On fits to correlated and autocorrelated data

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Motivations

(Particle) physics physical information often from fits to data

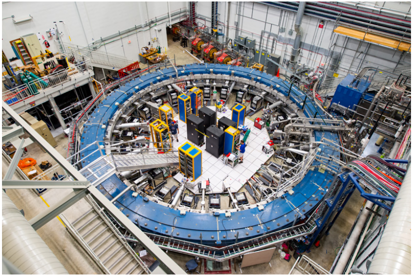
absence of direct signals for new physics → intensity frontier

precision is key word

Experiment

→ obtain data w/ stat.syst. errs

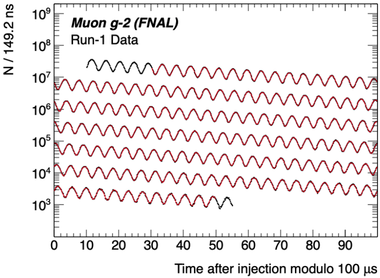
[Muon g-2 @ FermiLab]



Fit to data

driven by theory understanding

[Muon g-2 collab.]



Motivations

(Particle) physics physical information often from fits to data

absence of direct signals for new physics → intensity frontier

precision is key word

HPC

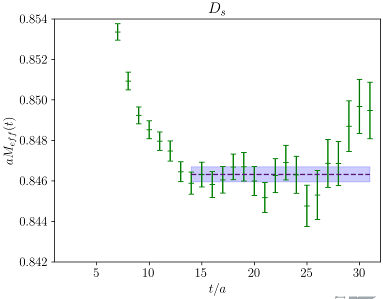
→ obtain data w/ stat.syst. errs

[Leonardo @ CINECA]

Fit to data

driven by theory understanding

[Gambino et al '22]



Lattice field theories

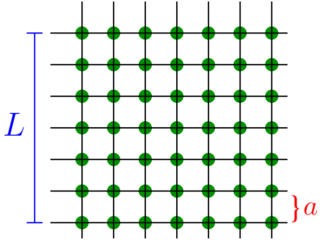
Due to confinement → non-perturbative formulation is necessary

lattice spacing a → regulate UV divergences

finite size L → infrared regulator

Continuum theory $a \to 0$, $L \to \infty$

Euclidean metric → Boltzman interpretation of path integral



$$\langle O \rangle = \mathcal{Z}^{-1} \int [DU] e^{-S[U]} O(U) \approx \frac{1}{N} \sum_{i=1}^{N} O[U_i]$$

Very high dimensional integral → Monte-Carlo methods

Markov Chain of gauge field configs $U_0 \to U_1 \to \cdots \to U_N$

0. $N_{\rm x}$ true expectation values Y_i
1. run a simulation with N configurations
2. measure estimators $y_i(t)$ at Monte Carlo time t

   e.g. a two-point correlator with i labelling source-sink separation
3. calculate averages $\bar{y}_i = \frac{1}{N}\sum_t y_i(t)$

   $\lim_{N\to\infty} \bar{y}_i = Y_i$

Central-limit theorem: $\bar{y}_i$ normally distributed around Y_i, $\delta\bar{y} = \bar{y} - Y$

$$P_C(\bar{y}) = (2\pi)^{-N_{\rm x}/2} (\det C)^{-1/2} \exp\Big(-\frac{1}{2}(\delta\bar{y}, C^{-1}\delta\bar{y})\Big)$$

Cov. matrix $\langle \delta\bar{y}_i \delta\bar{y}_j \rangle \equiv \int \mathrm{d}\bar{y}\ P_C(\bar{y})\ \delta\bar{y}_i\delta\bar{y}_j = C_{ij}$

$C = O(1/N)$ and $\delta\bar{y} = O(N^{-\frac{1}{2}})$

Notation: $(z, y) = z_i y^i$ and $||y||^2 = (y, y)$

χ^2 DISTRIBUTION

Null Hypothesis (NH): Y_i described by $\bar{y}_i$
statistical tests based on $\chi^2 = (\delta\bar{y}, C^{-1}\delta\bar{y}) = ||C^{-1/2}\delta\bar{y}||^2$

1. what is $\langle\chi^2\rangle$? $\rightarrow$ reduced χ^2
   $\langle\chi^2\rangle = N_{\mathrm{x}}$ degrees of freedom
   criterion 1) if $\chi^2 \simeq \langle\chi^2\rangle$ then NH valid (more later..)

