Bayesian Analysis of Many-Pole Fits of Hadron Propagators in Lattice QCD

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We use Bayes’ probability theorem to analyze many-pole fits of hadron propagators. An alternative method of estimating values and uncertainties of the fit parameters is offered, which has certain advantages over the conventional methods. The probability distribution of the parameters of a fit is calculated. The relative probability of various models is calculated.

1. Introduction

A common procedure in Lattice QCD is to calculate a correlation function in a certain channel and then fit it as a sum of several exponentials [1]. The parameters of the fits are estimated by minimizing $\chi^2$. To find the errors, ideally the calculations should be repeated many times, but this is impractical. Usually the jackknife or the bootstrap is performed. Instead here we use Bayes’s theorem to derive the parameters’ probability distribution for given data from the probability of the data for given parameters. Usually one determines the number of poles by comparing $\chi^2$. To find the errors, ideally the calculations should be repeated many times, but this is impractical. Usually the jackknife or the bootstrap is performed. Instead here we use Bayes’s theorem to derive the parameters’ probability distribution for given data from the probability of the data for given parameters. Usually one determines the number of poles by comparing $\chi^2$. To find the errors, ideally the calculations should be repeated many times, but this is impractical. Usually the jackknife or the bootstrap is performed. Instead here we use Bayes’s theorem to derive the parameters’ probability distribution for given data from the probability of the data for given parameters. Usually one determines the number of poles by comparing $\chi^2$. To find the errors, ideally the calculations should be repeated many times, but this is impractical. Usually the jackknife or the bootstrap is performed. Instead here we use Bayes’s theorem to derive the parameters’ probability distribution for given data from the probability of the data for given parameters. Usually one determines the number of poles by comparing $\chi^2$.

1.1. Bayes’ theorem and its applications

Bayes’ theorem reads:

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

where $P(A|B)$ is the conditional probability that proposition $A$ is true, given that proposition $B$ is true. Bayes’ theorem reads:

$$P(T|D, I)P(D|I) = P(D|T, I)P(T|I),$$

where $T$ is the theoretical model to be tested, $D$ is the data, and $I$ is the prior information.

II. Calculate the average values $\overline{E}_i$ and the standard deviations $\sigma_{E_i}$ (similarly for $c_i$)

$$\overline{E}_n = \int dE_n E_n P(E_n|D),$$

$$\sigma_{E_i}^2 = \int dE_n (E_n - \overline{E}_n)^2 P(E_n|D),$$

provided $P(E_n|D)$ is normalized.

III. Compare several models $T_i$, (for example one pole, two pole and three pole models). We cannot find the absolute probability of a theory, since we do not have the “complete set” of theories. But we can calculate the relative probabilities of two theories:

$$\frac{P(T_i|D)}{P(T_j|D)} = \frac{P(T_i)P(D|T_i)}{P(T_j)P(D|T_j)}$$

provided $P(E_n|D)$ is normalized.
\(P(D|T)\) can be obtained from \(P(D\{c, E\})\) by integrating over all parameters of the theory:

\[
P(D|T) = \int \{dc\}{dE} P\{c, E\} P(D\{c, E\}).
\]

(4)

For the prior probability \(P\{c, E\}\) of the parameters of a model in section 3 we make the “least informative” assumption that \(P(c, E) dc\, dE \sim dc/c\, dE/E\). This form is scale invariant. Priors \(P\{c, E\}\) should be normalized.

The direct probability \(P(D\{c, E\})\) of the data \(D\) can be calculated relatively easily if the data is Gaussian distributed. We generate “fake” data to be used in the analysis. We use an \(n\)-pole model, add noise \(e(t)\) to generate a sample of \(N\) “propagators” \(g_\alpha(t) = \sum_{i=1}^{N} c_\alpha e^{-E_\alpha t} + e(t)\) \((\alpha = 1, ..., N)\), calculate the average \(G(t)\) and estimate the covariance matrix \(C(t, t')\) from the data. Here \(t\) is the discrete, “lattice” time. We vary the number of “propagators” to control the noise level in the data. Here we use \(N = 360\) and \(N = 3600\), which corresponds to a decrease in the noise level by a factor of 3.

