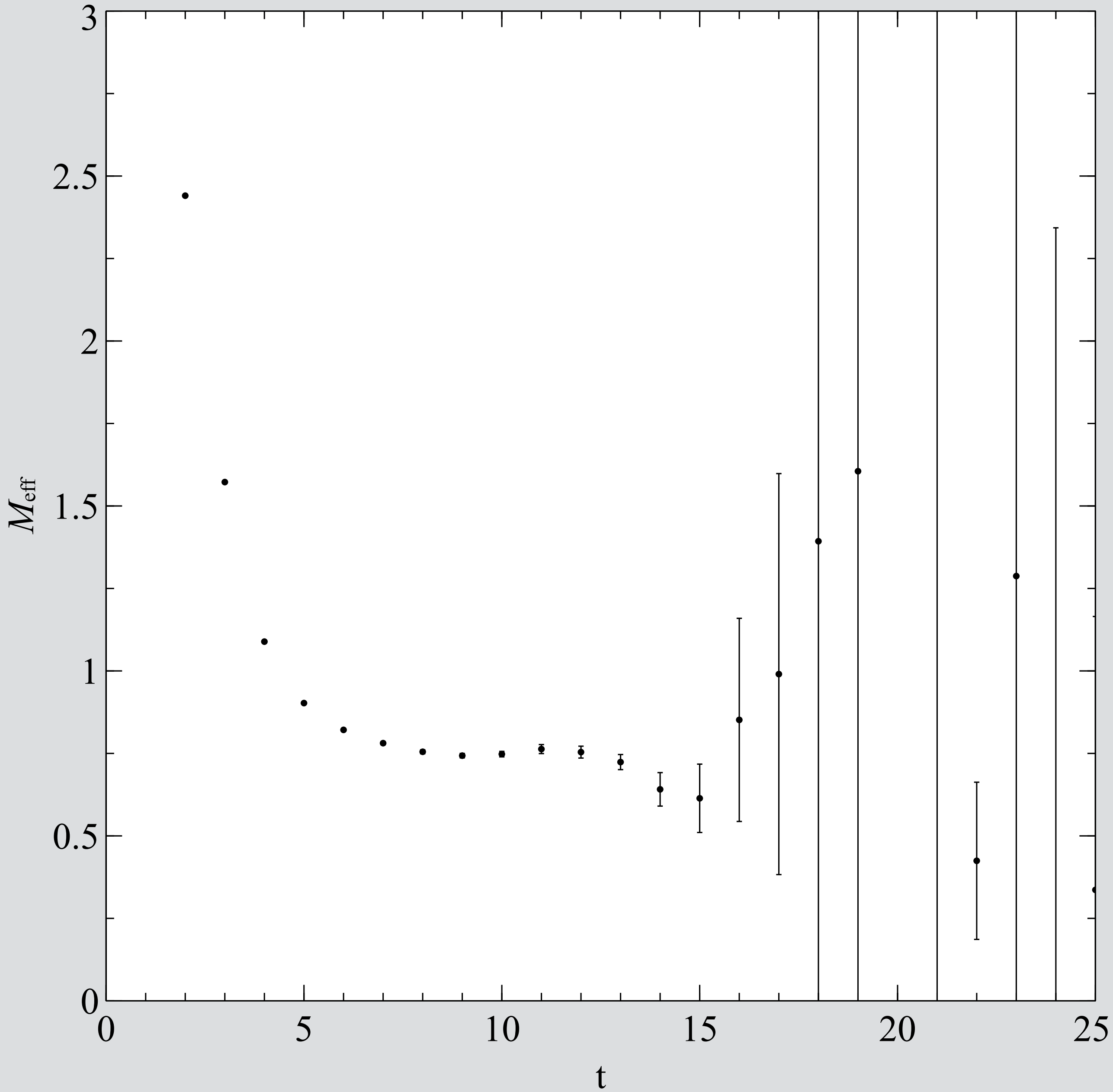
$$y_t = \sum_{n=0}^{\infty} Z_n^2 e^{-E_n t}$$

