On fits to correlated and auto-correlated data

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Abstract

Observables in particle physics and specifically in lattice QCD calculations are often extracted from fits. Standard χ^2 tests require a reliable determination of the covariance matrix and its inverse from correlated and auto-correlated data, a challenging task often leading to close-to-singular estimates. These motivate modifications of the definition of χ^2 such as uncorrelated fits. We show how the goodness-of-fit measured by their p-value can still be estimated robustly for a broad class of such fits.

1   Introduction

In particle physics, physical information is often extracted from fits to correlated data. When their covariance matrix is known well, the minimization of the so-called correlated χ^2 is the ideal method to obtain the best estimate of the fit parameters from the statistical point of view. In many cases model functions are guided by theoretical principles, but in practice one has to examine their validity case by case, and often specific model functions or data points are discarded based on a measure of their goodness-of-fit. For N_x data points normally distributed, and for correlated fits to model functions depending on N_A parameters, the expectation value of χ^2 (at the minimum) equals the number of degrees of freedom, $N_x - N_A$. When there is a large number of data points, a reduced χ^2 close to 1 (defined by the ratio of the observed χ^2 over $(N_x - N_A)$), provides a first good indication that a given model describes well the data. In addition, the goodness-of-fit is judged by computing the probability Q, often called p-value, of observing a χ^2 larger or equal than the observed χ^2, which we call χ^2_{obs}. The p-value is easily obtained in closed analytic form due to the exact cancellation between the covariance matrix, C, of the underlying data and C^{-1} used in the definition of the correlated χ^2. It depends only on χ^2_{obs} and on $N_x - N_A$.

However, data sets with limited statistics often lead to close-to-singular C^{-1}. Moreover, for data generated from Monte-Carlo (MC) methods, specifically from Markov chains, additional complications arise from the presence of auto-correlations, namely correlations along the Monte-Carlo history (or "time"). Hence for all cases where reliable estimations of the inverse of the covariance matrix are not possible, and correlated fits can not be performed, the standard χ^2-test is not applicable. In this work we point out a robust solution to the problem.

Our object of study is primarily lattice QCD, where Monte-Carlo methods based on Markov chains are an essential ingredient to obtain non-perturbative predictions. Field configurations are generated by successive repetitions of a predefined update scheme, and as a consequence, expectation values of correlation functions, obtained from averages over measurements on these field configurations, are both correlated and auto-correlated. The Γ-method is the preferable choice to estimate the statistical errors of primary and derived observables [1] obtained from a Markov process, but it is difficult to turn it into a practical method for general matrix elements of the covariance matrix.[1]

Because of these issues and the general difficulty in estimating covariances for large number of data points [2], ad hoc modifications of C^{-1} are often used, like so-called SVD cuts (see e.g. [3,4]) or uncorrelated fits. We will show how the expected value of χ^2 and the goodness-of-fit can be estimated robustly for all these cases. In fact, we emphasize that this can also be done when the weights of the data points are independent of the covariance matrix, which may be a good strategy when fits are used to perform extrapolations away from the region where data exists.

Our text is organized as follows: in Section 2 we present the derivation of the formulae for the expectation value of χ^2 and the correponding p-value; in Section 3 we describe how to handle auto-correlations, while in Section 4 we present a numerical test in a toy model, before concluding.

2   Method

We want to test whether data Y_j at kinematic coordinates x_j are described by model functions $\Phi(x, a)$, depending on the parameters a^α,

$$Y_j = \Phi(x_j, A) = \phi_j(a) \,, \tag{2.1}$$

with A^α the exact values of the model parameters: the so-called null-hypothesis. In our convention Greek indices run from 1 to N_A, Roman ones run from 1 to N_x, repeated indices are summed over,

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[1] A theoretical method is easily given if 1) N_x is not too large, 2) the exponential auto-correlation time, τ_{exp}, can be estimated, and 3) the MC chain is very long compared to it. Then the window size of Ref. [1] can be chosen a few times τ_{exp} and fixed independently of i, j for the estimate of C_{ij} given in the reference. Also jackknife with sufficiently large bin-size can be used in such, very restricted, cases.

and we use the natural scalar product $(r, s) = r_i s_i$ and norm $||r|| = (r, r)^{1/2}$. We also often use the matrix-vector notation to suppress Roman indices. Given data $\bar{y}_j$ with normal distribution,

$$P_C(\bar{y}) = (2\pi)^{-N_x/2} (\det C)^{-1/2} \exp\left(-\frac{1}{2}(\delta\bar{y}, C^{-1}\delta\bar{y}) \right), \qquad \delta\bar{y} = \bar{y} - Y, \tag{2.2}$$

with covariance matrix C, we want to find robust estimates for the fit parameters and have a measure for the likelihood that our model is compatible with the data. Expectation values are defined in the usual manner. In particular we have

$$\langle \delta\bar{y}_i \delta\bar{y}_j \rangle \equiv \int \mathrm{d}\bar{y} \, P_C(\bar{y}) \, \delta\bar{y}_i \delta\bar{y}_j = C_{ij}. \tag{2.3}$$

One possibility when such a normal distribution is approximately realized is when $\bar{y}_j$ are averages over Monte Carlo data of length N and N is sufficiently large. In this case, all elements of C are of order $1/N$, and $\langle \bar{y}_i \rangle \to Y_i$ in the limit $N \to \infty$.

The natural measure for the distance of the model to the data is

$$\chi^2(a) = ||W(\bar{y} - \phi(a))||^2, \tag{2.4}$$

in terms of a symmetric and positive $N_x \times N_x$ weight matrix W_{ij}. A reasonable requirement is that χ^2 remains finite as $N \to \infty$, which means that W should be of $O(N^{1/2})$: common choices for W^2 are the inverse covariance matrix C^{-1} or the inverse of its diagonal projection $W_{ij} = \delta_{ij} \sqrt{[C^{-1}]_{ii}}$ (no summation over i). The latter definition of χ^2 leads to so-called uncorrelated fits. However, one can also consider weight matrices W which scale weaker with N, e.g. $O(N^0)$. We will remark on that later.

As usual, from the minimization of the χ^2 function we obtain the best estimate of the parameters

$$\chi^2(\bar{a}) = \operatorname*{Min}_a \chi^2(a), \quad \bar{a} = \bar{a}(\bar{y}). \tag{2.5}$$

Our goal is to derive an expression for the expectation value

$$\langle \chi^2(\bar{a}) \rangle = \int \mathrm{d}\bar{y} \, P_C(\bar{y}) \, \chi^2(\bar{a}(\bar{y})), \tag{2.6}$$

predicted by the normal distribution of the data and under the assumption that Eq. (2.1) holds.

