Evolutionary Fitting Methods for the Extraction of Mass Spectra in Lattice Field Theory

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Abstract

We present an application of evolutionary algorithms to the curve-fitting problems commonly encountered when trying to extract particle masses from correlators in Lattice QCD. Harnessing the flexibility of evolutionary methods in global optimization allows us to dynamically adapt the number of states to be fitted along with their energies so as to minimize overall $\chi^2/(\text{d.o.f.})$, leading to a promising new way of extracting the mass spectrum from measured correlation functions.

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1 Introduction

Curve fitting plays a central role in the analysis of lattice simulation data. One of the most important and common uses of curve fitting in lattice gauge theory is the extraction of hadronic masses and matrix elements from measured correlation functions.

The problem of extracting the mass spectrum from the correlators measured in Lattice QCD simulations is well known [1,2]. The simulation produces data $\overline{G_i} = \overline{G(t_i)}$ for the expectation values of the correlator G(t) at a finite number of discrete (Euclidean) time steps t_i , $1 \leq i \leq N$. On the other hand, from theory the exact form of the propagator is known to be given by an infinite series²

$$G(t) = \sum_{n=0}^{\infty} Z_n e^{-E_n t} , \qquad (1)$$

where we will assume that the energy levels are ordered, $E_n \leq E_{n+1}$. The problem is then to determine an infinite number of amplitudes $Z_n > 0$ and energies $E_n > 0$ from only a finite number of data points $\overline{G_i}$, an obviously ill-posed problem.

To make the problem well-posed, we have to add some further physical constraints. The piece of theoretical information that is normally used is that the sequence of the Z_n is bounded from above, and therefore the correlator will be dominated by the lowest few terms at all but the smallest values of t due to the exponential suppression by E_n . We can therefore truncate the series in equation (1) after a finite number of terms, provided we only attempt to fit

 $^{^{2}}$ For periodic boundary conditions, hyperbolic functions will appear instead of the exponential. For a static particle, the energy is simply the particle mass.

at $t > t_{min}$ large enough for the truncation to include all terms that make a significant contribution.

In doing so, we are faced with a choice: Either take a fixed number n_{max} of terms of the sum in (1) and adjust t_{min} so as to obtain a good fit, or fix t_{min} and vary n_{max} so as to extract the largest possible amount of significant information. The problem with the first strategy is that we are throwing away valuable information contained in the data points at $t < t_{min}$, leading to large statistical errors if t_{min} is chosen too big. These need to be balanced against large systematic errors arising if t_{min} is chosen too small for the given $n_{max}[1]$. In this paper we will therefore adopt the second approach and attempt to fit all data points (excluding only the single point at t = 0 for practical reasons) with a variable number n_{max} of exponentials.

Naively, one might want to try to simply run a series of fits using a state-of-the art fitting method such as Levenberg-Marquardt [3,4] at a number of different n_{max} , and with a variety of initial parameter values, and choose the fit that produces the lowest χ^2 per degree of freedom. This method can be made to work in the case of one single correlator if the problem of finding an appropriate starting point in a potentially multi-modal landscape is somehow solved. However, for many questions in lattice QCD it is necessary to fit multiple correlators, which may or may not share some of the energy levels E_n . In this case, the fast combinatorial growth with n_{max} of the number of possibilities of assigning shared or separate fit parameters E_n to the fitting functions for the different correlators renders the application of this naive method to those problems largely impossible. The problem of choosing appropriate initial parameter values further exacerbates this approach. The current state of the art using the variable- n_{max} approach is that taken in [1] where it is used in the context of a Bayesian method [5] of *constrained curve fitting*. The latter works by adding prior information about the fit parameters and using it to constrain the fit to a smaller subset of likely parameter values out of the space of all possible values. Only those parameters whose fitted values are largely independent of the priors used to constrain them are considered to be determined by the data, while the others are disregarded as having been imposed by the priors.

While it is thus possible to determine which fitted quantities are independent of, or only weakly dependent on, the priors and thus determined from the data, the idea of using some external knowledge as an input could be seen as incompatible with the notion of a first-principles determination of the quantities of interest from QCD itself, without any recourse whatsoever to empirical models. Moreover, in some cases appropriate priors may not be available. Under those circumstances, it becomes desirable to be able to extract some estimate of the parameters to be fitted from the data themselves, and to use this estimate as a prior in the context of a Bayesian constrained fit. A number of methods to do this, such as the *sequential empirical Bayes method* [6], have been used in the existing literature.