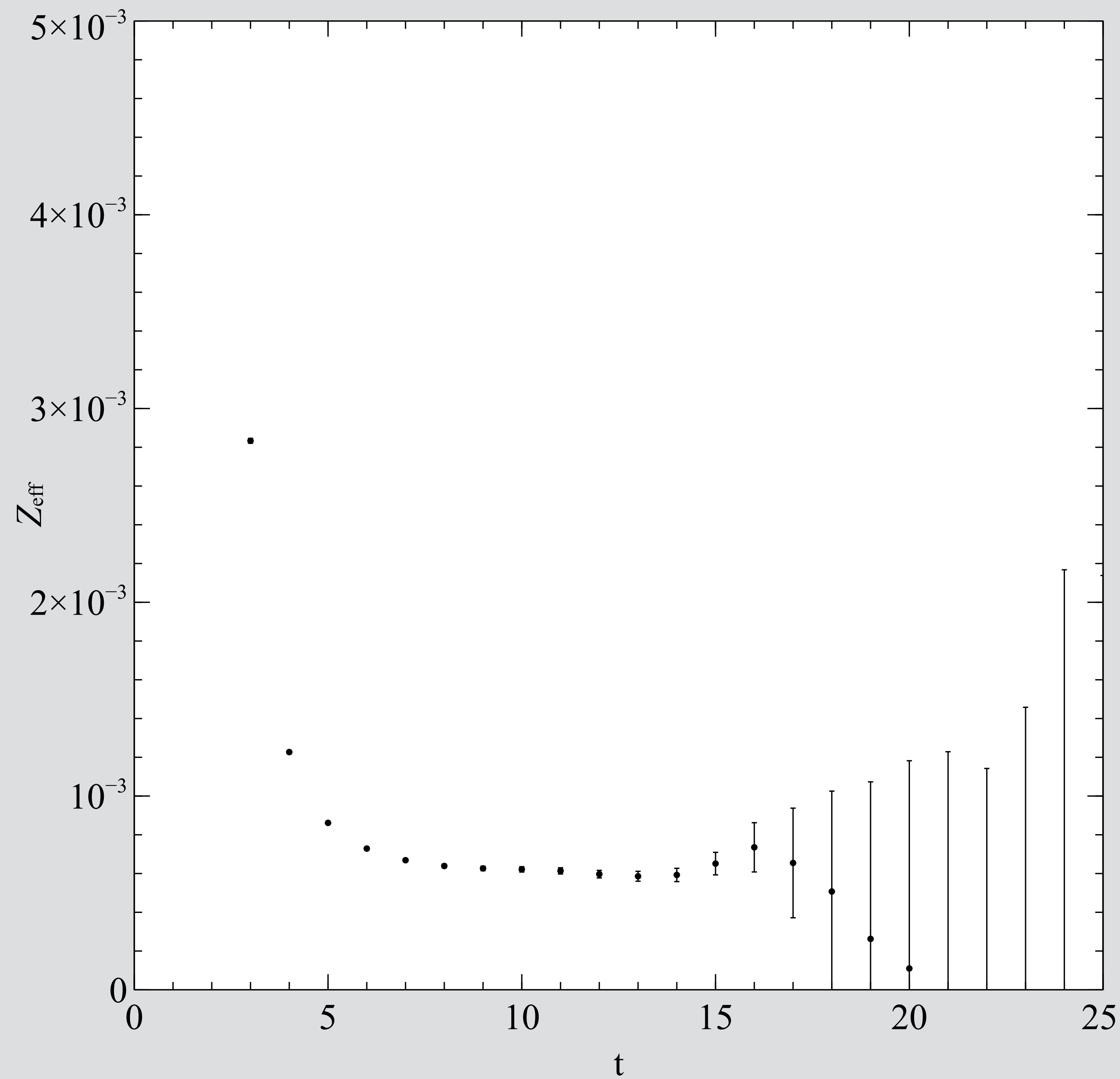
effective mass

$$M_{\text{eff}} = \ln\left(\frac{C_t}{C_{t+1}}\right)$$

scaled correlator

$$Z_{\text{eff}} = C_t e^{M_{\text{eff}}}$$





[Bouchard, Chang, Orginos, Richards]