The probability distribution of \(G(t)\) is

\[
P(G\{c, E\}) = e^{-\chi^2(c, E)/2},
\]

(5)

where \(\chi^2\) is calculated using the full covariance matrix \(\chi^2\). The individual \(g_\alpha(t)\) need not be Gaussian distributed, as long as we average over enough of them so that \(G(t)\) are Gaussian distributed of the “fake” data is ensured.

3. Estimating the Parameters.

3.1. 1 pole data.

We generate data \(D\) for the one pole model with \(c_1 = 0.15\) and \(E_1 = 0.485\). We use the one pole model to fit the data. Here we assume the prior probability of the data \(P\{c, E\}\) to be constant. Then the posterior probability of the parameters \(P\{c, E\}|D\) is up to a constant equal to the direct probability of the data given by equation (4). The posterior probability density for \(E_1\)

\[
P(E_1|D) = \frac{\int dc_1 e^{-\chi^2(c_1, E_1)/2}}{\int dc_1\, dE_1 e^{-\chi^2(c_1, E_1)/2}}.
\]

(6)

It begs for the Monte Carlo integration with the Metropolis algorithm.

We generate a set of points \((c_1, E_1)\). Every point is characterized by \(\chi^2(c_1, E_1)\). We sample the vicinity of the minimum of \(\chi^2(c_1, E_1)\) [maximum of \(exp(-\chi^2(c_1, E_1))\)] (Fig. 1).

![Figure 1. \(\chi^2\) vs. the point number \(n\).](image1)

We make a scatter plot \(c_1\) vs. \(E_1\) (Fig. 2) to visualize this distribution. The density of the points is proportional to the weight \(exp(-\chi^2(c_1, E_1))\).

![Figure 2. Scatter plot of \(\chi^2\) in \((c, E)\) space.](image2)

Taking integrals (3) is equivalent to making a histogram with steps big enough to make the distribution smooth (Fig. 3).

![Figure 3. Probability distribution \(P(E)\).](image3)
0.4851(1) and \( c = 0.1499(2) \). The present approach conserves computational time compared to the jackknife. If one uses simulated annealing to fit the data, one covers the same regions in the \((c_i, E_i)\) space as needed to calculate probability distributions \( 3 \). With the probability distributions one immediately obtains the parameters and errors, whereas with the jackknife the fitting has to be repeated \( N \) times.

3.2. 2 Pole data

We repeat the analysis performed in section 3.1 for two-pole data when the poles are well separated: \( c_1^{in} = 0.1, c_2^{in} = 0.1, E_1^{in} = 0.5, E_2^{in} = 0.6 \). We use the two-pole model to fit the data. The probability distributions for the energies and coefficients are obtained and the parameters are estimated just as in section 3.1.

The only complication is that now we have to deal with the 4-d space of parameters \((c_1, E_1, c_2, E_2)\). We perform a Monte Carlo integration as described above. The 4-d probability distribution is visualized by projecting it onto two planes \((c_1, E_1)\) and \((c_2, E_2)\). Each blob in Fig. 4 is a projection of the 4-d distribution on a 2-d plane. Each blob represents the probability distribution for one pair of \((c_i, E_i)\) after the second pair has been integrated out.