A completely different state-of-the-art approach that does not rely on prior information while allowing for extraction of a spectrum from multiple sets of data for improved statistics is the *variational method* [7,8,9]. Here one sets out by fixing a channel corresponding to a specific set of quantum numbers, and finds a set of appropriate linearly independent operators O_i for the channel. One then calculates all diagonal $\langle O_i O_i \rangle$ and off-diagonal $\langle O_i O_j \rangle$, $i \neq j$, correlators between these operators, each operator having a corresponding form for the sink that annihilates the state created by the operator at the source. One may then use the variational method on this cross-correlator matrix $C_{ij}(t)$ to find a superposition of the original operators that corresponds to the lowest energy state of the channel. Assuming a meson channel, the diagonal correlator of this operator may be fit by a single exponential function whose mass in the exponent is the ground state energy. Operators corresponding to excited states, whose diagonal correlators ideally correspond to functions only of the excited state masses, may be produced in a similar manner [10].

While very powerful, the variational method has a number of features that limit the scope of its applicability. Firstly, the use of the variational method is facilitated by the selection of operators such that the correlator matrix is hermitian [8,11]. However, in lattice simulations it is often desirable to suppress unwanted but usually present contributions from high-frequency modes by means of quark smearing of the operators [12,13,14]. In this case, hermiticity of the correlator matrix requires smearing to be applied both at the source and the sink of the correlator, which in most cases is very expensive computationally. Secondly, the variational approach also requires both source and sink operators to have the exact quantum numbers of the channel of interest, instead of the less stringent usual requirement that both operators overlap with the state of interest and that at least one of them have its exact quantum numbers. This requirement limits the selection of correlators that are usable with the variational method. Finally, the variational method requires all off-diagonal correlators to be calculated. The number of needed correlators thus grows as N^2 , with N the number of operators in the channel of interest. Since automated generation of group theoretical operators for a given symmetry channel [11,15,16] means that the number of operators that could be used may be rather large, this quadratic growth in computational complexity imposes further limitations. Thus correlator selection may be done more judiciously without the restrictions imposed by the variational method.

A different problem arises in the case where one desires to fit correlators corresponding to channels with *different* lattice quantum numbers. An example of this occurs when the continuous rotational symmetries of a quantum theory get broken when discretizing it to a lattice. In the continuum, the rotational group has representations corresponding to arbitrary integer or half-integer angular momenta J, but on the lattice one only retains the finite symmetry of the octahedral group. A particle of angular momentum J will therefore appear in one or more of the lattice channels labeled by those irreducible representations of the octahedral group to which the value of J subduces [17]. Thus a particle of integral spin will appear in some known subset of the irreps A_1, A_2, E, T_1 and T_2 of the octahedral group. Therefore, the extraction of the physical spectrum is complicated by the fact that a physical state's mass may lie in several lattice symmetry channels. One needs to identify in which irreps the physical state lies not only to aid in identifying its physical angular momentum J via its subduction signature, but also to extract its mass as the latter is contained in the data in all channels in which it appears. Since a state either lies within a lattice symmetry channel or it does not, the process of state identification and fitting requires an algorithm that is inherently discontinuous. As the number of resolvable states in lattice simulations increases, the need for a systematic solution to this second problem will as well.

Evolutionary fitting algorithms, while widely used in other areas of research [18,19,20,21,22,23,24,25], are not currently in common use in lattice QCD. In this paper, we present an application of evolutionary algorithms [26,27,28,29]

to the problem of extracting mass spectra from hadronic correlators. We believe that the advantages of evolutionary algorithms are particularly pertinent to this problem: evolutionary algorithms allow dynamic variation of the functional form of the fit function (such as the number of states to be fitted) in a natural way so as to minimize χ^2 per degree of freedom; the data themselves thus tell us how many states can be reliably extracted. In addition, evolutionary algorithms are inherently global optimizers and as such largely eliminate any residual dependence of the result on the initial guesses used as starting values, which may be a problem when using conventional local optimizers. Furthermore, based as they are on the Darwinian principle of adaptation by mutation and natural selection [30], evolutionary fitting methods excel at extracting information from data without the need for any external prior information. Finally, evolutionary fitting is able to fit multiple correlator datasets with either identical or differing quantum numbers.

In this paper we aim to introduce lattice theorists to the possibilities and features of evolutionary fitting algorithms and to present some preliminary results from our practical implementation of such an algorithm. Section 2 gives a general overview of the concepts and ideas of evolutionary algorithms. Section 3 details an evolutionary algorithm that can be used to fit a single hadronic correlator, and section 4 outlines the adaptations to the algorithm that are necessary in order to fit across multiple datasets. Some possible variations of the basic algorithm are explained in section 5.

