The Additional Interpolators Method for Variational Analysis in Lattice QCD

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In this paper, I describe the Additional Interpolators Method, a new technique for variational analysis in lattice QCD. It is shown to be an excellent method which uses additional interpolators to remove backward in time running states that would otherwise contaminate the signal. The proof of principle, which also makes use of the Time-Shift Trick (Generalized Pencil-of-Function method), will be delivered at an example on a 64\(^4\) lattice close to the physical pion mass.

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Introduction.— In Lattice QCD, the variational method \cite{1-4} has become a widely used method to separate physical states. Its main application is spectroscopy (recent examples are, e.g., \cite{5-19}), but it has also been successfully used to extract specific physical states in hadron structure calculations (e.g., \cite{15-19}). In this paper, I describe a new technique for variational analysis, the Additional Interpolators Method (AIM). It is important for studies where the backward (in time) propagating states are not negligible compared to the forward propagating ones in the time range of interest. By adding interpolators, one can explicitly account for the backward propagating states and then eliminate them with a properly chosen interpolator. For the proof of principle, the additional interpolators are obtained “for free” using the Time-Shift Trick (Generalized Pencil-of-Function method), which I will also briefly review in this paper.

The Variational Method.— The standard variational method is widely used to separate physical states in spectroscopy but also in hadron structure calculations. It uses several interpolators \(I_i\), \(i = 1, \ldots, N_T\) to separate the physical states \(s_i\), \(i = 1, \ldots, N_s\), with energies \(E_i\). Typically, one assumes that the number of significantly contributing physical states is equal to the number of interpolators \(N_T = N_s \equiv N\). The interpolators couple to the physical states through

\[
\langle s_i|I_j|0 \rangle = a_{ij}.
\]

On a lattice with (anti)periodic boundary conditions, the correlation matrix is

\[
C_{ij}(t) = \langle I_i(t)|I_j(0) \rangle = \sum_k \langle 0|I_i|s_k \rangle \langle s_k|I_j|0 \rangle \exp(-E_k t)
\]

\[
+ \sum_k \langle 0|I_j|s_k \rangle \langle s_k|I_i|0 \rangle \exp(-E_k (T-t))
\]

\[
= \sum_k a_{ik}^t a_{kj} \exp(-E_k t)
\]

\[
+ \sum_k b_{ik}^t b_{kj} \exp(-E_k (T-t)),
\]

where \(T\) is the temporal extent of the lattice and I have introduced \(b_{ij} \equiv \langle 0|I_j^\dagger|s_i \rangle\). The first term in Eq. (1) contains the forward moving and the second term the backward moving states. Neglecting the backward moving states (which is often a good approximation), Eq. (1) becomes

\[
C_{ij}(t) = \sum_k a_{ik}^t a_{kj} \exp(-E_k t).
\]

One proceeds by solving the generalized eigenvalue problem

\[
C_{ij}(t_0) v_{ij}^{(k)} = \lambda^{(k)} C_{ij}(t_0) v_{ij}^{(k)},
\]

where I denote the \(k\)th eigenvalue and -vector with \(\lambda^{(k)}\) and \(v_{ij}^{(k)}\), respectively. This is equivalent to finding the eigenvectors - and -values of the matrix

\[
G_{ij}(t_0, t_1) \equiv C_{ik}^{-1}(t_0) C_{kj}(t_1)
\]

\[
= \sum_k a_{ik}^{-1} a_{kj} \exp(-E_k(t_1 - t_0)).
\]

One sees immediately that the eigenvalues are \(\exp(-E_k(t_1 - t_0))\) and the \(i\)th eigenvector, with components \(v_{ij}^{(k)}\), fails for lattices with (anti)periodic boundary conditions when the backward running states are so light that they do not decay sufficiently fast and contribute significantly on the left side. In Figure 1 we show this problem for pions on a 64\(^4\) ensemble with Wilson gauge action, \(N_f = 2\) flavors of dynamical Wilson (Clover) fermions, \(\beta = 5.29\) (corresponding to \(a \approx 0.07\) fm) and \(\kappa = 0.13640\), where the pion has a mass of approximately 150 MeV. For ensembles like this one, but also at much larger pion masses, the variational method has to be modified to yield reasonable results.

