Padé and Padé-Laplace Methods for masses and matrix elements

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Motivation

- Crucial problem in lattice field theory is extracting masses E_n and matrix elements $\langle n|\hat{O}|0\rangle$ from correlation functions

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

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

- Multiexponential fits tend to be unstable, while variational methods work well, but require range of operators O_i at source and sink
- Desirable to have methods that can solve this problem with just one operator at source and sink
- Useful to consider methods used for similar purposes in other fields, such as laser fluorescence spectroscopy [1].

Padé Method [2]

- The Z transform of the correlator $C = \{C(ka) \mid k \in \mathbb{N}\}$ is given by

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

with $\lambda_n = \mathrm{e}^{-E_n a}$.

- Poles and residues give masses and matrix elements!
- In practice, only finitely many $C(ka)$ are known.
- Consider Padé approximants to $\mathcal{Z}[C](z)$ and use their poles and residues as estimates of λ_n, A_n.
- Naive implementation is equivalent to Prony's method in exact arithmetic [2].
- Results tend to be unstable (complex poles, Froissart doublets, ...)
- Solution: robust Padé approximants [3], which give an estimate of how many states can be identified from the data.
- Even with robust methods, results quickly deteriorate in the presence of noise [4].

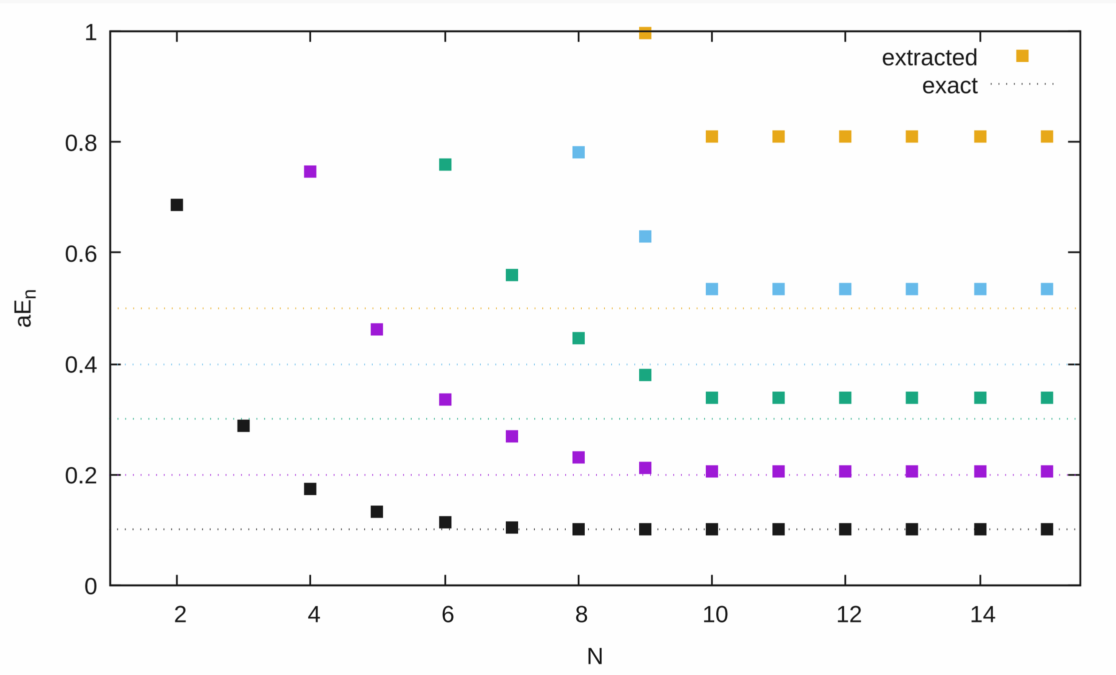

FIGURE 1: Results from the Padé Method with robust approximants applied to synthetic data. Dashed horizontal lines denote the exact values of the masses, points the extracted results as a function of the number N of poles tried.