2 Evolutionary Algorithms

Evolutionary computing and genetic algorithms [26,27] are a very active field in computer science and numerical optimization (cf. e.g. the review [28] and references therein). By borrowing concepts from evolutionary biology, evolutionary computing is able to harness the power of natural selection by mutation and selective breeding for the purpose of solving function optimization and related problems. The nomenclature is borrowed from evolutionary biology as well: candidate solutions are called "organisms", whose internal encodings are their "genotypes", the target function is referred to as "fitness", and each step of the algorithm produces a new "generation".

A number of fine distinctions between "genetic algorithms", "evolution strategies", "evolutionary programming" and related evolutionary algorithms and methods is sometimes employed in the literature [29]; here we will use the term "evolutionary algorithm" broadly to mean any global optimization method that relies on some form of random mutation combined with selective breeding in a population of candidate solutions [28]. From this point of view, an evolutionary algorithm consists of the following ingredients:

- A search space \mathcal{G} ,
- a fitness function $f: \mathcal{G} \to \mathbb{R}$, assumed to be bounded from above,
- a mutation function $M_{\eta}: \mathcal{G} \to \mathcal{G}$, and
- a selection function $S_{\eta'}: \mathcal{G}^N \to \mathcal{G}^N$

Here N is the (fixed) size of the population. Both the mutation and the selection function depend on some uncorrelated white noise η, η' that acts as a source of randomness. The update step on a population $P_{\tau} \in \mathcal{G}^N$ is then

$$P_{\tau+1} = S_{\eta'}(M_{\eta}(P_{\tau})) .$$
 (2)

The mutation function acts on each individual in a population separately, while the selection function performs comparisons in fitness between individuals, and may also involve crossover or "sexual" reproduction, which creates a new individual from a pair of "parent" individuals.

The simplest selection procedure to use is straightforward "elitist" selection of the fittest $N_{elite} < N$ individuals from a population of size N, followed by repopulation with their pairwise offspring (where a child is formed by random interpolation between the parameter values from either parent for each parameter). More sophisticated selection procedures (such as "roulette wheel", "rank" or "tournament" selection [28]) could be used instead. Adding additional, less fit, members to the elite on the basis of genetic distance may be helpful in maintaining genetic diversity and avoiding premature convergence.

If we require that the mutation function leaves the fittest individual in a population alone, thereby ensuring

$$\max_{p \in M_{\eta}(P)} f(p) \ge \max_{p \in P} f(p) , \qquad (3)$$

and that the selection procedure never decreases the maximum fitness within a population,

$$\max_{p \in S_\eta(P)} f(p) \ge \max_{p \in P} f(p) , \qquad (4)$$

it follows that the sequence $f_{\tau} = \max_{p \in P_{\tau}} f(p)$ is bounded from above and monotonically increasing, and hence will converge.

Evolutionary algorithms are inherently global optimizers, as opposed to local

optimizers such as steepest descent or Newton methods. This global nature is largely due to their inherent parallelism, since all organisms in a population search the fitness landscape in parallel, and also because crossover allows information learned by different organisms to be combined and propagate throughout the population. Another important feature of evolutionary algorithms is their ability to optimize by varying discrete parameters (such as the functional form of a candidate solution) in a natural and straightforward way, something which local optimizers relying on certain smoothness assumptions about the target function cannot easily do.

While evolutionary algorithms have not yet become a standard tool in lattice QCD, they have previously been used for the purpose of nonperturbative Landau gauge fixing [31,32,33,34] and (in combination with an accept-reject step to achieve detailed balance) as a simulation algorithm [35,36]. In other fields of physics, evolutionary fitting algorithms have been used among other things to discriminate between different SUSY models [18], to analyze resonances in $p(\gamma, K^+)\Lambda$ reactions [19], to fit stellar spectra [20], to determine the mass loss rate of stellar winds [21], to search for extrasolar planets [22,23], to build diatomic potentials using a variational method [24], and to solve black-box system characterization problems in engineering [25]. In most of these cases, just as in this work, it has been observed that combining the evolutionary algorithm with a conventional (local) optimization step gave the best results.

We believe that the flexibility and global nature of evolutionary algorithms makes them an excellent tool for the purpose of curve fitting, especially when the exact form of the fitting function (such as the number of exponentials to use in our case) is subject to some kind of data-dependent uncertainty.

3 Evolutionary Fitting of a Single Correlator

In this and the following section we present some details of our version³ of an evolutionary algorithm for fitting correlation functions in lattice QCD.