The condition for $\bar{a}$,

$$(W\phi^\alpha(\bar{a}), W(\bar{y} - \phi(\bar{a}))) = 0, \quad \text{with } \phi^{\alpha_1 \cdots \alpha_m}(a) \equiv \frac{\partial^m \phi(a)}{\partial a^{\alpha_1} \cdots \partial a^{\alpha_m}}, \tag{2.7}$$

can be rewritten as

$$\mathcal{P} W (\bar{y} - \phi(\bar{a})) = 0, \tag{2.8}$$

with $\mathcal{P}$ the projector onto the space spanned by $\{W \phi^\alpha\}$, namely

$$\mathcal{P}W\phi^\alpha = W\phi^\alpha, \; \mathcal{P} = \mathcal{P}^2, \; \operatorname{tr}\mathcal{P} = N_A, \tag{2.9}$$

and we have

$$\chi^2(\bar{a}) = ||(1 - \mathcal{P})W(\bar{y} - \phi(\bar{a}))||^2. \tag{2.10}$$

2.1 Expectation value of χ^2

We expand ϕ around $a = \bar{a}$,

$$\phi(A) = \phi(\bar{a}) + \phi^\alpha(\bar{a})\delta\bar{a}^\alpha + \frac{1}{2}\phi^{\alpha\beta}(\bar{a})\delta\bar{a}^\alpha\delta\bar{a}^\beta + O(\delta\bar{a}^3), \quad \delta\bar{a}^\alpha \equiv \bar{a}^\alpha - A^\alpha, \tag{2.11}$$

and obtain, using $(1 - \mathcal{P})W\phi^\alpha(\bar{a}) = 0$,

$$\chi^2(\bar{a}) = ||(1 - \mathcal{P})W\,\delta\bar{y}||^2 + (W\delta\bar{y}, (1 - \mathcal{P})W\phi^{\alpha\beta})\delta\bar{a}^\alpha\delta\bar{a}^\beta + \mathrm{O}(N^{-1})\,. \qquad (2.12)$$

Taking $\delta\bar{a} = \mathrm{O}(N^{-1/2}) = \delta\bar{y}$, the expected value of χ^2 is then

$$\langle\chi^2(\bar{a})\rangle = \mathrm{tr}[C_{\mathrm{w}}(1 - \mathcal{P})] + \mathrm{O}(N^{-1})\,, \quad C_{\mathrm{w}} = WCW\,. \qquad (2.13)$$

We stress the fact that in the result above even an approximate knowledge (up to statistical errors) of the covariance matrix is sufficient. The corrections to eq. (2.13) are seen to be $\mathrm{O}(N^{-1})$ in the following way. Expanding $\delta\bar{a}(\delta\bar{y})$ in terms of $\delta\bar{y}$ (and therefore in terms of $N^{-1/2}$), we have $\langle(W\delta\bar{y}, (1 - \mathcal{P})W\phi^{\alpha\beta})\delta\bar{a}^\alpha\delta\bar{a}^\beta\rangle = g_{ijk}\langle\delta\bar{y}_i\delta\bar{y}_j\delta\bar{y}_k\rangle + \mathrm{O}(N^{-1})$ where $g = \mathrm{O}(N)$ due to the two factors of W. In the assumed symmetric (normal) distribution $\langle\delta\bar{y}_i\delta\bar{y}_j\delta\bar{y}_k\rangle$ vanishes and skewed corrections to it are down by a factor $N^{-1/2}$ leading overall to $\mathrm{O}(N^{-1})$. However, in practice the estimate of C_{w} from the data themselves introduces order $N^{-1/2}$ uncertainties, as well as the projector $\mathcal{P}$ which is a function of $\bar{a}^\alpha$. The essential point is that $\langle\chi^2(\bar{a})\rangle$ can easily be computed also with auto-correlated data, as we will show in the next section.

For the special choice of an "uncorrelated fit", i.e. $W_{ij} = \delta_{ij}\sqrt{[C^{-1}]_{ii}}$, we have $[C_{\mathrm{w}}]_{ii} = 1$ and

$$\langle\chi^2(\bar{a})\rangle = N_{\mathrm{x}} - \mathrm{tr}[C_{\mathrm{w}}\mathcal{P}]\,. \qquad (2.14)$$

Similarly, for a "correlated fit" with $W^2 = C^{-1}$, $[C_{\mathrm{w}}]_{ij} = \delta_{ij}$, we reproduce the standard result $\langle\chi^2(\bar{a})\rangle = N_{\mathrm{x}} - N_{\mathrm{A}}$.

Above we used $W = \mathrm{O}(N^{1/2})$. However, one could also consider more generic functions[2], which may for example depend additionally or alternatively on the kinematic coordinates x_i. This changes nothing in the above, since $\delta\bar{a}$ remains $\mathrm{O}(N^{-1/2})$. In Appendix C we discuss several other generalizations of the fit functions assumed above.

At this point, it is natural to define the reduced-χ^2 for fits with arbitrary W as $\chi^2/\langle\chi^2(\bar{a})\rangle$ with eq. (2.13) for $\langle\chi^2(\bar{a})\rangle$. Although a reduced-$\chi^2$ of order 1 is already a first indication of whether a given model fits well the data, the real discriminator for the goodness of a fit is the p-value.

2.2 Quality-of-fit

The probability for having a value of $\chi^2(\bar{a})$ which is larger or equal than a given value χ^2_{obs} is

$$Q = \int \mathrm{d}\bar{y}\, P_C(\bar{y})\, \theta\big(\chi^2(\bar{a}(\bar{y})) - \chi^2_{\mathrm{obs}}\big)\,. \qquad (2.15)$$

It is useful to decide whether the model can be statistically rejected (the null hypothesis). In practice χ^2_{obs} stands for the value of $\chi^2(\bar{a})$ that one has in the particular fit to the existing data and Q gives the probability of finding a fit worse than the one that one found, i.e. with a larger value of $\chi^2(\bar{a})$. If Q is too low, then one has significant reasons to doubt that the model describes the data, and usually dismisses the fit and modifies the model or the fit ranges. The probability Q is often called quality-of-fit or p-value.