correlator fit

interested in ground state state parameters

loosely constrain ground state
tight(er) constraints for excited states

example priors

$$\tilde{E}_0 = 0.74(20) \qquad \tilde{Z}_0 = 0.026(20)$$

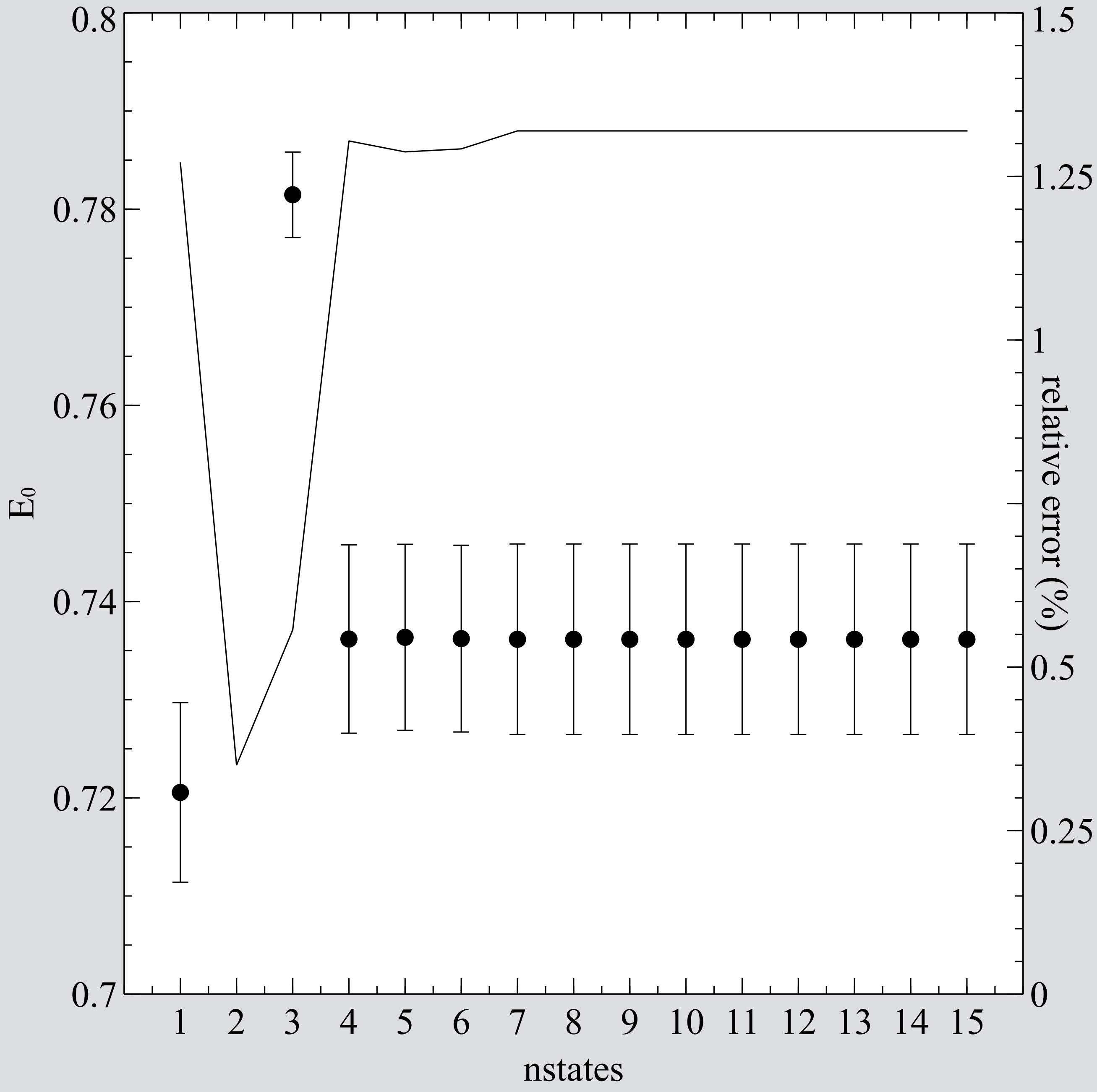
$$\tilde{\Delta}_n = -0.5(1.0) \qquad \tilde{Z}_n = 0.00(5)$$

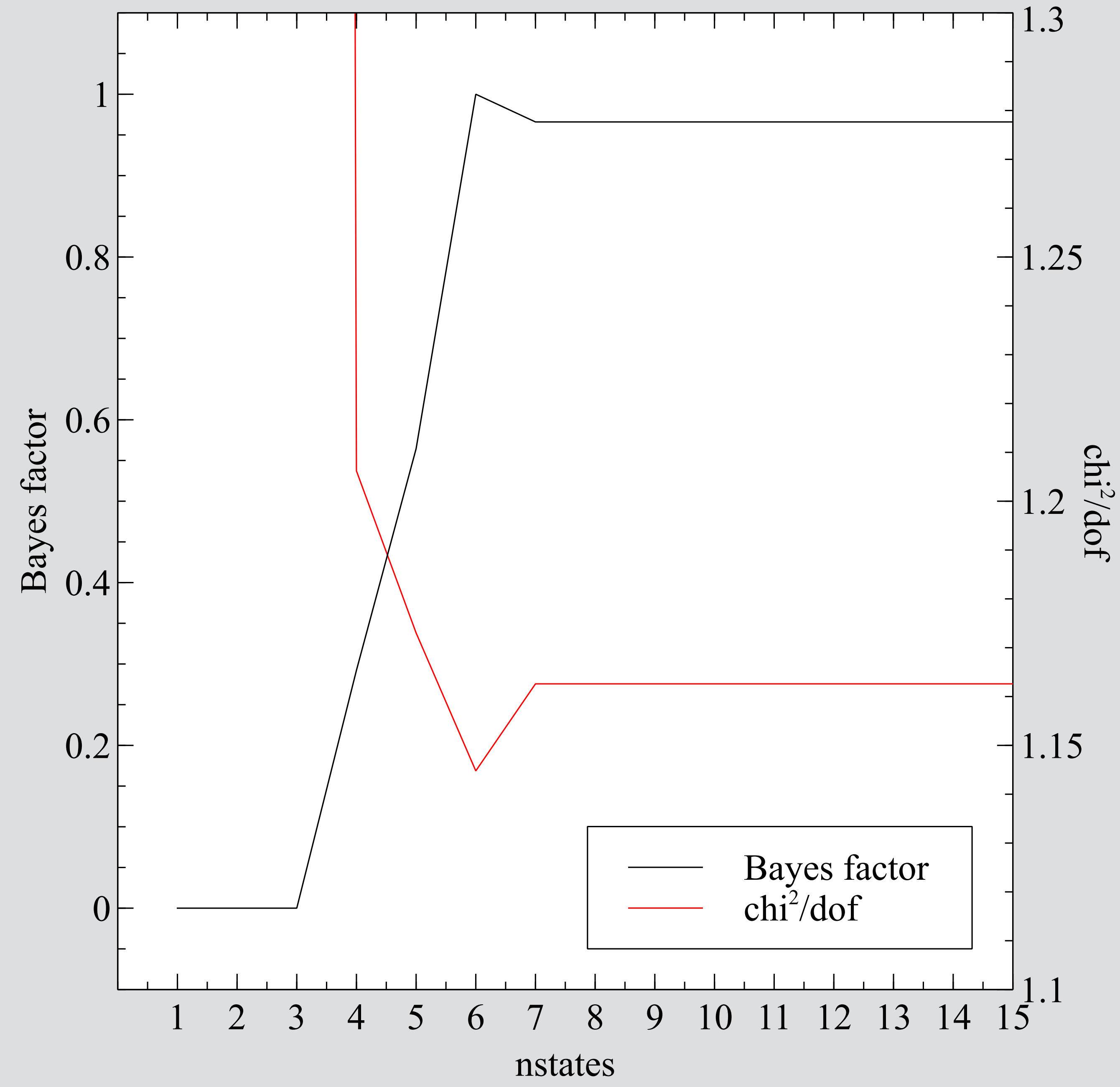
where $\tilde{E}_n = \tilde{E}_0 + e^{\tilde{\Delta}}$ (better way to enforce hierarchy?)