For the purpose of fitting a diagonal meson correlator⁴, the search space is

$$\mathcal{G} = \left\{ G \in \mathcal{C}(\mathbb{R}) \, \middle| \, \exists \, n_{max} > 0, \, Z_n > 0, \, E_n > E_{n-1} > 0 : \right.$$
$$G(t) = \sum_{n=0}^{n_{max}} Z_n \left(e^{-E_n t} + e^{-E_n (T-t)} \right) \right\},$$

where T is the temporal extent of the periodic lattice. The fitness function is $f(G) = -\chi^2(G)/n_{dof}(G)$, where the correlated χ^2 [39,40] is

$$\chi^2(G) = \sum_{t_i, t_j} (\overline{G_i} - G(t_i))(\sigma^{-1})_{ij} (\overline{G_j} - G(t_j)) , \qquad (5)$$

with the covariance matrix defined by

$$\sigma_{ij} = \overline{G_i G_j} - \overline{G_i} \,\overline{G_j} \,, \tag{6}$$

and where

$$n_{dof}(G) = (t_{max} - t_{min} + 1) - 2n_{max} \tag{7}$$

is the number of degrees of freedom of the fit given by G.⁵

An organism $G \in \mathcal{G}$ can therefore be represented by a list of n_{max} pairs (Z_n, E_n) , ³ For a practical implementation, we have chosen PYTHON [37], augmented by SciPy [38], because of its object-orientation and the flexible list and tuple types it natively provides.

⁴ For baryonic and off-diagonal correlators, the functional form needs some adjustments. Nevertheless, the general method works the same in those cases.

⁵ Where a fitness function $f : \mathcal{G} \to [0;1]$ is desired, functions such as $f(G) = e^{-\chi^2(G)/n_{dof}(G)}$ or $f(G) = 1/(1 + \chi^2(G)/n_{dof}(G))$ can be used instead.

and it is this representation on which the mutation and breeding algorithms outlined below work.

There are two kinds of mutation steps needed to search the entire search space \mathcal{G} . The first amounts to increasing or decreasing n_{max} of an individual organism. When making these length mutations it is valuable to keep the sum $\sum_n Z_n$ of all amplitudes fixed.⁶ One reason for this is that the coefficient sum $G(0) = \sum_n Z_n$ can become relatively stable across the population early on, so that changing n_{max} by simply dropping the pair $(Z_{n_{max}}, E_{n_{max}})$ or adding a random pair will tend to produce an unfit organism, regardless of whether some potentially desirable organism of the new length exists. Moreover, a situation can occur where spurious near-degenerate states are kept because the change in overall amplitude from just removing a single one of them increases χ^2 more than is offset by the simultaneous increase in n_{dof} caused by the mutation. The second type of mutation performs a random modification of a pair (Z_n, E_n) . A natural way to implement this is the addition of a pair of independent Gaussian random variables to the original pair.

Since mutations can become somewhat disruptive of already accumulated genetic information in the later stages of evolution, it may be useful to make the rate of mutation dependent on χ^2/n_{dof} in such a way as to increase the search area early on, before contracting it to a more local search around the optima already found as the algorithm converges.

⁶ This may be accomplished, for instance, by sharing the amplitude of a removed term between the remaining amplitudes, and by decreasing the amplitudes of the existing exponentials so as to keep the overall amplitude fixed when adding a new term.

Mutation steps can also be combined with a finite number of steps of a local optimization routine (such as Levenberg-Marquardt).⁷ We have found that the addition of this latter step can greatly accelerate convergence by giving beneficial mutations an improved chance of survival.⁸

Putting these ingredients together, we arrive at the following mutation algorithm:

- (I) Generate a random number $p \in [0; 1]$.
- (II) If $p < p_0^{len}(1 e^{-\alpha^{len}\chi^2/n_{dof}})$ (where p_0^{len} , α^{len} are tunable parameters):
 - (a) Generate a random number $p' \in [0; 1]$.
 - (b) If p' < (1 − 1/n_{max}), decrease n_{max} by one, removing one randomly chosen exponential (Z_n, E_n) from the fit, and redistributing the amplitude in Z_n between the neighboring exponentials.
 - (c) Else increase n_{max} by one and add a new, randomly generated (Z_n, E_n) pair to the fit, decreasing the amplitudes of the pre-existing exponentials so as to keep the total amplitude fixed.
- (III) Generate a random number $p'' \in [0; 1]$.
- (IV) If $p'' < p_0^{parm}$ (where p_0^{parm} is a tunable parameter):
 - (a) Generate n_{max} pairs of Gaussian deviates $(\Delta Z_n, \Delta E_n)$ with zero mean and standard deviation $\sigma = \sigma_0^{parm} (1 e^{-\alpha^{parm}\chi^2/n_{dof}})$ (where σ_0^{parm} and α^{parm} are tunable parameters).