Using the variables $z = C^{-1/2}\delta\bar{y}$ it is given by

$$Q(\chi^2_{\mathrm{obs}}, \nu) = \int \mathrm{d}z\, (2\pi)^{-N_{\mathrm{x}}/2}e^{-\frac{1}{2}||z||^2}\, \theta\big((z, \nu z) - \chi^2_{\mathrm{obs}}\big)\,, \qquad (2.16)$$

in terms of the positive, symmetric matrix

$$\nu = C^{1/2}W(1 - \mathcal{P})WC^{1/2}\,. \qquad (2.17)$$

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[2] Consider for example a linear extrapolation of $\Phi(x, a) = a_0 + a_1 x + \mathrm{O}(x^2)$, to $x = 0$, i.e. we want to determine a_0. When the data set is not rich enough to include higher order terms in ϕ, it can be a good strategy to choose a weight $W_{ii} \propto 1/x_i^n$, e.g. with $n = 2$.

The latter takes over the role of the number of degrees of freedom in correlated fits, where $CW = 1$ and $\text{tr}[\nu] = N_\text{x} - N_\text{A}$. Denoting the strictly positive eigenvalues of ν by $\lambda_i(\nu)$, $i = 1 \ldots N_\nu \leq N_\text{x} - N_\text{A}$, we have

$$Q(\chi_\text{obs}^2, \nu) = \int \theta\Big(\sum_{j=1}^{N_\nu} \lambda_j(\nu) z_j^2 - \chi_\text{obs}^2 \Big) \prod_{i=1}^{N_\nu} \frac{\mathrm{d}z_i}{(2\pi)^{1/2}} \, e^{-\frac{1}{2}z_i^2} \,. \qquad (2.18)$$

In this form, Q is easily evaluated by a MC over z_i drawn from a Gaussian distribution. A sample of order thousand random numbers is sufficient for a precision of Q of order 0.01, and our proposal is to use this as estimate for the quality-of-fit.

The difficult part is not the statistical error in the MC estimate of eq. (2.18) but the fact that ν has to be estimated from the data $\bar{y}$ and thus the eigenvalues $\lambda_i(\nu)$ are uncertain themselves. This leads to the expectation that the statistical error ΔQ of Q is order $N^{-1/2}$. In contrast to the case of a correlated χ^2 fit no enhancement by small eigenvalues (of the estimated ν) will occur in ΔQ. Instead the contribution of modes with small eigenvalues are suppressed. In sect. 4 we will demonstrate in a toy model that ΔQ is small and can be neglected in practice.

In general one should decide whether a fit is to be discarded based on the quality-of-fit. For example, if $Q(\chi_\text{obs}^2, \nu) = 0.05$ there is only a 5% chance that one finds such a χ_obs^2 or worse but the fit-function describes the data on average. One will then dismiss fits with $Q(\chi_\text{obs}^2, \nu) \leq 0.05$ or with a different threshold. When one performs a correlated fit and has a large number of data, more precisely when $N_\text{x} - N_\text{A} = \langle \chi^2(\bar{a}) \rangle \gg 1$, then $Q(\chi_\text{obs}^2, \nu)$ is close to a step function $1 - \theta(\chi_\text{obs}^2/\langle \chi^2(\bar{a}) \rangle)$. But this is not the case in general. To understand this behavior, we examine the region where Q makes the transition from $Q \approx 1$ to $Q \approx 0$. Its width can be estimated by the variance of $\chi^2(\bar{a})$. Using eqs. (2.12, 2.13) we obtain

$$\langle [\chi^2(\bar{a}) - \langle \chi^2(\bar{a}) \rangle]^2 \rangle = \langle (\chi^2(\bar{a}))^2 \rangle - \langle \chi^2(\bar{a}) \rangle^2 = 2\text{tr}(\nu^2) + \mathrm{O}(N^{-1/2}) \,, \qquad (2.19)$$

valid for arbitrary weights W. For a correlated fit with $WCW = 1$, the width is suppressed by $1/(N_\text{x} - N_\text{A})$ relative to $\langle \chi^2(\bar{a}) \rangle^2$. For a large number of data points, a step-function behavior is approached. However, in general this is not the case. Assume for example that the eigenvalues of ν are geometrically distributed, namely $\lambda_j = \lambda_0 r^j$ with $r < 1$. Then we have

$$\frac{\langle [\chi^2(\bar{a}) - \langle \chi^2(\bar{a}) \rangle]^2 \rangle}{2 \langle \chi^2(\bar{a}) \rangle^2} = \frac{\sum_{j=1}^{N_\nu} (\lambda_j(\nu))^2}{(\sum_{j=1}^{N_\nu} \lambda_j(\nu))^2} = \frac{1-r}{1+r} + \mathrm{O}(r^{N_\nu+1}) \,. \qquad (2.20)$$

In general the width is therefore not suppressed at all and it is necessary to examine the p-value. For an illustration the reader may look ahead at Q-functions in our toy model in Fig. 3.

3 Auto-correlated Monte Carlo data

In the above formulae the covariance matrix is assumed to be known, but in practice we have to replace it by an estimate from the Monte Carlo data, often in presence of non-negligible auto-correlations, which we discuss next.

We consider explicitly the case where MC data from Markov chains with different update schemes or different equilibrium distributions enter the fit. Extensions to multiple MC chains with the same update scheme, often called replica, are straightforward. On a single MC chain labelled by $\mathcal{E}$ we assume to have estimators $p_i^\mathcal{E}(t)$ at MC time t of several quantities labelled by i, such that

$$\bar{p}_i^\mathcal{E} = \frac{1}{N_\mathcal{E}} \sum_{t=1}^{N_\mathcal{E}} p_i^\mathcal{E}(t) \qquad (3.1)$$

converges to P_i for $N_\mathcal{E} \to \infty$. In general, the Y-variables in our fits are functions

$$Y_j = \eta_j(P) \qquad (3.2)$$

of primary observables P, estimated by $\bar{y}_j = \eta_j(\bar{p})$. Note that if different chains yield estimators for the same observable P_i, we just replace P_i by the (weighted) average over the different chains. This average is then considered as part of the function η_j.