$$e^{\tilde{\Delta}} \approx 800\mathrm{MeV} \qquad \tilde{Z}_n \approx \mathcal{O}(\tilde{Z}_0)$$

(this ensemble has ~400MeV pions)

stability plots



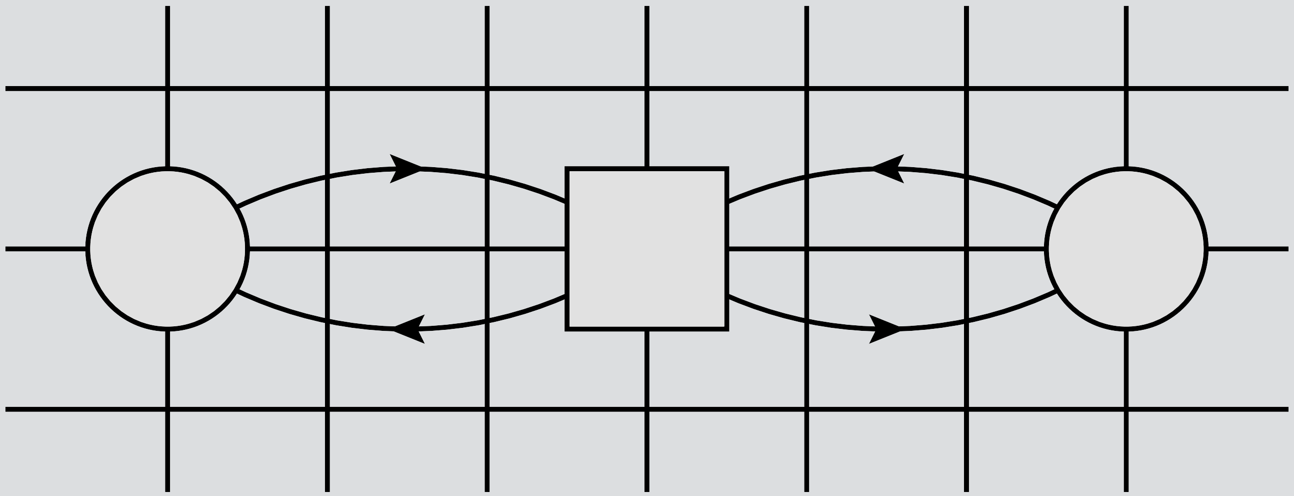


some fit details:
364 cfgs x 16 sources
time range 1 to 17

Is there an equivalent to Bayes factor (or any IC) to compare fits to subsets?

heavy flavor physics

neutral meson mixing example



$D^0 \leftrightarrow \bar{D}^0$

$B_d^0 \leftrightarrow \bar{B}_d^0$

$B_s^0 \leftrightarrow \bar{B}_s^0$ (also kaon)