The \(\cosh\) Method.— The straightforward way to account for the backward running states is to replace the exponential decays by \(\cosh\)s and \(\sinh\)s, see below. As an example, I use two interpolators for the pion (\(\pi\)) and excited pion (\(\pi^+\)
states, $\mathcal{I}_1 = \Pi = \bar{d}\gamma_5 u$ and $\mathcal{I}_2 = A_0 = \bar{d}\gamma_5 \gamma_4 u$. The adjoint interpolators which couple to the antiparticle are:

$$
\Pi^\dagger = (\bar{d}\gamma_5 u)^\dagger = \bar{u}\gamma_5 d
$$

$$
A_0^\dagger = (\bar{d}\gamma_5 \gamma_4 u)^\dagger = \bar{u}\gamma_4 \gamma_5 d = -\bar{u}\gamma_5 \gamma_4 d.
$$

Since the up and down quarks are identical in our simulations, one finds

$$
\langle \pi^+ | \Pi^\dagger | 0 \rangle = \langle \pi^- | \Pi | 0 \rangle
$$

$$
\langle \pi^+ | A_0^\dagger | 0 \rangle = -\langle \pi^- | A_0 | 0 \rangle,
$$

and equivalently for the excited pion. In other words, $b_{1i}^j = a_{11}$ and $b_{2i}^j = -a_{12}$. The relative minus sign between these expressions is responsible for the fact that $\langle \Pi | \Pi^\dagger \rangle$ and $\langle A_0 | A_0^\dagger \rangle$ have a sinh-like time dependence, while $\langle A_0 | \Pi^\dagger \rangle$ and $\langle \Pi | A_0^\dagger \rangle$ are cosh-like. Assuming that the $a_{ij}$ are real, Eqs. (3) become

$$
\langle \Pi(t) | \Pi^\dagger(0) \rangle = 2a_{11}^2 \exp(-E_x T/2) \cosh(E_x \bar{t}) + 2a_{22}^2 \exp(-E_x T/2) \cosh(E_x \bar{t})
$$

$$
\langle A_0(t) | A_0^\dagger(0) \rangle = 2a_{12}^2 \exp(-E_x T/2) \cosh(E_x \bar{t}) + 2a_{21}^2 \exp(-E_x T/2) \cosh(E_x \bar{t})
$$

$$
\langle A_0(t) | \Pi^\dagger(0) \rangle = -2a_{11}a_{12} \exp(-E_x T/2) \sinh(E_x \bar{t}) - 2a_{21}a_{22} \exp(-E_x T/2) \sinh(E_x \bar{t})
$$

$$
\langle \Pi(t) | A_0^\dagger(0) \rangle = 0.
$$

where I have used $E_x \equiv E_\pi$, and $\bar{t} \equiv t - T/2$ for brevity. Eqs. (3) have to be solved numerically and it turns out that the solution is numerically not very stable and needs some “supervision”. Once the $a_{ij}$ have been found, one can again construct optimal interpolators for the forward running states by $T_{opt}^{(j)} = T_j^i a_{ji}^{-1}$. One finds for an arbitrary operator $\mathcal{O}$:

$$
\langle \mathcal{O}(t) | T_{opt}^{(j)}(0) \rangle
$$

$$
= \langle \mathcal{O}(t) | T_j^i(0) | 0 \rangle a_{ji}^{-1}
$$

$$
= \sum_k \langle 0 | \mathcal{O} | s_k \rangle \langle s_k | T_j^i | 0 \rangle a_{ji}^{-1} \exp(-E_k t)
$$

$$
+ \sum_k \langle 0 | T_j^i | s_k \rangle \langle s_k | \mathcal{O} | 0 \rangle a_{ji}^{-1} \exp(-E_k (T - t))
$$

$$
= \langle 0 | \mathcal{O} | s_i \rangle \exp(-E_i t)
$$

$$
+ \sum_k \langle s_k | \mathcal{O} | 0 \rangle b_{kj} a_{ji}^{-1} \exp(-E_k (T - t)),
$$

and the example above showed that $ba^{-1}$ is not necessarily the unit matrix. Therefore, while the forward running contribution is optimized for the wanted state, the backward running part contains several or all states, which prevents simple exponential or cosh fits.

The Additional Interpolators Method.— The method that I propose here is to add extra interpolators that account for the backward running states. In other words, we treat the backward running states as forward running particles with negative mass. Usually, the heavier backward running states will be negligible on the left side since they decay too fast. The number of backward running states that contribute significantly is $N_b \ll N_s$. One then needs $N_T = N_s + N_b$ interpolators to account for the forward and the significant backward running states. I define $\tilde{b}_{kj} = b_{kj} \exp(-E_k T/2)$ and sort the states so that the first $N_b$ states are the ones that are non-negligible to rewrite Eq. (1) as

$$
C_{ij}(t) = \sum_{k=1}^{N_s} a_{ik}^j a_{kj} \exp(-E_k t)
$$

$$
+ \sum_{k=1}^{N_b} \tilde{b}_{ik}^j \tilde{b}_{kj} \exp(E_k t).
$$

With

$$
d_{kj} \equiv \begin{cases} 
 a_{kj}, & 1 \leq k \leq N_s \\
 b_{(k-N_s)j}, & N_s < k \leq N_T 
\end{cases}
$$

and

$$
\tilde{E}_k \equiv \begin{cases} 
 E_k, & 1 \leq k \leq N_s \\
 -E_{k-N_s}, & N_s < k \leq N_T, 
\end{cases}
$$

this becomes the standard variational problem. I define the optimal interpolator as $T_{opt}^{(j)} = T_j^i d_{ji}^{-1}$. Then, for an arbitrary
The results are similar and the eigenvalues agree within the error bars in the region of the plateau. So while the results are comparable, I consider the method more robust than the cosh method and therefore able to go two time steps further to the right.