3.1 Γ-method

The preferred method for dealing with auto-correlations in the error estimate of $\bar{p}_i^{\mathcal{E}}$ is the so-called Γ-method [1,5] (different error estimators are discussed in Appendix D). It inherits its name from the matrix valued auto-correlation function

$$\Gamma_{ij}^{\mathcal{E}}(t) = \langle \Delta p_i^{\mathcal{E}}(t + t_0)\, \Delta p_j^{\mathcal{E}}(t_0)\rangle_{\mathcal{E}}, \quad \Delta p_i^{\mathcal{E}}(t) = p_i^{\mathcal{E}}(t) - P_i. \tag{3.3}$$

Here the average $\langle . \rangle_{\mathcal{E}}$ may be defined as the t_0-average of an infinitely long chain. Linearizing the error propagation and applying the chain rule as in [1] leads to the same simple form above ($\Delta p \to \Delta y$) also for the auto-correlation function of derived quantities, with the linearized fluctuations given by

$$\Delta y_i^{\mathcal{E}}(t) = \sum_k \left.\frac{\partial \eta_i}{\partial p_k}\right|_{p=P} \Delta p_k^{\mathcal{E}}(t). \tag{3.4}$$

Since the covariance matrix of the variables $\bar{y}_i^{\mathcal{E}}$ reads

$$C_{ij}^{\mathcal{E}} = \frac{1}{N_{\mathcal{E}}} \sum_{t=-\infty}^{\infty} \Gamma_{ij}^{\mathcal{E}}(t), \tag{3.5}$$

the expected χ^2, eq. (2.13), becomes

$$\langle \chi^2(\bar{a})\rangle = \sum_{\mathcal{E}} \frac{1}{N_{\mathcal{E}}} \sum_{t=-\infty}^{\infty} \mathrm{tr}\left[\Gamma^{\mathcal{E}}(t)\, W(1-\mathcal{P})W\right], \tag{3.6}$$

in presence of auto-correlations. With finite length MC data the above formulae need to be supplemented by summation windows in t, over which the MC estimate of $\Gamma_{ij}^{\mathcal{E}}(t)$, denoted by $\Gamma_{ij}^{\mathcal{E},\mathrm{MC}}(t)$, should be summed [1,5,6]. Hence a good approximation to eq. (3.6) is found in the form

$$\langle \chi^2(\bar{a})\rangle = E_f \pm \Delta E_f, \quad E_f = \sum_{\mathcal{E}} E_f^{\mathcal{E}}(w_{\mathcal{E}}), \tag{3.7}$$

$$E_f^{\mathcal{E}}(w_{\mathcal{E}}) = \frac{1}{N_{\mathcal{E}}} \sum_{t=-w_{\mathcal{E}}}^{w_{\mathcal{E}}} \mathrm{tr}[\Gamma^{\mathcal{E},\mathrm{MC}}(t)\, W(1-\mathcal{P})W], \tag{3.8}$$

or, assuming $W^{-2} = \mathrm{diag}(C)$ (uncorrelated fit),

$$\langle \chi^2(\bar{a})\rangle = N_{\mathrm{x}} - E_s \pm \Delta E_s, \quad E_s = \sum_{\mathcal{E}} E_s^{\mathcal{E}}(w_{\mathcal{E}}), \tag{3.9}$$

$$E_s^{\mathcal{E}}(w_{\mathcal{E}}) = \frac{1}{N_{\mathcal{E}}} \sum_{t=-w_{\mathcal{E}}}^{w_{\mathcal{E}}} \mathrm{tr}[\Gamma^{\mathcal{E},\mathrm{MC}}(t)\, W\mathcal{P}W]. \tag{3.10}$$

In both cases the standard automatic windowing procedure of Ref. [1] or the one of Ref. [6] may be applied simply replacing $\Gamma_F(t)$ in Ref. [1] by $\mathrm{tr}[\Gamma(t)\, W\mathcal{P}W]$ or $\mathrm{tr}[\Gamma(t)\, W(1-\mathcal{P})W]$, while nothing changes in the discussions in Refs. [1,6]. Note that the knowledge of the full covariance matrix is not required. Its presence is captured by the traces in eq. (3.8) and eq. (3.10). We may use the same automatic determination of the windows ensemble by ensemble and possibly the addition of a tail [6] due to large auto-correlations and will have balanced statistical and systematic errors (from the truncation of the t-sum) of size

$$\Delta E_{f,s}^2 \approx 2 \sum_{\mathcal{E}} \frac{2w_{\mathcal{E}} + 1}{N_{\mathcal{E}}} \left[E_{f,s}^{\mathcal{E}}(w_{\mathcal{E}})\right]^2. \tag{3.11}$$

Assuming that the required $w_{\mathcal{E}}$ are not much different, for strong correlations (not auto-correlations) eq. (3.8) will be more precise, while in the opposite case eq. (3.10) will be better. Obviously one may just evaluate both and take the one with the smaller error.

The covariance matrix may be estimated from $\Gamma_{ij}^{\mathcal{E},\mathrm{MC}}$ by truncating the t-sum in eq. (3.5) to the summation windows $w_{\mathcal{E}}$ obtained from the automatic procedure for $E_{f,s}^{\mathcal{E}}$. The p-value is then obtained from eq. (2.18). In Sect. 4 we demonstrate in a toy model that this is a valid approach, namely the p-value is stable against increasing the window size. Note that only modes with $\lambda(\nu) > 0$ enter eq. (2.18).

Two remarks on the error estimates, eq. (3.11) are in order. These are of the type error-of-the-error. As is common [1, 5, 6], we use the Madras-Sokal approximation, which consists of neglecting the connected parts of a dynamical four-point function. We are not aware of a general argument on the quality of this approximation, but F. Virotta found that it works quite well in a simple interacting field theory [7]. Secondly eq. (3.11) neglects the statistical error of $\mathcal{P}$ which is a function of $\bar{a}$ and of the same order of $\Delta E_{f,s}$. In Appendix A we provide the analytic formula for its evaluation and in all our experiments we find it to be subdominant compared to the terms in eq. (3.11).

