

Padé and Padé-Laplace Methods for masses and matrix elements

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The problem of having to reconstruct the decay rates and corresponding amplitudes of the single-exponential components of a noisy multi-exponential signal is common in many other areas of physics and engineering besides lattice field theory, and it can be helpful to study the methods devised and used for that purpose in those contexts in order to get a better handle on the problem of extracting masses and matrix elements from lattice correlators. Here we consider the use of Padé and Padé-Laplace methods, which have found wide use in laser fluorescence spectroscopy and beyond, emphasizing the importance of using robust Padé approximants to avoid spurious poles. To facilitate the accurate evaluation of the Laplace transform required for the Padé-Laplace method, we also present a novel approach to the numerical quadrature of multi-exponential functions.

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1. Introduction

A crucial problem in lattice field theory is the extraction of particle masses E_n and matrix elements $\langle n|\hat{O}|0\rangle$ from measured correlation functions via their spectral representation,

$$C(t) = \langle O(t)O^*(0) \rangle = \sum_{n=1}^{\infty} A_n e^{-E_n t}$$

with $A_n = |\langle n|\hat{O}|0\rangle|^2$.

While this can in principle be achieved by fitting the measured data, multiexponential fits tend to be unstable and typically require stabilization with Bayesian priors. While variational methods work well for a prior-free determination of masses and matrix elements, they require a full correlator matrix with a range of operators O_i at both source and sink, which is not always a feasible option.

It is therefore desirable to have at one's disposal methods that can solve this problem with just one operator at source and sink. To this end, it is useful to consider methods used for similar purposes in other fields, such as laser fluorescence spectroscopy [1]. Previously, Prony's method found its way into the lattice toolkit in a similar manner from NMR spectroscopy [2].

2. The Padé Method

The correlator $C(t)$ is measured only on discrete timeslices, $C(ka)$, $k \in \mathbb{N}$. A natural object to study is thus the Z transform of $C = \{C(ka) \mid k \in \mathbb{N}\}$ given by

$$\mathcal{Z}[C](z) = \sum_{k=0}^{\infty} C(ka)z^{-k} = \sum_{n=1}^{\infty} \frac{A_n z}{z - \lambda_n} \quad (1)$$

with $\lambda_n = e^{-E_n a}$. One immediately notes that the poles and residues of $\mathcal{Z}[C]$ give the masses and matrix elements.

However, in practice, only finitely many values $C(ka)$ of the correlator are known, which renders the series defining $\mathcal{Z}[C]$ inaccessible. Nevertheless, one can consider Padé approximants to $\mathcal{Z}[C]$ and use their poles and residues as estimates of λ_n , A_n . Interestingly, a naive implementation of this idea is equivalent to Prony's method in exact arithmetic [3].

However, the results tend to be very unstable in the presence of even minimal round-off error: common issues include the emergence of pairs of complex-conjugate poles off the real axis, and of Froissart doublets (a pole and a nearby zero which fail to cancel each other, typically signalled by anomalously small residuals). A solution to these problems is given by the method of robust Padé approximants [4], which use the singular-value decompositions to give an estimate of how many states can be identified from the data.

Even with robust methods, the results obtained using the Padé method are known to quickly deteriorate in the presence of noise [5, 6]. This is borne out by numerical tests on synthetic data. In Fig. 1, we plot the reconstructed energy levels on a synthetic data set with equally spaced energy levels as a function of the number of poles used for the Padé approximant; it can be clearly seen that the lowest few energy levels exponentially approach their true values as the number of poles is increased, until the robust procedure eventually saturates the number of extracted poles. In contrast,