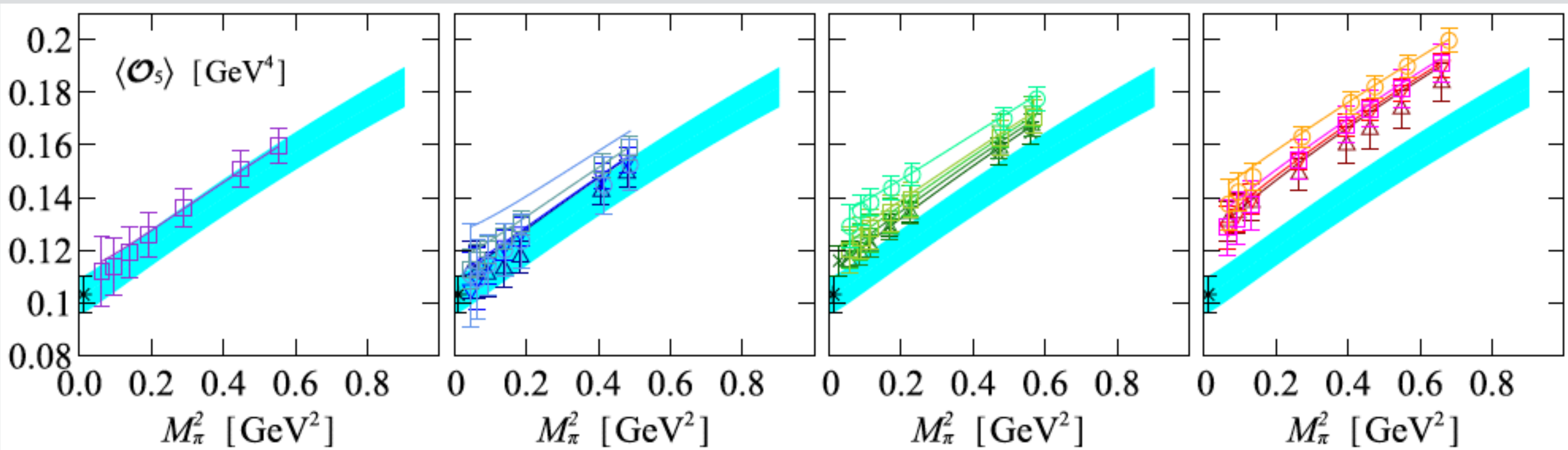
constrain electroweak free parameters (CKM)
eliminate NP parameter spaces

fantastic paper [hep-lat/1602.03560] (I'm an author)

[Fermilab Lattice and MILC Collaborations]

chiral-continuum fits (data)

D-meson mixing chiral-continuum extrapolation



0.045fm 0.06fm 0.09fm 0.12fm

different shades for light sea-quark masses (uncorrelated)
x-axis labels valence light-quark masses (correlated)
cyan band is the continuum extrapolation
black point labels physical pion mass