4 Numerical illustration

4.1 Toy model

As an illustration, we consider the free one-component scalar theory with standard action,

$$S = a^d \sum_x \left[\frac{1}{2} \partial_\mu \phi(x) \partial_\mu \phi(x) + \frac{m^2}{2} \phi^2(x) \right] \tag{4.1}$$

on a $T \times L^d$ torus (periodic boundary conditions) discretized on a hyper-cubic lattice with spacing a and standard discrete forward derivative ∂_μ. Our observables are the often used time-momentum correlation functions

$$G_{\phi\phi}(t, \mathbf{p}) = a^d \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \langle \phi(t,\mathbf{x})\phi(0) \rangle, \quad G_{\phi^2\phi^2}(t) = a^d \sum_{\mathbf{x}} \langle \phi^2(t,\mathbf{x})\phi^2(0) \rangle. \tag{4.2}$$

In absence of interactions, the Green function $G_{\phi\phi}$ on a torus with finite time extent T is given by

$$G_{\phi\phi}(t, \mathbf{p}) = \sum_{n=-\infty}^{\infty} \Delta(t + nT, \mathbf{p}), \tag{4.3}$$

in terms of the infinite T propagator

$$\Delta(t, \mathbf{p}) = \frac{e^{-|t|\,\omega(\mathbf{p})}}{2\sinh(a\omega(\mathbf{p}))/a}, \tag{4.4}$$

where $\omega(\mathbf{p})$ satisfies the lattice dispersion relation

$$2[\cosh(a\omega(\mathbf{p})) - 1] = a^2 m^2 + 2 \sum_{i=1}^d (1 - \cos(ap_i)), \tag{4.5}$$

and $p_i = \frac{2\pi}{L} k_i$, $k_i = 0, 1, \dots L/a - 1$. A further correlator is

$$G_{\phi^2\phi^2}(t) = \frac{2}{L^d} \sum_{\mathbf{p}} G_{\phi\phi}(t, \mathbf{p})^2 + \frac{1}{L^d} \left[\sum_{\mathbf{p}} G_{\phi\phi}(0, \mathbf{p}) \right]^2, \tag{4.6}$$

where the second term is a disconnected contribution which dominates at long distances.

On a given MC configuration, one may estimate $G_{\phi\phi}$ from

$$E_{\phi\phi}(t, \mathbf{p}) = \tilde{\phi}(t, \mathbf{p})\, \tilde{\phi}(0, -\mathbf{p})\,, \quad \tilde{\phi}(t, \mathbf{p}) = \frac{a^d}{L^{d/2}} \sum_{\mathbf{z}} e^{-i\mathbf{p}\cdot\mathbf{z}} \phi(z_0, \mathbf{z})\,, \tag{4.7}$$

and for the case of negligible auto-correlations, i.e. measurements separated by MC time much larger than the exponential auto-correlation time, the covariance matrix of N measurements of the estimators $E(t, \mathbf{p})$ takes the simple form $(g(t) \equiv G_{\phi\phi}(t, \mathbf{p}))$

$$N \times \mathrm{Cov}(t, t') = g(t)g(t') + \delta_{\mathbf{p},0}\, g(t - t')g(0)\,. \tag{4.8}$$

We note that off-diagonal matrix elements are exponentially suppressed by $e^{-|t-t'|m}$ and there is the typical strong exponential noise/signal enhancement at large $t \approx t'$. For the noisy $G_{\phi^2\phi^2}$ correlator, we employ an estimator with a maximal volume average,

$$E_{\phi^2\phi^2}(t) = \frac{a^{d+1}}{TL^d} \sum_{z_0=0}^{T-a} \overline{\phi^2}(z_0 + t)\, \overline{\phi^2}(z_0)\,, \quad \overline{\phi^2}(z_0) \equiv \sum_{\mathbf{z}} \phi^2(z_0, \mathbf{z})\,, \tag{4.9}$$

4.2 Simulation

To illustrate our method on auto-correlated data similar to standard lattice QCD calculations, we simulated the free theory in 1+1 dimensions with the following algorithm. We performed a MC iteration composed of a Hybrid Monte Carlo (HMC) trajectory of length 4 molecular dynamics units [8] followed by one Metropolis sweep. Both the integration of the equations of motion in the HMC and the width of the Metropolis proposal were tuned to have $\approx 80\%$ acceptance. The Metropolis sweep was added to avoid exceedingly large auto-correlations, specific to the free theory [9]. Setting $am = 0.075$, we simulated a lattice of size 160×40 and generated several
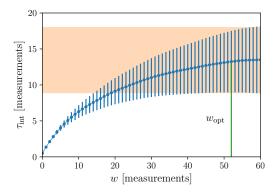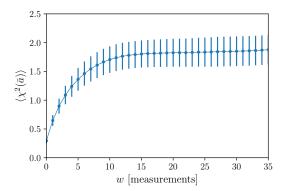

Figure 1: Determination of the integrated auto-correlation time, τ_{int}, of $\langle\phi^2\rangle$ with the window size w_{opt} determined by $\tau_{\mathrm{int}} = 4w_{\mathrm{opt}}$.

replica of 2000 consecutive configurations with the algorithm describe above. For this setup auto-correlations (cf. the upper panel of Fig. 1) are under control but not negligible, thus mimicking a common situation in lattice QCD.

We now investigate the determination of the lowest energy level by a fit to the correlation function $G_{\phi^2\phi^2}^{\mathrm{conn}}(t) = G_{\phi^2\phi^2}(t) - \langle\phi^2\rangle^2$. It is asymptotically dominated by the (2-particle state, each with momentum $\mathbf{p} = \mathbf{0}$) level $aE_{\mathrm{exact}} = 2a\omega(\mathbf{0}) = 2\cosh^{-1}(1 + a^2m^2/2) \approx 0.15$. The higher levels are two-particle states with non-zero momentum of $|\mathbf{p}| \geq 2\pi/L$. This leads to a gap of $a\Delta E \approx 0.2$. We study the typical approach to the problem of extracting the lowest level through fits to the functional form $A_{\mathrm{fit}} e^{-m_{\mathrm{fit}} t}$ to $G_{\phi^2\phi^2}^{\mathrm{conn}}(t)$. Of course these suffer from the contaminations $\mathrm{O}(\exp(-t\Delta E))$ which are neglected in the fit function. Furthermore the signal-to-noise problem
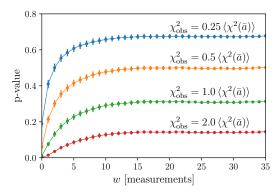
Figure 2: Fits of $G^{\mathrm{conn}}_{\phi^2\phi^2}(t) = G_{\phi^2\phi^2}(t) - \langle\phi^2\rangle$ in a fit-range $t/a \in [4, 26]$. Several replica are considered and error bars are obtained from the fluctuations over the replica. The left and right panels show the estimator $E_f(w)$, eq. (3.8), and the p-value for several choices of χ^2_{obs} as a function of the window size w in units of measurements.

is quite severe for $G^{\mathrm{conn}}_{\phi^2\phi^2}(t)$. We therefore consider fits only up to an upper cut, which we set to $t_{\max}/a = 26$.