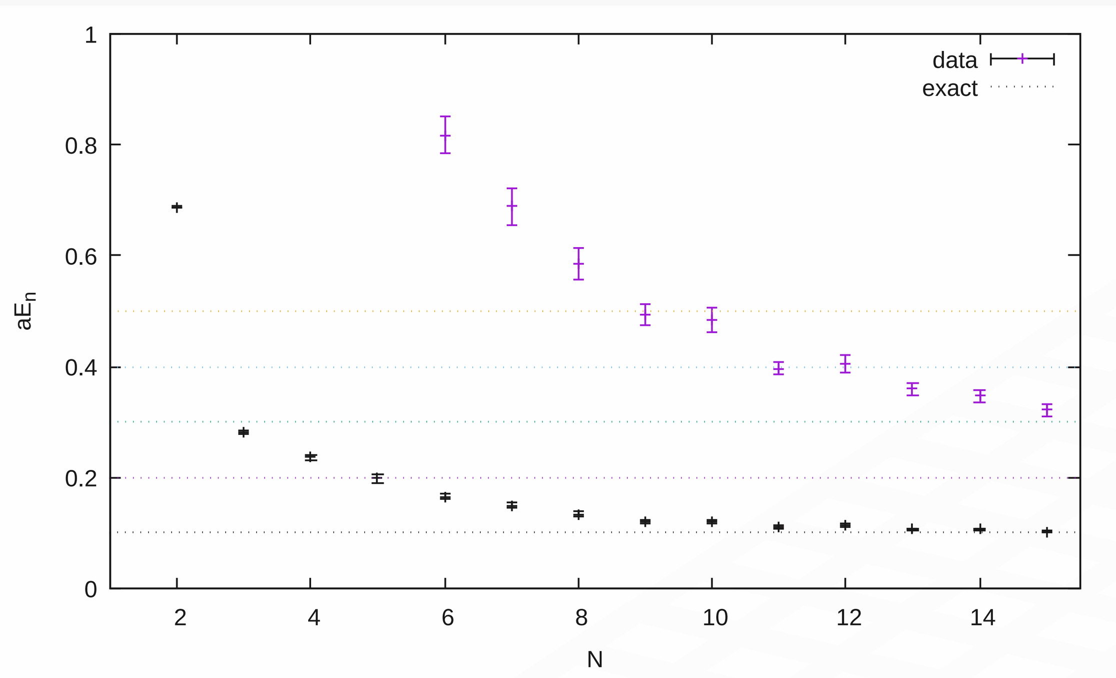

FIGURE 2: Same as Figure 1, but with a 1% noise applied to the synthetic data.

Padé-Laplace Method [1]

- Laplace transform of correlation function $C(t)$ given by

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

- Compute Padé approximants to $\mathcal{L}[C](p)$ from moments

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

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

- Robust methods even more important due to errors from numerical integration.
- Due to the averaging inherent in the Laplace transform, the results are more resistant to noise than for the Padé method.