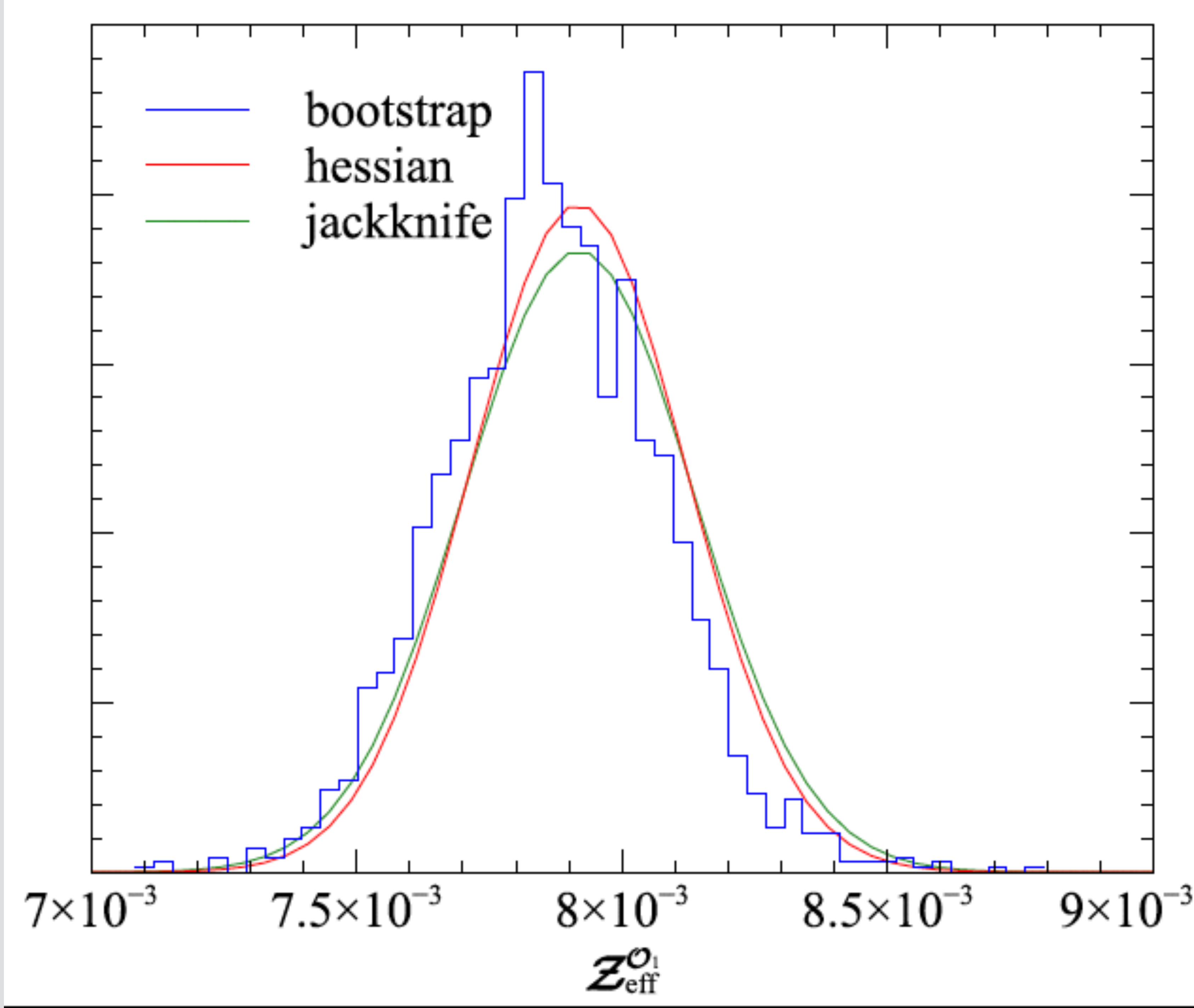
bootstrap correlator fits

- different data sets with different number of observations
- preserve correlations between data sets

method

- correlate cfg draws
- resample priors

posterior consistent with bootstrap and jackknife!



chiral perturbation theory (model)

$$F_i = F_i^{\text{logs.}} + F_i^{\text{analytic}} + F_i^{\text{HQ disc.}} + F_i^{\kappa} + F_i^{\text{renorm}}$$

F_i^{logs}	NLO chiral	extrapolate
F_i^{analytic}	NLO + NNLO analytic terms (N3LO)	
$F_i^{\text{HQ disc}}$	a^2 and a^3 heavy-quark discretization	various systematic uncertainty
F_i^{κ}	heavy-quark tuning error	
F_i^{renorm}	two-loop renormalization error	

model parameters

~ 40 constrained parameters

$$f_\pi, g_{DD^*\pi}, r_1, r_1/a, \text{etc...}$$

~ 25 unconstrained parameters

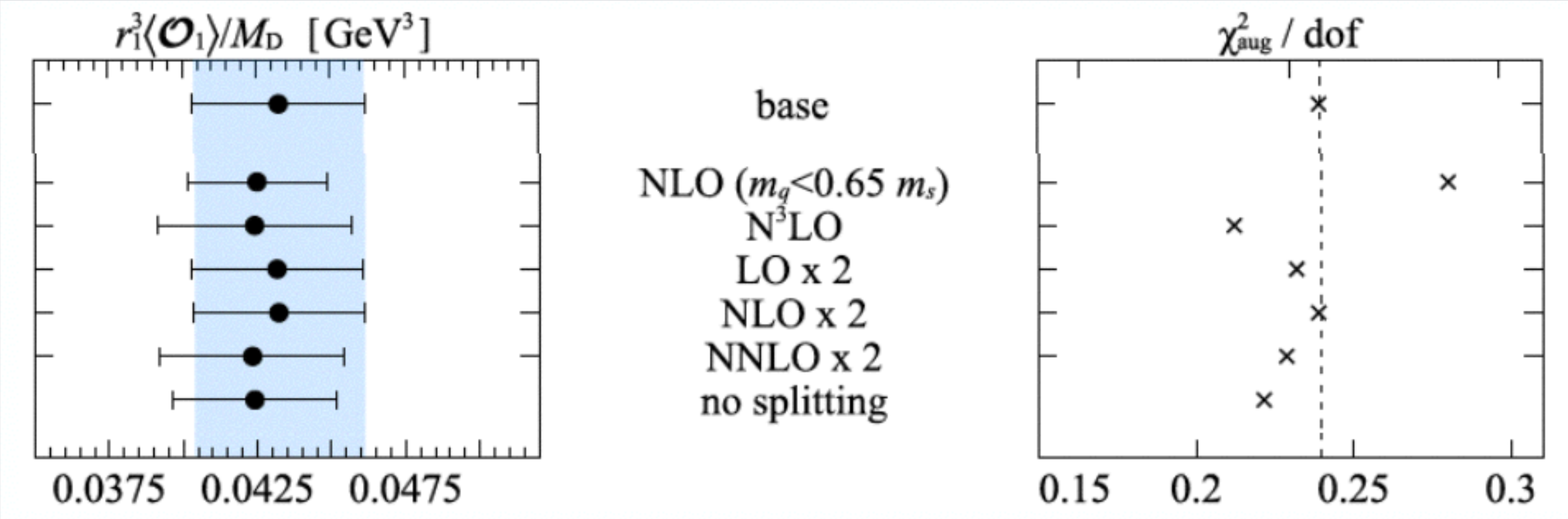
LO and NLO LECs

~ 100 possibly constrained parameters

NNLO LECs, systematic error coefficients

~170 parameters
510 data points

example of “free” priors



parameters are unconstraining by doubling prior width
errors saturation demonstrated by N3LO fit

maybe constraining?