2. probability of finding χ^2 larger than observed χ^2_{obs}? $\rightarrow$ p-value
   $Q(\chi^2_{\mathrm{obs}}) = \int \mathrm{d}\bar{y}\ P_C(\bar{y})\ \theta(\chi^2(\bar{y}) - \chi^2_{\mathrm{obs}}) = \gamma(k/2, \chi^2_{\mathrm{obs}}/2)$
   γ incomplete Γ-function
   criterion 2) if $Q(\chi^2_{\mathrm{obs}}) > 0.05$ then NH valid

Exact cancellation of C in P_C and χ^2 $\rightarrow$ simple analytic results

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Problems

In practical calculations we estimate C

1. Lattice QCD (fermions) simulations expensive
   $O(100)$ independent samples

2. Limit $N \to N_{\mathrm{x}}$ cov. matrix singular [Michael '94]

3. Markov chains induce autocorrelations
   consecutive configurations correlated along Monte-Carlo time
   statistical independent information reduced [Madras-Sokal '88]
   error $\sigma^2 = 2\tau_{\mathrm{int}}/N \mathrm{var}$

For fits we need C^{-1}, but hard to estimate in practice
$\to$ uncorrelated fits, or SVD-cuts/regularized C^{-1}

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Model function

Null-hypothesis: Y_j described by model function $\Phi(x_j, A) = \phi_j(A)$

Notation: A_α parameters, $\alpha = 1, \ldots N_{\mathrm{A}}$

Best fit parameters $\bar{a}$ from correlated fits

minimize $\chi^2(a) = ||C^{-\frac{1}{2}}(\bar{y} - \phi(a))||^2 \rightarrow \left.\frac{\partial \chi^2(a)}{\partial a_\alpha}\right|_{a=\bar{a}} = 0$

at minimum $\bar{a}(\bar{y})$ and $\chi^2(\bar{a})$

If C ill-conditioned, $\chi^2(a) = ||W(\bar{y} - \phi(a))||^2$

e.g. $W_{ij} = \delta_{ij}/\sqrt{C_{ii}}$ uncorrelated fits, or SVD cuts...

We want robust statistical tests to judge quality of fit

1. what is $\langle \chi^2(\bar{a}) \rangle$? $\rightarrow$ reduced χ^2
2. how likely finding χ^2 larger than χ^2_{obs}? $\rightarrow$ p-value

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$\langle \chi^2(\bar{a}) \rangle$

We evalute $\langle ||W(\bar{y} - \phi(\bar{a}))||^2 \rangle$ [MB, Sommer '22]

notation: $\delta\bar{a} = \bar{a} - A$ and $\phi^\alpha(a) = \partial\phi(a)/\partial a_\alpha$

1. Use minimum condition to define projector $\mathcal{P}$ span $W\phi^\alpha(\bar{a})$

   $\big(W\phi^\alpha(\bar{a}), W(\bar{y} - \phi(\bar{a}))\big) = 0 \quad \rightarrow \quad \mathcal{P}W(\bar{y} - \phi(\bar{a})) = 0$

   $\chi^2(\bar{a}) = ||(1 - \mathcal{P})W(\bar{y} - \phi(\bar{a})||^2$

2. Expand $\phi(\bar{a})$ about A

   $\phi(\bar{a}) = \phi(A) + \phi^\alpha(\bar{a})\delta\bar{a}_\alpha + O(\delta\bar{a}^2)$

   $\bar{y} - \phi(\bar{a}) = \bar{y} - \phi(A) + \phi^\alpha\delta\bar{a}_\alpha + O(\delta\bar{a}^2) = \delta\bar{y} + \phi^\alpha\delta\bar{a}_\alpha + O(\delta\bar{y}^2)$

3. $\chi^2(\bar{a}) = ||(1 - \mathcal{P})W\delta\bar{y}||^2 + O(\delta\bar{y}^3) + O(\delta\bar{y}^4)$

Taking $W = O(N^{1/2})$, i.e. a function of $C^{-1/2}$

   $\langle O(\delta\bar{y}^3) \rangle = 0$ up to corrections

$$\langle \chi^2(\bar{a}) \rangle = \mathrm{tr}[(1 - \mathcal{P})WCW] + O(N^{-1})$$

P-VALUE

$Q(\chi^2_{\rm obs}) = \int \mathrm{d}\bar{y}\ P_C(\bar{y})\ \theta(\chi^2(\bar{y}) - \chi^2_{\rm obs})$

1. a useful relation is given by change of variables $z = C^{-1/2}\delta\bar{y}$

$$\langle f(\delta\bar{y})\rangle = \int \mathrm{d}\bar{y}\ P_C(\bar{y})\ f(\delta\bar{y}) = \int \mathrm{d}z\ (2\pi)^{-N_{\rm x}/2} e^{-\frac{1}{2}||z||^2} f(C^{1/2}z)$$

2. replace $\chi^2(\bar{a})$ with $||(1-\mathcal{P})W\delta\bar{y}||^2 = (z, \nu z)$
   matrix $\nu = C^{1/2}W(1-\mathcal{P})WC^{1/2}$

$$Q(\chi^2_{\rm obs}) = \int \mathrm{d}z\ (2\pi)^{-N_{\rm x}/2} e^{-\frac{1}{2}||z||^2} \theta((z,\nu z) - \chi^2_{\rm obs})$$

Integral in Q evaluated numerically (easy)

Summary

[MB, Sommer '22]

For arbitrary W, i.e. uncorrelated fits, SVD cuts, correlated fits ...

robust statistical tests based on p-value (and reduced χ^2)