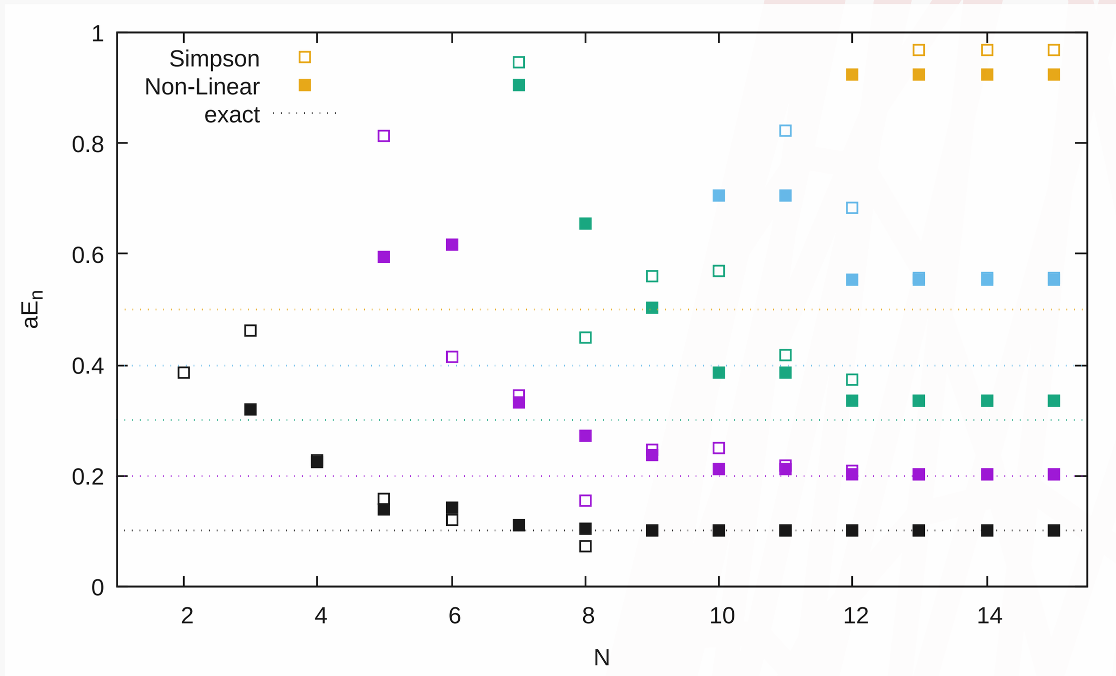

FIGURE 3: Results from the Padé-Laplace Method with robust approximants applied to synthetic data. Dashed horizontal lines denote the exact values of the masses, points the extracted results as a function of the number N of poles tried. Empty points use Simpson's rule for the numerical integration, filled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

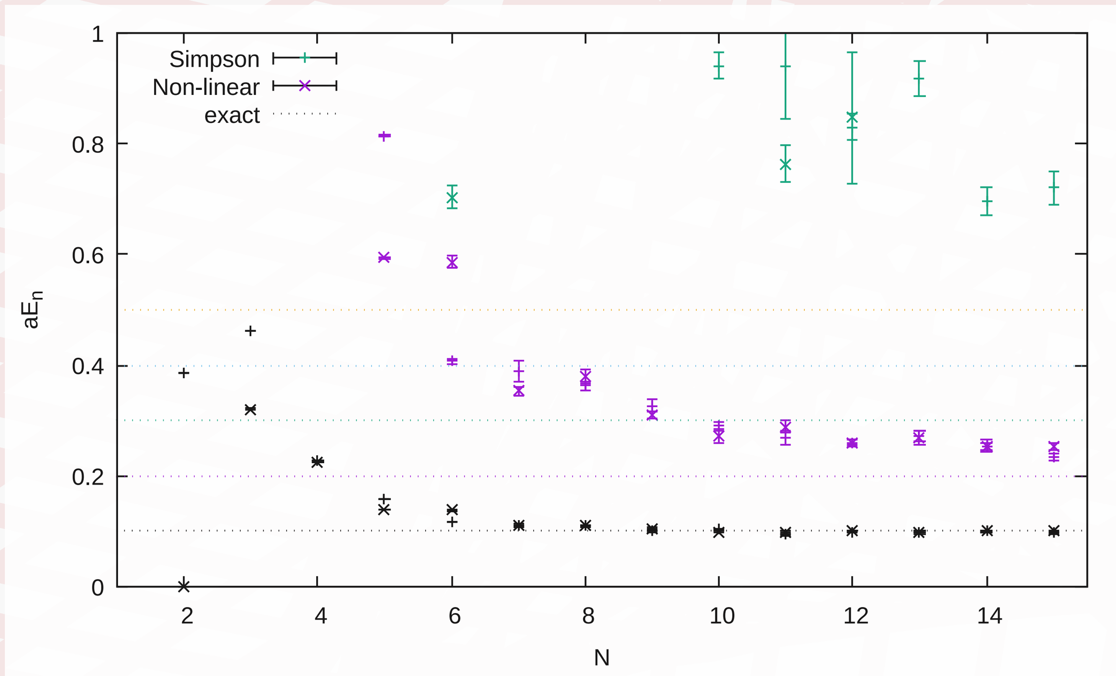

FIGURE 4: Same as Figure 3, but with a 1% noise applied to the synthetic data.

Non-Linear Quadrature Formulae

- When computing moments (3) numerically, e.g. using trapezoidal rule, numerical error introduces additional instability to the Padé approximants.
- Consider non-linear approximations

$$\int_a^b \mathrm{d}x\, f(x) \approx (b-a)\, q(f(a), f(b)) \tag{4}$$

As long as (4) is exact on all multiples of at least one function, integration error is no worse than trapezoidal rule (and better for functions close to such multiples).

- Specifically, a non-linear quadrature formula exact on functions of the form $A\mathrm{e}^{-mx}$ is given by

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

- Can develop higher-order non-linear quadrature rules using multiple nodes.

References

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