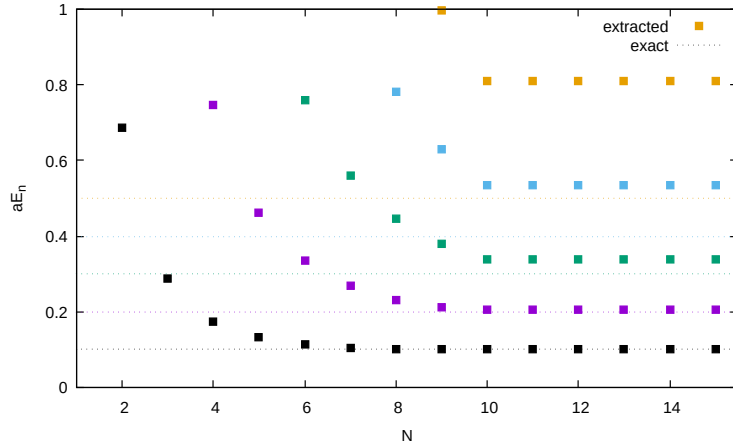


Figure 1: Results from the Padé Method with robust approximants applied to synthetic data. Dashed horizontal lines denote the exact values of the masses, points the extracted results as a function of the number N of poles tried.

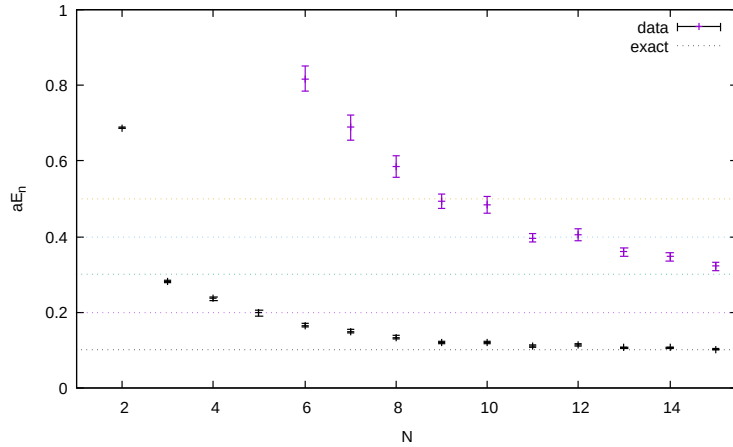


Figure 2: Same as Figure 1, but with a 1% noise applied to the synthetic data.

Fig. 2 shows the results of applying the same procedure to the same toy model, but with a 1% noise applied to the synthetic data; here, the exponential approach to the true value is much slower, and only one excited state can be extracted, albeit with a large systematic error on its energy.

3. The Padé-Laplace Method

To avoid the shortcomings of the Padé method, the Padé-Laplace method was proposed by Yeramian and Claverie in [7]. It is based on noting that the Laplace transform of the correlation function $C(t)$ is given by

$$\mathcal{L}[C](p) = \int_0^\infty dt C(t)e^{-pt} = - \sum_{n=1}^{\infty} \frac{A_n}{p + E_n} \quad (2)$$

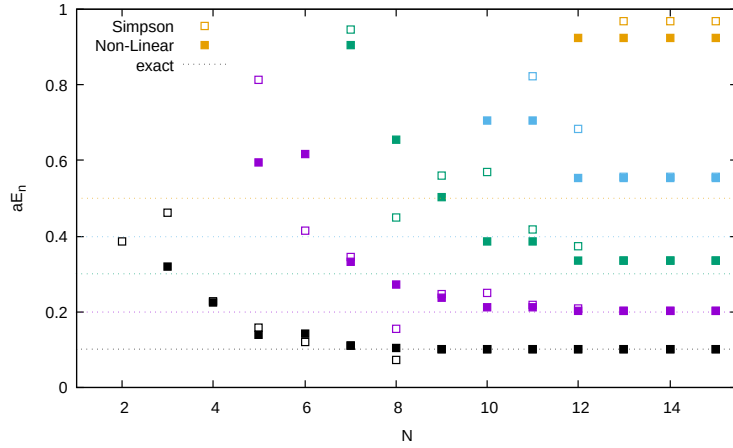


Figure 3: Results from the Padé-Laplace Method with robust approximants applied to synthetic data. Dashed horizontal lines denote the exact values of the masses, points the extracted results as a function of the number N of poles tried. Open symbols use Simpson’s rule for the numerical integration, filled symbols a novel non-linear quadrature formula specialized to exponentially-decaying integrands.

so that the poles and residues of the Laplace transform again yield the masses and matrix elements of interest.