C and $C^{1/2}$, i.e. large (not small) eigenvalues of C

For correlated fits $[W = C^{-1/2}] + [\mathrm{tr} P = N_\mathrm{A}]$, imply:

$\mathrm{tr}[(1-\mathcal{P})WC] = \mathrm{tr}[1-\mathcal{P}] = N_\mathrm{x} - N_\mathrm{A} =$ degrees of freedom

similarly $\mathrm{tr}\nu = N_\mathrm{x} - N_\mathrm{A}$, so p-value takes standard form

C never known, only its estimator $\bar{C}$: consequences?

estimator of $\langle\chi^2\rangle$ with error $O(N^{-1/2})$

estimator of p-value, no closed-form for error

bootstrap? to be explored [MB, Kelly in prep]

Autocorrelations - I

[Madras-Sokal '88][Wolff '03][Schaefer et al. '11]

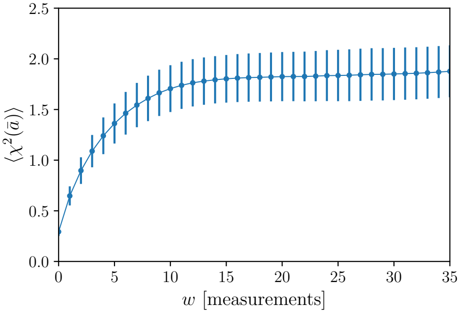
Assume $y_i(t)$ measured on single ensemble at Monte Carlo time t

autocorrelation function $\Gamma_{ij}(t) = \langle \Delta y_i(t+t_0)\, \Delta y_j(t_0) \rangle$

covariance matrix $C_{ij} = \frac{1}{N} \sum_{t=-\infty}^{\infty} \Gamma_{ij}(t)$

Expected χ^2 in presence of autocorrelations

$\langle \chi^2(\bar{a}) \rangle = \frac{1}{N} \sum_{t=-\infty}^{\infty} \mathrm{tr}\big[\Gamma(t)\, W(1-\mathcal{P})W\big]$



[MB, Sommer '22]

Estimator E of $\langle \chi^2 \rangle$

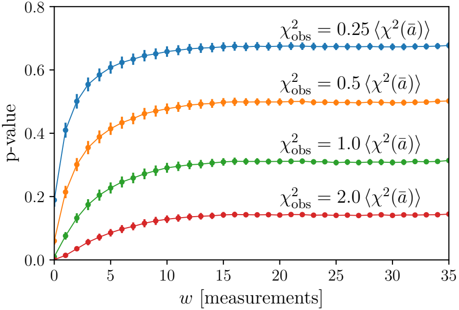
1. estimator of Γ
2. truncate sum (W) 3.

$\Delta E^2 \simeq \frac{2}{N}(2W+1)E^2$

example in toy model

Autocorrelations - II

Autocorrelation effects from matrix $\nu = C^{1/2} W (1 - \mathcal{P}) W C^{1/2}$



Uncorrelated fit

Error on p-value from several replicas

Example in toy model

P-VALUE

Correlated fits

large d.o.f.

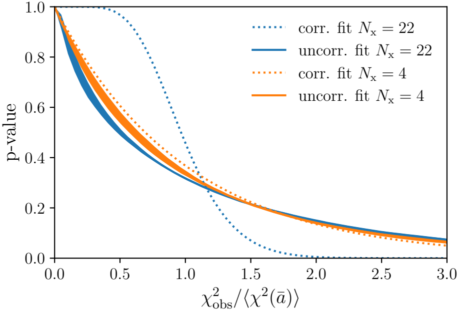
p-value sharp drop for $\frac{\chi^2}{\text{d.o.f}} \simeq 1$

$\rightarrow$ $\chi^2/\text{d.o.f} \simeq 1$ valid criterion

small d.o.f.

$\chi^2/\text{d.o.f} \simeq 1$ not good

$\rightarrow$ p-value preferable



Uncorrelated fits

$\chi^2/\text{d.o.f} \simeq 1$ meaningless; $\chi^2/\langle\chi^2\rangle \simeq 1$ not good criterion

$\rightarrow$ p-value from our method preferred choice

Conclusions

Lattice QCD

- predictions often involve fits to correlated and autocorrelated data
- correlated fits always preferred, but estimator of C is often singular
- alternatives: uncorrelated fits, SVD cuts...

Our work novel analytic control of $\langle \chi^2 \rangle$ and p-value

- unlocks robust statistical tests (only C,$C^{1/2}$ involved)

Autocorrelations are easily incorporated

- Γ-method, jackknife/bootstrap with binning

Thanks for your attention

A DIFFERENT METHOD

Bootstrap generates new 'fake' resampled ensembles

for each ensemble minimize χ^2

build histogram $\rightarrow$ well-defined "probability" density of χ^2? No

re-centering χ^2 allows to build proper density [Kelly Lattice '19]

well-defined p-value, valid for arbitrary W

More work under preparation [MB, Kelly in prep]

formal proof of equivalence of two ideas

extension of recentering to jackknife

study of $1/N$ neglected terms