We demonstrate the determination of $\langle\chi^2(\bar{a})\rangle$ in Fig. 2 for a typical such fit. Neglecting auto-correlations ($w = 0$) leads to a significant underestimate of $\langle\chi^2(\bar{a})\rangle$. However, this is no issue, because one can easily sum up to an appropriate window size w, even with only 2000 measurements as used here. In fact, the window summation of $\langle\chi^2(\bar{a})\rangle$ saturates earlier than the one of typical observables, e.g. $\langle\phi^2\rangle$, Fig. 1.
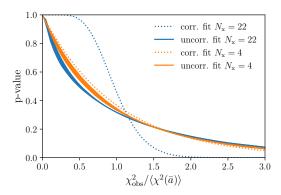
4.3 p-value

We can identify statistically good fits as those which have an acceptable p-value, say $Q \gtrsim 0.05$. For a correlated fit with a known covariance matrix we have $\nu = \mathcal{P}$, and thus $\langle\chi^2(\bar{a})\rangle = N_{\mathrm{x}} - N_{\mathrm{A}}$. Furthermore, its p-value is simply given by

$$Q(\chi^2_{\mathrm{obs}}, \mathcal{P}) = \gamma\big((N_{\mathrm{x}} - N_{\mathrm{A}})/2, \chi^2_{\mathrm{obs}}/2\big) \tag{4.10}$$

in terms of the upper incomplete γ-function. In Fig. 3 we compare this particular case to $Q(\chi^2_{\mathrm{obs}}, \nu)$, eq. (2.18), for uncorrelated fits. Several replica of 2000 measurements are used. For each replicum the computation of $\langle\chi^2(\bar{a})\rangle$ employs the automatic windowing procedure [1] for E_f. The determined window w_{opt} is used to estimate the matrix ν from the covariance matrix. The uncertainty of Q due to the statistical fluctuations of ν is then estimated from the width of the replica-distribution. This very small uncertainty is given by the widths of the solid lines in the left panel of Fig. 3.

While in correlated fits with a *large number of degrees of freedom*, a criterion $\chi^2/\langle\chi^2(\bar{a})\rangle \approx 1$ is a good discriminator between good and bad fits, in general the p-value needs to be considered. Indeed, for uncorrelated fits, it is even more important to base the acceptance on the p-value as demonstrated by Fig. 3. Acceptable p-values are still present for χ^2_{obs} significantly above $\langle\chi^2(\bar{a})\rangle$ – also for large $N_{\mathrm{x}} - N_{\mathrm{A}}$. The right panel of the figure shows the Q-function for a different case, namely a fit to $G_{\phi\phi}$, where we use the analytic covariance matrix without uncertainties. Again values of $\chi^2_{\mathrm{obs}}/\langle\chi^2(\bar{a})\rangle$ above 1.5 still have rather good p-values. Since Q is easily evaluated, there is no drawback in always basing the acceptance of a fit on it. Also auto-correlations are easy to control: Fig. 2 shows the dependence of Q on the summation window of the auto-correlation functions. One may again just use the w_{opt} determined in the analysis of $\langle\chi^2(\bar{a})\rangle$.
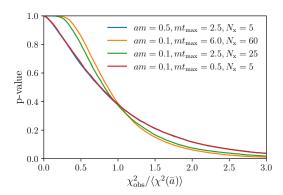
Figure 3: The p-value as a function of the observed χ^2, χ^2_{obs}, divided by $\langle\chi^2(\bar{a})\rangle$.
Left: Fits of $G^{\mathrm{conn}}_{\phi^2\phi^2}(t)$ are done in a range $t \in [t_{\min}, t_{\max}]$ where $t_{\min}/a$ of 4 and 22 are considered, with $t_{\max}/a = 26$. For correlated fits the exact formula eq. (4.10) is illustrated by dashed lines. For uncorrelated fits we evaluated eq. (2.18). The statistical error of the p-value curves for uncorrelated fits, estimated from several replica, is given by the widths of the curves.
Right: The p-value of uncorrelated fits to $G^{\mathrm{conn}}_{\phi\phi}(t)$ is evaluated from the exact covariance matrix eq. (4.8).

4.4 Determination of the fit window

At this point we turn to the typical problem of finding the minimal value of the lower end of the fit range, $t_{\min}$, for which the single exponential ansatz describes well the data. We want to compare the use of the uncorrelated fits to correlated ones, but the covariance matrices estimated with the statistics of our test-runs are (typically) not positive. Therefore we generated a long MC chain with 40000 measurements solely to estimate C, and use $W = C^{-1/2}$ in the definition of the correlated χ^2. Of course, this is not a viable procedure in general while uncorrelated fits are always possible.
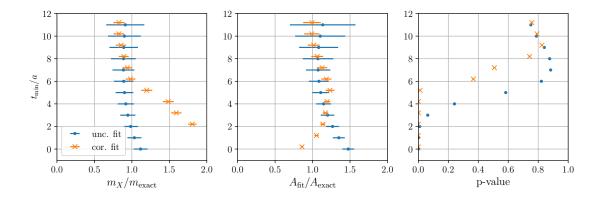

Figure 4: In the left and middle panels we show the fitted masses and amplitudes normalized by their exact asymptotic value as a function of $t_{\min}$ with $t_{\max}/a = t_{\min}/a + 18$. Results for correlated and uncorrelated fits are represented by orange crosses and blue dots respectively. In the right panel we plot the p-values.

In Fig. 4 we show one out of several replica of 4000 measurements each. We compare the results of fits to $G^{\mathrm{conn}}_{\phi^2\phi^2}(t)$ to the true asymptotic values of the parameters. When the p-values becomes acceptable the fitted parameters agree reasonably well with their exact asymptotic values.[3] This illustrates that uncorrelated fits can be judged by the computed p-value. In contrast, the naive

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[3] We repeated the exercise for larger L with all other parameters the same. In that case the gap, ΔE, is smaller and the good fits need larger $t_{\min}$. The parameters, in particular the amplitude A_{fit}, are then further off when the p-value is not satisfactory.

goodness of fit criterion, $\langle \chi^2(\bar{a}) \rangle / (N_{\mathrm{x}} - N_{\mathrm{A}}) \lesssim 1$ is useless, since $\langle \chi^2(\bar{a}) \rangle < 1$ for all fits shown. We remind the reader that the correlated fits could be done only by estimating the covariance matrix with a 10-folded statistics.

Quite often the data fluctuate more and in a correlated fashion around the true correlation function. One can then have fits with acceptable p-values, i.e. the fits describe the data over a certain range of a kinematical parameter (here t), but this does not guarantee that the asymptotic values of the model parameters (here A and E_{exact}) are determined. In our numerical experiment we have seen that in six out of ten cases A_{fit} differed from the exact value by 30% to 50% and more than two standard deviations, even when the p-value was acceptable. In that sense, the shown replicum is a lucky case.