renormalization and matching uncertainty

- power counting estimate ~ 4% to 6.5%

posteriors

$$\rho_{11}^{[1]} = 0.07(99) \quad \rho_{12}^{[1]} = -0.11(96)$$
$$\rho_{22}^{[1]} = 0.40(96) \quad \rho_{21}^{[1]} = -0.23(99)$$
$$\rho_{33}^{[1]} = -0.75(96) \quad \rho_{31}^{[1]} = -1.13(91)$$
$$\rho_{44}^{[1]} = -0.08(96) \quad \rho_{45}^{[1]} = -0.03(99)$$
$$\rho_{55}^{[1]} = -0.04(98) \quad \rho_{54}^{[1]} = -0.10(86)$$

posterior correlations

	p1	p2	p3	p4	p5
ME1	-0.79	0.02	-0.08	0.0	-0.04
ME2	0.05	-0.66	0.1	0.03	0.04
ME3	-0.01	0.06	-0.8	-0.04	-0.03
ME4	0.0	0.02	-0.05	-0.65	-0.05
ME5	-0.04	0.02	-0.04	-0.05	-0.87

$$p_i = \alpha_s^2 \left(\beta_i \rho_{ii}^{[1]} + \beta_j \rho_{ij}^{[1]} \right)$$

$$\mathrm{ME}_i = \text{entire fit function} - p_i$$

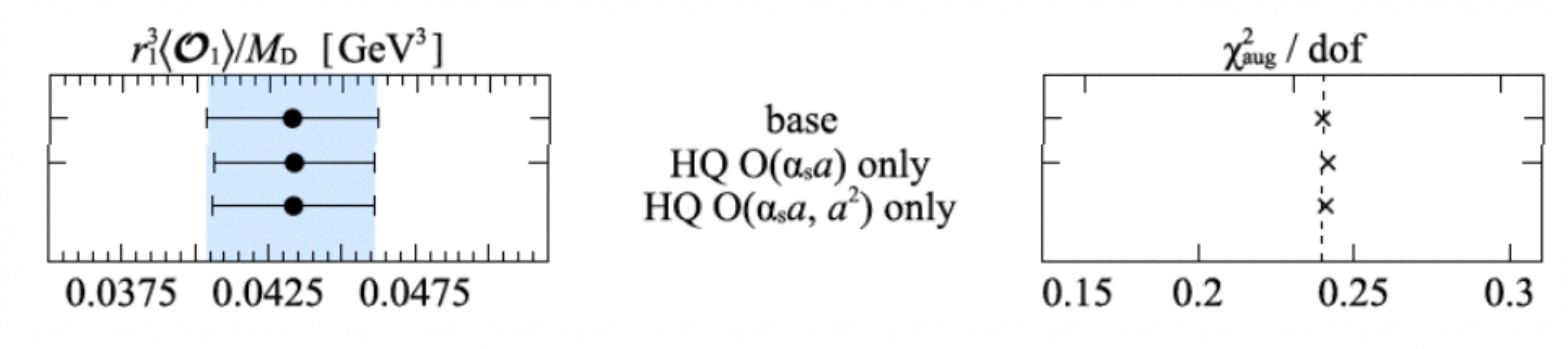
partial variance from fit

$\langle \mathcal{O}_1 \rangle$	$\langle \mathcal{O}_2 \rangle$	$\langle \mathcal{O}_3 \rangle$	$\langle \mathcal{O}_4 \rangle$	$\langle \mathcal{O}_5 \rangle$
3.7%	2.2%	3.8%	2.1%	4.1%