The full functional form of the Laplace transform is not available from numerical data, but we can compute Padé approximants to $\mathcal{L}[C]$ by noting that the Taylor coefficients of $\mathcal{L}[C]$ are just the moments of $C(t)$,

$$\left. \frac{d^k}{dp^k} \mathcal{L}[C](p) \right|_{p=p_0} = \int_0^\infty dt (-t)^k C(t) e^{-p_0 t} \quad (3)$$

and use their poles and residues as estimates for E_n, A_n .

Since the integrals for the moments cannot be analytically evaluated given the numerical data $C(ka)$, the moments need to be estimated using quadrature formulae. As a result, robust methods are even more important in the case of the Padé-Laplace method due to the numerical errors arising from numerical integration.

Due to the averaging over different times that is inherent in the Laplace transform, the results from the Padé-Laplace method tend to be more resistant to noise than those from the Padé method. As an example, Fig. 3 shows the results of applying the Padé-Laplace method to the same synthetic data as in Fig. 1; a similar approach to the true value can be observed as the number of poles tried is raised, although the approach is less monotonic, largely due to the effects of numerical error from the quadrature formula used, as can be seen from the difference between the results using Simpson’s rule (shown as open symbols) and those using a novel non-linear quadrature formula of the kind discussed in the next section (shown as filled symbols). On the other hand, Fig. 4 shows the results of applying the Padé-Laplace method to the same noisy synthetic data as in Fig. 2; here, the approach to the true value is faster than for the Padé method, and the first excited state can be extracted much more reliably (while higher excited states are still drowned out by the noise).

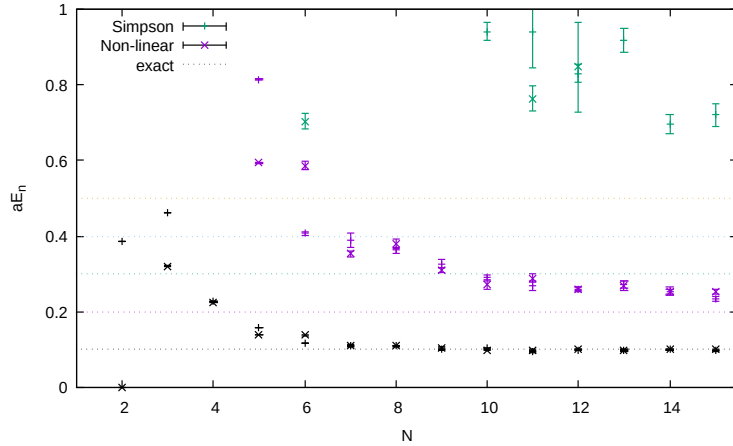


Figure 4: Same as Figure 3, but with a 1% noise applied to the synthetic data.

4. Non-Linear Quadrature Formulae

When computing moments (3) numerically, e.g. using the trapezoidal rule or Simpson’s rule, the numerical error from quadrature introduces an additional source of instability to the Padé approximants. To avoid this source of error as far as possible, it is useful to consider quadrature formulae that give exact results when applied to functions of the form (1).

Unfortunately, the traditional quadrature formulae all are exact by design on linear spaces of polynomials, while the functions we are interested in integrating here form a non-linear family. We therefore need to go beyond traditional quadrature formulae and consider non-linear approximations

$$\int_a^b dx f(x) \approx (b-a) q(f(a), f(b)) \quad (4)$$

to definite integrals. The core result [8] in this context is that as long as (4) is exact on all multiples of at least one function, its integration error is no worse than that of the trapezoidal rule (and better for functions close to such multiples).

Specifically, a non-linear quadrature formula that is exact on functions of the form Ae^{-mx} is given by

$$q(f(a), f(b)) = \frac{f(a) - f(b)}{\log \frac{f(a)}{f(b)}} \quad (5)$$

and one can systematically develop higher-order non-linear quadrature rules using multiple nodes. For further details and proofs, the reader is referred to Ref. [8].

5. Conclusions and Outlook

The Padé-Laplace method has seen wide usage in other areas of science ranging from biophysics [1] and medical research [9] to climate science [10] and food science [11]. Its application to lattice QCD data is therefore warranted. It remains to be seen how helpful the newly developed non-linear quadrature rules will be in this context.

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