![Figure 4. Scatter plot of \( \chi^2 \) projected on \((c_1, E_1)\) and \((c_2, E_2)\) planes and combined on one plane.](image)

Table 1 contains the values of \( \chi^2 \) obtained when 1 and 2 pole data are fit with 1 and 2 pole models.

| data # of propagators model | 1 pole | \( \chi^2/dof \) |
|-----------------------------|--------|-----------------|
| 1 pole 360 | 1 pole | 0.61 |
| 2 pole 360 | 2 pole | 0.57 |
| 1 pole 3600 | 1 pole | 1.2 |
| 2 pole 3600 | 2 pole | 1.3 |
| 2 pole 360 | 1 pole | 0.87 |
| 2 pole 3600 | 2 pole | 0.99 |
| 1 pole 3600 | 1 pole | 2.0 |
| 1 pole 3600 | 1 pole | 1.2 |

Table 1. Values of \( \chi^2 \) for fitting 1 and 2 pole data of different noise levels with 1 and 2 pole models.

4. Model selection

Unless one has some prior knowledge, determining the number of poles present in the data based on comparing \( \chi^2 \) for models with different numbers of poles is very often ambiguous.

Table 3 contains the values of \( \chi^2 \) obtained when

\[
P(D|1pole) = \int dc_1dE_1 \frac{e^{-\chi^2(c_1,E_1)}}{c_1E_1} \quad (7)
\]

The integration is tricky since we are dealing with a function that varies rapidly in the multidimensional space. We use scatter plots to determine the areas of integration. Table 3 contains integration results for the total probability ratio \( R = \frac{P(1pole|D)}{P(2pole|D)} \). With a sufficiently low noise level the total probabilities ratio picks the correct model. If we estimate the parameters of the 2 pole data with 3600 propagators using equation \( 6 \), we get the input parameters back within the error bars. The jackknife here gives unreasonably large errors because \( \chi^2 \) has several minima in the \((c_1, c_2, E_1, E_2)\) space. It can be seen from the graph of \( \chi^2 \) vs. \( n \) (Fig. 7), and they can be also clearly identified on the scatter plot (Fig. 8). Two
| R   | # of propagators | data |
|-----|------------------|------|
| 1 pole | 360              | 3    |
| 2 pole | 3600             | 0.02 |

Table 2
Total probabilities ratio R.

minima (1 and 3) have the same \( \chi^2 \). When we perform the jackknife, the blind fitting finds either minimum 1 or 3, which results in the unreasonably large error estimates.

![Figure 7. \( \chi^2 \) has multiple minima.](image)

![Figure 8. Three minima of \( \chi^2 \) from Fig.7 projected on the two-dimensional plane \((c,E)\).](image)

5. Analysis of SU(2) data

Here we analyze hadron propagators in the pseudoscalar channel. The detailed description of these data is given in [4,5]. The coupling constant \( \beta = 2.5 \), lattice spacing \( a = 0.09 \pm 0.012 \) fm, the lattice size is \( 12^3 \times 24 \). The propagators analyzed here were calculated with \( \kappa = 0.146 \) for 360 configurations. The point source is at \( t = 5 \). The fit is performed in the time range 6-20.

We repeat the analysis for 60 and 360 configurations to study the data with different noise levels. For 60 configurations the \( \chi^2/dof \) is 1.0 for the 3 pole fit and 1.17 for the 4 pole fit, and the total probabilities ratio is \( \frac{P(3\text{pole}|D)}{P(4\text{pole}|D)} \sim 1 \). For 360 configurations the \( \chi^2/dof \) is 0.52 for the 3 pole model fit and 0.69 for the 4 pole model fit, and the total probabilities ratio for 360 configurations is \( \frac{P(3\text{pole}|D)}{P(4\text{pole}|D)} \sim 10 \). Here again, for low noise data we are able to choose between two models based on a qualitative estimate given by the total probabilities ratio.

6. Conclusion

A new method has been introduced that can be used to analyze many-pole fits of hadron propagators in Lattice QCD. It has been used to estimate the many-pole model parameters and their uncertainties. It works in the presence of multiple minima when the jackknife (at least in its simple minded form) fails. It cuts the computational time. The new method has been used to calculate relative probabilities for different models, which can be crucial in making the optimal choice of a model. The scatter plots, which have been introduced as an auxiliary tool for the multidimensional integration, can be used as an independent tool for the many pole fit analysis.

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