While we observe smaller statistical errors in the parameters from correlated fits for a fixed set of data points, uncorrelated fits tend to give acceptable p-values for smaller $t_{\min}$. No particular difference is then observed in the precision of the estimated best fit parameters.

5 Conclusions

Estimating the covariance matrix C from limited correlated and auto-correlated data, in particular the lower part of its spectrum, often proves to be challenging. Here we investigated a method that bypasses the need for the inverse covariance matrix and is numerically robust against fluctuations of its small eigenvalues.

By studying the expansion of the χ^2 function about its minimum, we have obtained expressions to compute the expected value of χ^2 and the corresponding p-value, for arbitrary positive weight matrices W. The formulae contain the covariance matrix in such a way that the upper part of the spectrum of C predominantly determines the expected χ^2 and the p-value. They therefore provide *robust* statistical tests for the fits.

We observe that it is important to use the p-value to discriminate between good and bad fits, not just the reduced χ^2. An investigation in a toy model illustrates how the method works with moderate statistics and with auto-correlations present.

Finally, we would like to emphasize that correlated fits are the preferred choice, when the correlation of the data is known. The issue is "just" that as yet a robust estimator of C^{-1} is missing when we have finite statistics, auto-correlated data.

A Statistical error of $\mathcal{P}$

Here we derive the explicit form of the projector and other useful relations. We begin from the minimum condition, which we rewrite as

$$\mathcal{P} W \delta \bar{y} = W \phi^\alpha(\bar{a}) \delta \bar{a}^\alpha + \mathrm{O}(N^{-1}). \tag{A.1}$$

By multiplying on the left by $\phi^{\beta \mathrm{T}}(\bar{a}) W$, we obtain

$$\delta \bar{a}^\alpha = [H^{-1}]^{\alpha\beta} (W \phi^\beta, W \delta \bar{y}), \quad H^{\alpha\beta} = (W \phi^\alpha(\bar{a}), W \phi^\beta(\bar{a})), \tag{A.2}$$

which tells how to propagate the errors from the data to the fitted parameters. More specifically the covariance matrix of $\bar{a}^\alpha$ reads

$$C^{\alpha\beta} = [H^{-1}]^{\alpha\alpha'} (W\phi^{\alpha'}, C_{\mathrm{w}}W\phi^{\beta'}) [H^{-1}]^{\beta'\beta} . \tag{A.3}$$

Now combining together eq. (A.2) and eq. (A.1) one quickly obtains

$$\mathcal{P} = W\phi^\alpha(\bar{a}) [H^{-1}]^{\alpha\beta} (\phi^\beta)^{\mathrm{T}}(\bar{a})W \tag{A.4}$$

which satisfies all the properties outlined in the main text. The partial derivative

$$\frac{\partial\langle\chi^2(\bar{a})\rangle}{\partial\bar{a}^\alpha} = 2\mathrm{tr}\big[C_{\mathrm{w}}\mathcal{K}^\alpha(1-\mathcal{P})\big] , \tag{A.5}$$

combined with eq. (A.3) gives us the explicit form of the contribution to the error of $\langle\chi^2(\bar{a})\rangle$ that originates from the dependence of $\mathcal{P}$ upon $\bar{a}^\alpha$, which we neglect. In the derivation of the result above, we have used

$$\mathcal{P}^\alpha = \frac{\partial\mathcal{P}}{\partial\bar{a}^\alpha} = \mathcal{K}^\alpha(1-\mathcal{P}) + (1-\mathcal{P})(K^\alpha)^{\mathrm{T}} , \quad \mathcal{K}^\alpha = W\phi^{\alpha'}(\bar{a}) [H^{-1}]^{\alpha'\beta'} (\phi^{\beta'\alpha})^{\mathrm{T}}(\bar{a})W . \tag{A.6}$$

B   Reference implementations

A reference implementation in MATLAB/Octave and Python is publicly available at this link https://github.com/mbruno46/chiexp. Documentation on the syntax can be consulted online, https://mbruno46.github.io/chiexp, from the git repository, locally after downloading it or by using the corresponding `help` functions in the MATLAB or Python interactive sessions.

C   Generalizations

In the main text we have considered the case of data described by a single fit function, but more complicated cases can be easily accommodated.

When different sets of data $Y^{(1)}, Y^{(2)}$ (with different sizes M_1 and M_2) are described by different models $\phi^{(1)}, \phi^{(2)}$ with a few common parameters, it suffices to extend $N_{\mathrm{x}} = M_1 + M_2$ to incorporate all points, such that

$$\begin{aligned}
\bar{y}_i &= \{\bar{y}_1^{(1)}, \ldots, \bar{y}_{M_1}^{(1)}, \bar{y}_1^{(2)}, \ldots, \bar{y}_{M_2}^{(2)}\} , \\
\phi_i(a) &= \{\phi_1^{(1)}(a), \ldots, \phi_{M_1}^{(1)}(a), \phi_1^{(2)}(a), \ldots, \phi_{M_2}^{(2)}(a)\} .
\end{aligned} \tag{C.1}$$

If the two data sets are correlated, e.g. they originate from the same MC ensembles, but estimating the full $N_{\mathrm{x}} \times N_{\mathrm{x}}$ covariance matrix and its inverse turns out to be impractical, the method proposed in this manuscript allows to arbitrarily regularize the covariance matrix in the definition of χ^2 (e.g. just consider the diagonal blocks $M_1 \times M_1$ and $M_2 \times M_2$) and still have a reliable statistical interpretation of the associated fit.

Similarly, there are situations where we might want to include the error of the kinematic coordinates $\bar{x}_i$ (for instance they might be obtained from averages over MC chains which may also be correlated with the data points $\bar{y}_i$). Such cases are easily incorporated by considering the vectors

$$r_i = \{\bar{y}_1 - \Phi(X_1, A), \ldots, \bar{y}_{N_{\mathrm{x}}} - \Phi(X_{N_{\mathrm{x}}}, A), \bar{x}_1 - X_1, \ldots \bar{x}_{N_{\mathrm{x}}} - X_{N_{\mathrm{x}}}\} \tag{C.2}$$

in the definition of $\chi^2 = ||Wr||^2$. The matrix W^2 may correspond to various regularizations of the inverse of the extended covariance matrix

$$C = \left\langle \begin{matrix} \delta\bar{y}\delta\bar{y}^{\mathrm{T}} & \delta\bar{y}\delta\bar{x}^{\mathrm{T}} \\ \delta\bar{x}\delta\bar{y}^{\mathrm{T}} & \delta\bar{x}\delta\bar{x}^{\mathrm{T}} \end{matrix} \right\rangle , \tag{C.3}$$

and nothing changes in the derivation of $\langle\chi^2(\bar{a})\rangle$ and in the discussion on the goodness-of-fit for the model function ϕ. In the equations above X_i represent the true values of the kinematic coordinates, and $\delta\bar{x}_i = \bar{x}_i - X_i$.