⁷ Specifically, we take the functional form implied by the genotype and do a fixed number of steps of the Levenberg-Marquardt routine using the genotype's parameter values as the initial values. The new genotype's values are set to the result. Some random subset of the parameter values can be kept fixed in the routine if desired. ⁸ This kind of strategy has sometimes been referred to as a *hybrid genetic* or *memetic algorithm* [41].

- (b) Replace (Z_n, E_n) by $(Z_n + \Delta Z_n, E_n + \Delta E_n)$, unless this would lead to a negative new value for E_n or Z_n .
- (V) Optionally perform a local (e.g. Levenberg-Marquardt) optimization on the fit with probability p_0^{local} .

This mutation procedure depends on a number of tunable parameters. In a number of numerical tests on a set of synthetic data, we found that the point to which the algorithm ultimately converged did not depend on the values of these parameters, indicating good stability of the answer. The rate of convergence, on the other hand, did depend on the particular parameters chosen, although the dependence was small for "sensible" parameter choices. Generally, p_0^{len} should not be too small, in order to explore the full solution space; we found that $p_0^{len} = 0.5$ worked well. α^{len} did not appear to have a crucial influence on convergence, and was set to $\alpha^{len} = 0.2$ in subsequent runs. Since element mutations can be rather disruptive of already achieved partial convergence, p_0^{parm} has to be chosen reasonably small; we found $p_0^{parm} = 0.1$ a sensible choice. The convergence rate did not appear to strongly depend on α^{parm} and σ_0^{parm} , which were set to $\alpha^{parm} = 0.1$ and $\sigma_0^{parm} = 0.5$, respectively. On the other hand, performing a local optimization step can never be harmful, and p_0^{local} should be set as large as computational resources allow. It should be pointed out that the optimal choice of parameters will likely depend on the particular fitting problem investigated in each case, since the fitness landscapes can conceivably look very different for different data.

The breeding or crossover function returns a child organism from two parent organisms (par1 and par2), and works as follows:

(I) Let $n_{max}^{child} = \max(n_{max}^{par1}, n_{max}^{par2}).$

- (II) Generate n_{max}^{child} pairs of independent uniformly distributed random numbers $(x_i, y_i) \in [-\delta; 1+\delta]$.
- (III) For $n < \min(n_{max}^{par1}, n_{max}^{par2})$, choose the fit parameters of the child to be $(Z_n^{child}, E_n^{child}) = (x_n Z_n^{par1} + (1 - x_n) Z_n^{par2}, y_n E_n^{par1} + (1 - y_n) E_n^{par2})$; for other *n*, choose them equal to the longer parent's fit parameter values.

The fit parameter values of the child organism are therefore chosen in a hypercube spanned by the parent's fit values. Allowing for the possibility of extrapolation instead of interpolation by introducing a parameter δ is necessary to avoid rapid contraction towards central points. In agreement with [18], we found $\delta = 0.2$ sufficient to prevent this contraction. "Parthenogenesis" or "cloning" of an existing individual is possible by breeding an organism with itself.

Putting these elements together, we arrive at the following basic evolutionary step to generate the next generation from a given population:

- All organisms except the fittest one are subjected to mutations according to the mutation algorithm stated above.
- (II) Selection and breeding are carried out as follows:
 - (a) The fittest N_{elite} organisms are selected.
 - (b) Another $N_{diversity}$ organisms are selected at random in order to maintain genetic diversity and avoid premature convergence.
 - (c) For each possible combination of the selected organisms (including those containing the same organism twice), a child organism is created according to the breeding algorithm above, and these child organisms form the next generation.
 - (d) N_{mutant} copies of organisms from the elite are added to the population

and are subjected to targeted mutations as a form of local search around the elite.

By not subjecting the fittest organism to mutations and including parthenogenesis in the breeding step, we ensure that inequalities (3) and (4) are fulfilled, and that thus the algorithm will eventually converge.

The basic evolutionary step is repeated until χ^2/n_{dof} converges below a chosen threshold $[\chi^2/n_{dof}]_{max}$, or until a chosen maximum number τ_{max} of generations has been exceeded with no improvement in the best overall genotype for the last τ_{static} generations.

In order to be able to get a handle on the overall stability of the evolutionary fit, and also as an aid in a possible parallelization, we add a final wrinkle by partitioning the total population into "islands" of equal size, each of which forms a separate population to which the basic evolutionary step is applied independently of the other islands. To avoid individual islands with particularly unfavorable starting conditions getting stuck, a weak coupling between islands is introduced by replacing the least fit organism on each island with a randomly chosen immigrant from a randomly chosen island with probability p^{mig} before carrying out the selection step. We find that the lowest-lying states are identified rather consistently across all islands fairly early on; only for the most massive states discrepancies in number, energy and amplitude are found between different islands, sometimes even in late generations, indicating that the identification of these states is somewhat uncertain.