This shows that the method works indeed and one is left with an optimal interpolator for the ground or excited states, with no contamination from the backward running states, which greatly improves the further analysis.

In my example, I need $N_T = 3$ interpolators to account for the pion, the excited pion and the backward running pion. Since only data for the two interpolators $\Pi$ and $A_0$ was available, I had to use the Time-Shift Trick to obtain the third interpolator.

The Time-Shift Trick.— The Generalized Pencil-of-Function method or, more catchy, the Time-Shift Trick allows one to obtain additional interpolators “for free”. As the name suggests, new interpolators are constructed by time-shifting other interpolators. I will label the time-shift operator $T(\delta t) = T^\dagger(\delta t)$, with the amount of time shift $\delta t$. Its action on an operator $O(t)$ is defined by $T(\delta t)O(t) = O(t - \delta t)$ and due to time invariance one sees that

$$\langle O_2(t_2)|T(\delta t)|O_1(t_1)\rangle = \langle O_2(t_2)|O_1(t_1 - \delta t)\rangle = \langle O_2(t_2 + \delta t)|O_1(t_1)\rangle$$

and therefore

$$O(t)T(\delta t) = O(t + \delta t). \quad (4)$$

Using this, one can define a new interpolator $I_i' = T(\delta t)I_i$ and sees immediately that

$$\langle s_i|I_j'|0\rangle = \langle s_i|T(\delta t)I_j|0\rangle = \exp(-E_i\delta t)\langle s_i|I_j|0\rangle = \exp(-E_i\delta t)a_{ij}.$$

Therefore, $I_i'$ is, in general, a new linearly independent interpolator.

Proof of principle.— In this final paragraph, I show that the AIM and the Time-Shift Trick actually work with “real data”. I investigate the pion with the two interpolators $\Pi$ and $A_0$ and the time-shifted interpolator $\Pi T(\delta t)$ so that I can account for the pion, the excited pion and the backward running pion. Using Eq. (4), one obtains the correlation matrix

$$C(t) = \begin{pmatrix}
\langle \Pi(t)|\Pi^\dagger(0)\rangle & \langle \Pi(t)|A_0^\dagger(0)\rangle & \langle \Pi(t+\delta t)|\Pi^\dagger(0)\rangle \\
\langle A_0(t)|\Pi^\dagger(0)\rangle & \langle A_0(t)|A_0^\dagger(0)\rangle & \langle A_0(t+\delta t)|\Pi^\dagger(0)\rangle \\
\langle \Pi(t+\delta t)|\Pi^\dagger(0)\rangle & \langle \Pi(t+\delta t)|A_0^\dagger(0)\rangle & \langle \Pi(t+2\delta t)|\Pi^\dagger(0)\rangle
\end{pmatrix}.$$

I use this matrix in the standard variational method and find the eigenvalues of $C(t_0,t_1)$ in Eq. (2). To obtain optimal results, I vary $t_0, t_1$ and $\delta t$. It turns out that for this example, $t_1 - t_0 = 2$ and $\delta t = 14$ are good choices. For the sake of completeness, I compare these results to the results obtained with the cosh method, where I also kept $t_1 - t_0 = 2$. The results are shown in Figure 2. Both methods find perfect plateaus for the pion (the AIM also for the backward running pion) and reasonably nice plateaus for the excited pion. The error bars are similar and the eigenvalues agree within the error bars in the region of the plateau. So while the results are comparable, I prefer to use the AIM over the cosh method because of its nu-
merical stability and robustness (which also allows the AIM to reach higher $t_0$ than the cosh method). Furthermore, the AIM is faster than the cosh method, although this is usually not relevant with today’s computers.

The big advantage of the AIM over the cosh method, however, are the optimal interpolators. For each method, I construct the optimal interpolators as described above and show the correlators $\langle \Pi(t) | \tau^{(i)}_{\text{opt}} (0) \rangle$ in Figure 3. The AIM yields an optimal pion, i.e., one that has an exponential (linear in the logarithmic plot) behavior throughout the plot range. The backward running pion is also very good and the excited pion state is resolved better with the AIM than with the cosh method.

In conclusion, the AIM has proven to be a robust method that is at least as good as the cosh method in finding the energy eigenvalues but has its real strengths in the construction of optimal interpolators. The Time-Shift Trick was also very useful and can be applied wherever additional interpolators are needed, in many cases even at no extra computational cost.

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