D Alternative estimators of the covariance matrix

In this Appendix we discuss the replacement of the Γ-method by other error estimation techniques.

D.1 Jackknife and binning methods

When it is known that the (exponential) auto-correlation time is small compared to the run length $N_\mathcal{E}$, the covariance matrix may be estimated by Jackknife resampling of binned data, with bin length significantly larger than the auto-correlation time. Assuming that $N_\mathcal{E} = B_\mathcal{E} N_B^\mathcal{E}$, blocked measurements on a given ensemble are defined as

$$b_i^\mathcal{E}(k) = \frac{1}{B_\mathcal{E}} \sum_{t=1}^{B_\mathcal{E}} p_i^\mathcal{E}((k-1)B_\mathcal{E} + t), \quad k = 1, \ldots, N_B^\mathcal{E}, \tag{D.1}$$

while complementary or jackknife bins are

$$c_i^\mathcal{E}(k) = \frac{N_B^\mathcal{E} \bar{p}_i^\mathcal{E} - b_i^\mathcal{E}(k)}{N_B^\mathcal{E} - 1}. \tag{D.2}$$

An estimator of the covariance matrix is given by

$$C_{ij} = \sum_\mathcal{E} \frac{N_B^\mathcal{E} - 1}{N_B^\mathcal{E}} \sum_{k=1}^{N_B^\mathcal{E}} \Delta c_i^\mathcal{E}(k) \Delta c_j^\mathcal{E}(k), \quad \Delta c_i^\mathcal{E}(k) = c_i^\mathcal{E}(k) - \bar{p}_i^\mathcal{E}, \tag{D.3}$$

and the case of derived observables $Y_i = \eta_i(P)$ is obtained by replacing $c_i^\mathcal{E}(k)$ with $\eta_i(c^\mathcal{E}(k))$ in the equations above. The generalization of our previous results to jackknife estimators is straightforward: starting from the intermediate quantities

$$E_f^\mathcal{E}(k) = [\Delta c^\mathcal{E}(k)]^\mathrm{T} W(1 - \mathcal{P}) W \Delta c^\mathcal{E}(k), \tag{D.4}$$

$$E_s^\mathcal{E}(k) = [\Delta c^\mathcal{E}(k)]^\mathrm{T} W \mathcal{P} W \Delta c^\mathcal{E}(k), \tag{D.5}$$

the central value of $\langle \chi^2(\bar{a}) \rangle$ is obtained by replacing $E_{f,s}$ in eq. (3.7) and eq. (3.9) with

$$E_{f,s} = \sum_\mathcal{E} \frac{N_B^\mathcal{E} - 1}{N_B^\mathcal{E}} \sum_{k=1}^{N_B^\mathcal{E}} E_{f,s}^\mathcal{E}(k). \tag{D.6}$$

Using the results of Ref. [1] one can estimate their errors according to

$$[\Delta E_{f,s}]^2 \approx 2 \sum_\mathcal{E} \frac{1}{N_B^\mathcal{E}} [E_{f,s}^\mathcal{E}]^2, \tag{D.7}$$

whereas the p-value is estimated from the covariance matrix in eq. (D.3).

We refer the interested reader to Refs. [10, 11] for a discussion of bootstrap resampling, to directly estimate $\langle \chi^2(\bar{a}) \rangle$. When it is known that auto-correlations are negligible (e.g. because the data can be binned with a large bin size), this is certainly a valid approach. Our proposal based on the Γ-method allows to directly examine and control auto-correlation effects.

D.2 Priors and the Bayesian approach

Gaussian priors on the parameters, a special case of a Bayesian analysis, are easily taken into account by extending the r vectors to

$$r_i = \{\bar{y}_1 - \Phi(x_1, a), \ldots, \bar{y}_{N_x} - \Phi(x_{N_x}, a), a_1 - \widetilde{a}_1, \ldots, a_{N_{\mathrm{priors}}} - \widetilde{a}_{N_{\mathrm{priors}}}\} \tag{D.8}$$

and the covariance matrix to

$$C = \left\langle \begin{matrix} \delta\bar{y}\delta\bar{y}^\mathrm{T} & 0 \\ 0 & \mathrm{diag}[1/\sigma_{\widetilde{a}_1}^2, \ldots, 1/\sigma_{\widetilde{a}_{N_{\mathrm{priors}}}}^2] \end{matrix} \right\rangle, \tag{D.9}$$

with $\widetilde{a}^\alpha$ and $\sigma_{\widetilde{a}^\alpha}$ representing the prior and its width for the parameter a^α. One can easily verify that for correlated fits $\langle \chi^2(\bar{a}) \rangle = N_x + N_{\mathrm{priors}} - N_A$.

D.3 Master fields

Recently M. Lüscher has derived formulae [12] for statistical errors based on the invariance under translations of space-time, rather than of Monte-Carlo time. We write

$$\bar{y}_i = \frac{1}{V} \sum_s y_i(s) \,, \quad \lim_{V \to \infty} \bar{y}_i = Y_i \,, \tag{D.10}$$

with s labelling the sites for a given large-volume configuration, called master field. Following Ref. [13], the Γ method is then defined from the counter-part of $\Gamma^{\mathrm{MC}}(t)$, which we may now call $\Gamma^{\mathrm{MF}}_{ij}(s)$, and which is evaluated from the fluctuations $\delta\bar{y}_i(s) = y_i(s) - \bar{y}_i$. As described in Ref. [12], the variance of $\bar{y}_i$ may be obtained by summing $\Gamma^{\mathrm{MF}}_{ii}(s)$ up to distances $|s| < R$, thus introducing only an exponentially small bias of order $e^{-2m_\pi R}$. Our formulae then hold after replacing $\Gamma^{\mathrm{MC}}_{ij}$ with $\Gamma^{\mathrm{MF}}_{ij}$ e.g. in eq. (3.6) and after providing an appropriate windowing procedure.

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