Our main program thus employs a multi-island ecosystem for the evolutionary optimization and then tries to improve on the results of the best evolutionary fit by performing a Levenberg-Marquardt optimization upon it. If sufficiently many islands are being used, it is possible to do this as a constrained fit where desired, with the average and standard deviation of the parameter values derived from bootstrapping [42] the best island fits being employed as priors. Real parameter errors may be determined by bootstrapping the data configurations and rerunning the fit algorithm. However, as this could in principle produce different functional forms for different bootstrap configurations, and as this procedure may be quite expensive, one may choose instead to apply a Levenberg-Marquardt fit to the bootstrap configurations using the final functional form obtained from the evolutionary algorithm, as one would do in a conventional fit.

We have settled on the latter procedure for our implementation, and have found that the final Levenberg-Marquardt fit always returned within errors (as estimated by the bootstrapped Levenberg-Marquardt procedure) of the evolutionary fit, indicating that the evolutionary fit was already close to optimal. The errors from the bootstrapped Levenberg-Marquardt fit were usually (though not always, depending on how well genetic diversity between islands was preserved in each case) comparable to those estimated from the difference between the fits obtained on different islands.⁹ In the following, we use the error estimates from the final bootstrapped Levenberg-Marquardt fit as our estimate of the error in the fitted parameters.

To demonstrate the viability of our method, we have run a fit on two sets of synthetic data consisting of 200 artificial correlators for 48 timesteps, each constructed from a signal consisting of a sum of exponentials with known

⁹ For the purpose of these single correlator tests, we used a large ecosystem with 100 islands.



Fig. 1. Result of a fit to a set of pion-like synthetic correlators. Shown is a plot of the mass against the excitation number of the state. The horizontal lines are the input values used to create the synthetic data; the data points and errors are the fit results.

masses and amplitudes, and Gaussian noise. In one case ("pion-like", figure 1) the amplitude of the noise scaled linearly with the signal, in the other ("rho-like", figure 2) the noise amplitude was kept constant. It can be seen that the ground state mass and the mass of the first excited state are extracted with high reliability, while for the higher states good estimates are obtained. The increased error in the excited states is largely due to the noise component in the created data which makes it impossible to adequately resolve those states and not to a shortcoming in the algorithm itself.

The running time for our PYTHON implementation of each of the two bootstrapped fits was on the order of one to two hours on a single-processor Pen-



Fig. 2. Result of a fit to a set of rho-like synthetic correlators. Shown is a plot of the mass against the excitation number of the state. The horizontal lines are the input values used to create the synthetic data; the data points and errors are the fit results.

tium 4 workstation; implementing the same algorithm in a compiled language could cut this runtime down further. It should be stressed that the evolutionary fit works robustly without any human intervention, thus saving valuable human time at the expense of a moderate increase in computer time when compared to more conventional excited state fitting methods that often require a larger degree of user intervention.

Finally, in figure 3 we show the results from fits to actual pion and rho correlators from a quenched simulation using Wilson quarks, demonstrating the ability of our program to deal with real lattice data.



Fig. 3. Result of a fit to an actual meson correlator from a quenched simulation using Wilson quarks. The simulation $(N_{conf} = 100)$ was run on a $16^3 \times 32$ lattice at $\beta = 6.0$, $\kappa = 0.154$. The red points and error bars are the results of the fit; the blue bands are the approximate masses of the continuum states corresponding to the lowest and first excited states in the fitted channels extrapolated to the quark masses employed in the simulation. The largest fitted state does not correspond to a known continuum state and may be a lattice artifact.

4 Evolutionary Fitting of Multiple Correlators

In this section we discuss the generalizations of the evolutionary fitting algorithm required for fitting multiple datasets simultaneously. A more sophisticated genotype is required in this case, since now the same energy E_n can occur throughout some subset of the datasets. Hence, the fit for dataset number *i* will now be represented by a list of $n_{max}^{(i)}$ coefficients $(Z_n^{(i)}, I_n^{(i)})$, $n = 1, \ldots, n_{max}^{(i)}$ where $I \in \{1, \ldots, m_{max}\}$ is an integer index into a list of m_{max} energy states E_m indicating to which state the coefficient is associated.¹⁰ The list $E_1 \ldots E_{m_{max}}$ is common to all datasets.