constraining

heavy-quark discretization uncertainty

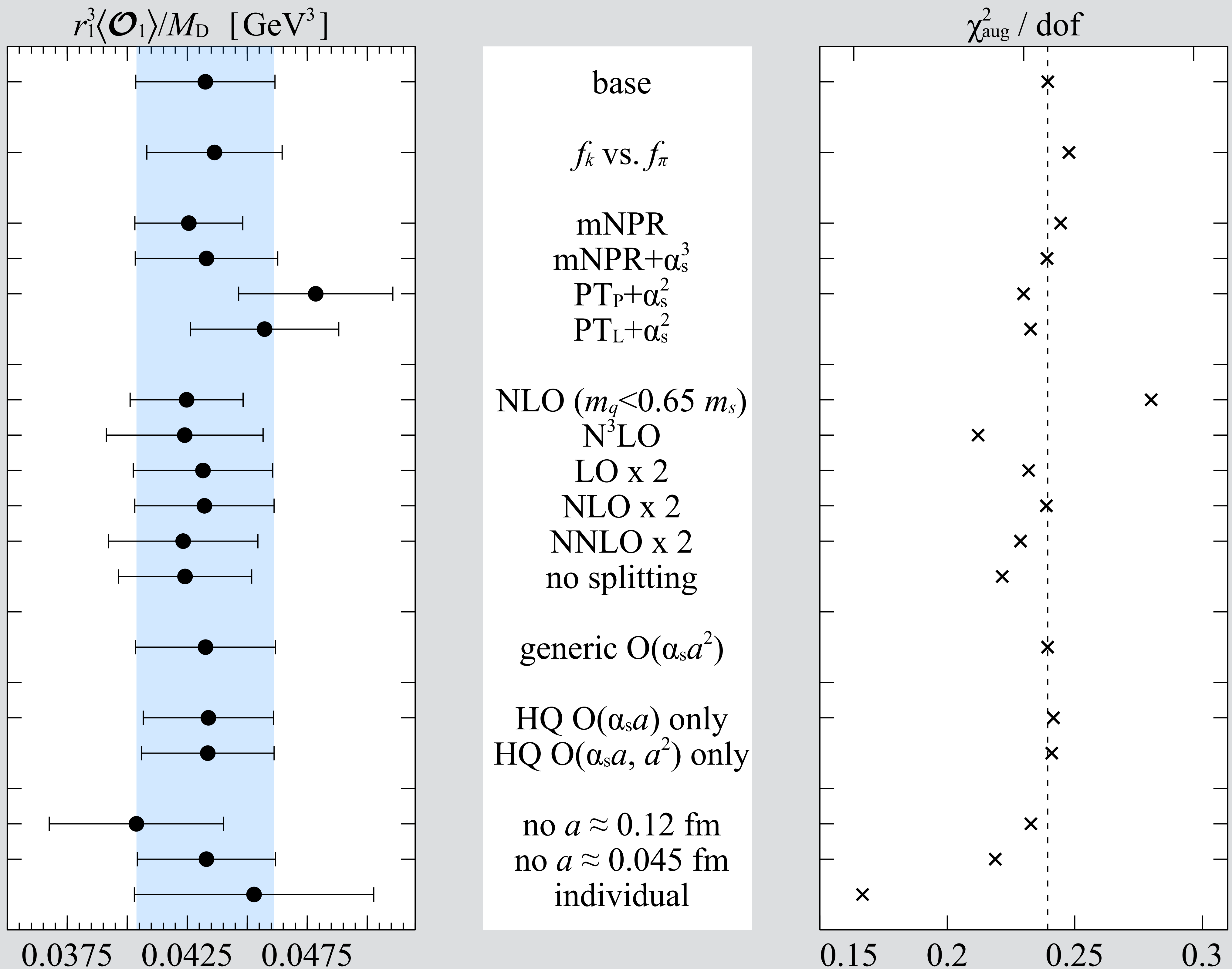
- power counting estimate ~ 3%



partial variance

$\langle \mathcal{O}_1 \rangle$	$\langle \mathcal{O}_2 \rangle$	$\langle \mathcal{O}_3 \rangle$	$\langle \mathcal{O}_4 \rangle$	$\langle \mathcal{O}_5 \rangle$
3.0%	2.3%	3.4%	2.4%	3.4%

fit stability



similar to nstate stability plot

complete error budget

	stat.	inputs	κ tuning	matching	chiral	LQ disc	HQ disc	r_1/a	r_1	fit total
$\langle \mathcal{O}_1 \rangle$	3.5	0.6	1.5	3.7	1.3	0.6	3.0	0.4	2.1	6.7
$\langle \mathcal{O}_2 \rangle$	1.8	0.5	0.4	2.2	0.8	0.4	2.3	0.4	2.1	4.4
$\langle \mathcal{O}_3 \rangle$	3.1	0.3	0.6	3.8	1.3	0.5	3.4	0.4	2.1	6.5
$\langle \mathcal{O}_4 \rangle$	2.2	0.6	0.4	2.1	0.9	0.3	2.4	0.4	2.1	4.6
$\langle \mathcal{O}_5 \rangle$	3.0	0.7	0.5	4.1	1.5	0.5	3.4	0.3	2.1	6.7

error breakdown from partial variances

$$\sigma_{\bar{p}}^2 = \frac{\partial y}{\partial \bar{p}}^T \Sigma_{\bar{p}} \frac{\partial y}{\partial \bar{p}}$$

missing systematic uncertainty

- finite volume ~0.1%
- isospin breaking ~ 0.01%
- electromagnetism ~ 0.2%

total error is unchanged at the reported precision when missing systematics are included in quadrature

software suite

www.github.com/gplepage

- lsqfit - least squares fitting with Bayesian priors
- gvar - manipulating Gaussian random variables
- vegas - Monte Carlo integration
- corrfitter - specialized for Lattice QCD

professionally written code
incredibly good documentation
I was not paid to advertise this