In summary, for a fit of i_{max} datasets the complete genotype is of the form:

Fit Genotype = (Dataset coefficients, Mass list) = ((Dataset 1 coefficients, ..., Dataset i_{max} coefficients), Mass list) (8)

with

Dataset *i* coefficients =
$$((Z_1^{(i)}, I_1^{(i)}), \dots, (Z_{n_{max}^{(i)}}^{(i)}, I_{n_{max}^{(i)}}^{(i)}))$$

Mass list = $(E_1, \dots, E_{m_{max}})$. (9)

Assuming the datasets are not correlated in any way, the new χ^2 is simply the sum of terms of the form in equation (5), one per dataset. The number of degrees of freedom changes from the form of equation (7) to:

$$n_{dof}(G) = n_{data} - m_{max} - \sum_{i=1}^{i_{max}} n_{max}^{(i)}$$
(10)

where n_{data} now counts all included timesteps in the fit of all datasets.

The presence of integer variables in the multi-dataset genotype requires some adaptations to the breeding algorithm used. For practical reasons, it is advantageous to use a fixed-length integer implementation with *n*-bit integers, where 2^n is the maximum number of distinct states we will allow in our fit. Crossover can be performed by exchanging the first m ($0 \le m \le n$) bits of two integers. Mutations are implemented by flipping each bit of the integer with some fixed probability.

¹⁰ The stored integer is interpreted modulo m_{max} to ensure it maps to an actual energy state.

The genotype (8) has a hierarchical structure as a list of lists ultimately containing floating point or integer numbers. Mutation and crossover can therefore be structured by recursing through these list structures, applying appropriate mutation and crossover operations at each level. The lists can be distinguished by the number (fixed or variable) and type (homogeneous or heterogeneous) of their elements, and by whether they are ordered or unordered. Elementwise mutation can be done on any kind of list. Lists of variable length can also be mutated by removing elements or adding a random new element, and ordered lists may be mutated by permuting their elements. Likewise for crossover, building two new lists by picking from the elements of the parent lists in order can be done for any list. Homogeneous lists allow more general subsets of the parents' elements to be chosen. Elementwise crossover may also be done, in order for heterogeneous lists or with random pairs of the parents' elements in the homogeneous case. All of the different mutation and crossover operations that are possible in each case can have different probabilities assigned to them and for lists of variable length, a range of valid list lengths may be specified.

In addition to these generic genetic operations, the multi-dataset fitting problem benefits from some operations specific to its structure. One notes that the genotype of equation (8) allows for multiple representations of the same fitting function, because the coefficient integers are taken modulo the number of masses in the fit, because either the masses or the indices to them may be in different orders, and because some masses may be unused or referred to multiple times for a single dataset. This degeneracy can have an adverse effect on the convergence of the algorithm. To encourage the algorithm to work toward a single representation of the solution, we employ a reduction mutation which sorts the mass list and removes unused masses. It also combines coefficients pointing to the same mass, places coefficient indices uniquely within the range $1, \ldots, m_{max}$, and orders them within each dataset by the associated mass index. In order to favor this operation, as well as any other mutation that may reduce redundancies, it is beneficial to count all masses and coefficients, whether redundant or not, in the count of the degrees of freedom in equation (10).

As in the single-correlator case, interspersing local optimization steps using the Levenberg-Marquardt method with the other mutations was found to be useful in accelerating convergence. Limiting the mutation to a fixed number of steps of the Levenberg-Marquardt algorithm and making it a relatively improbable mutation keeps the overall time evolution reasonable.

Special care needs to be taken in the multi-dataset case when adding or removing masses, since simply dropping a mass from the list will mean that any coefficients belonging to the dropped mass will now become associated with a different mass, which tends to have a catastrophic effect on fitness, especially for more evolved genotypes. A careful generalization of the way in which amplitudes are redistributed when changing the number of masses in the single-correlator case is therefore necessary. This is facilitated by first applying the reduction operation mentioned above before adding or removing a mass from the mass list. When removing a mass, one then loops through the dataset functions to see which ones have a coefficient corresponding to the removed mass. For any that do, the coefficient is deleted and its amplitude is redistributed between neighboring masses, either by increasing the coefficients for the closest masses already having coefficients in that dataset function, or by adding a new coefficient for an unrepresented neighboring mass. When adding a mass, at least one of the datasets receives a new coefficient associated with it, and the coefficients of the other masses in those datasets are lowered accordingly. As a final step, a Levenberg-Marquardt optimization step is carried out in order to give the new mutant a better chance of survival. There is obviously a tradeoff between the probability of such relatively expensive mutations and the maximum size of the population that can be employed.

As a test of the efficiency of the evolutionary algorithm in the multi-dataset case we have run fits of synthetic data. The result of such a test is shown in figure 4. Four hypothetical diagonal meson correlators were constructed to contain four masses among them. One correlator had coefficients for only two of the masses, two had coefficients for three of the masses, and one had coefficients for all four masses. The four datasets, with 48 timesteps each, were modified by adding Gaussian noise, the amplitude of which was chosen small enough to allow statistical discrimination of all states. A Levenberg-Marquardt fit to the synthetic data, using the masses and coefficients used to generate the data as the starting point, is shown in the last column of figure 4. As expected, the parameters shifted only marginally from their ideal values and χ^2/n_{dof} for the fit is very close to 1.

The multi-dataset algorithm was then run on the synthetic data. It was restricted to fit genotypes containing a maximum of eight masses with positive masses of value less than 10. Each dataset function was allowed to have up to six coefficients whose values were only restricted to being positive. Four islands were used, each containing 120 individuals (specifically $N_{elite} = N_{diversity} = 5$, $N_{mutants} = 20$). Figure 4 displays the best fit genotype from each generation along with its χ^2/n_{dof} . It is evident that the algorithm quickly succeeds at finding a good fit to the data. By generation 20 one has a fit with good χ^2/n_{dof} and characteristics almost identical to the model



Fig. 4. Best fit genotype and its χ^2/n_{dof} of each generation for a multi-dataset fit are shown. Four datasets were constructed to contain four masses with each dataset having coefficients for two to four of the masses. The model fit that generated the data is shown on the right. Each fit is displaced horizontally with different masses in separate columns with their corresponding coefficients in each of the datasets vertically aligned above them. The latter have been multiplied by powers of 10 for display purposes. The left side of the plot shows the results of the evolutionary algorithm, starting with the best fit of the first generation. Only generations with an improvement in the best fit genotype are plotted. For clarity a few of these fits have only their χ^2/n_{dof} displayed (open circles) to ensure that all data between subsequent drop lines corresponds to a single fit.

function, having the same number of masses and corresponding coefficients, except for the addition of a small (four orders of magnitude lower) coefficient added in the first dataset for the highest mass. Generation 64 shows that this functional form with an additional coefficient actually improves the fit, having a lower χ^2/n_{dof} than the optimized model function. Generations 100 onward *improve* even further in the fit by bifurcating the lowest mass to produce a fit of ever so slightly *greater* probability than the actual model function used to generate the data. This was the final result as of generation 2000. The total run was performed overnight on a single-processor Pentium 4 workstation.

Overall one notices that the algorithm adds masses initially as required before proceeding to coalesce masses and combine coefficients to improve the fit. The reduction mutation serves to encourage an ordering of masses from lowest to highest but generations 2 to 10 show it is not strictly required.

We are currently employing this program in a forthcoming analysis [43] of the meson spectrum of twisted-mass QCD [44] based on the representation theory of the octahedral group with generalized parity [45]. In figure 5, we show the results of a fit to actual data from the Wilson QCD action in the pion channel. The algorithmic parameters were the same as for the previous fit. Again, one observes that initially the number of states found fluctuates considerably, with states being added to improve the fit. At some point, too many states which are nearly degenerate have been introduced, and the population culls unnecessary bifurcations. One observes that by generation 200 the energy states have been largely found, further improvements occurring within the coefficients. The fitness of the best genotype traces this behavior.¹¹

¹¹ As an aside we note that for this fit and the fit to synthetic data shown in figure 4, the restriction $E_n < 10$ was initially imposed with an eye to restricting ourselves to physical masses and thereby preventing the occurrence of "runaway" solutions commonly encountered in this fitting task. We subsequently found this restriction to be unnecessary. We conjecture that the problem with runaway solutions may



Fig. 5. A simultaneous fit to actual data of eight diagonal pion (i.e. $\Lambda^{PC} = A_1^{-+}$) correlators from a quenched simulation using Wilson quarks ($\beta = 6.0, \kappa = 0.1554$, $20^3 \times 48,600$ configurations) is shown; the eight operators used are from [45]. Only the energies of the fittest organism of each generation are shown; the coefficients in each dataset, a further 28 parameters in the final fit, are not. The last column depicts the best fit found with bootstrap errors produced via Levenberg-Marquardt fits with its fixed functional form. Also shown (circles) is (the logarithm of) χ^2/n_{dof} of the best genotype, which indicates that by generation 25 one has technically a good fit ($\chi^2/n_{dof} \approx 1$).

To get an impression of how well the algorithm converges, we show histograms of χ^2/n_{dof} values of the final best fit for 160 twisted-mass meson channels in be due to trying to fit a poor functional form to the data, something which our algorithm avoids, thus removing the need for such a constraint. Subsequently, we merely constrain parameters to be positive.

figure 6. The 160 channels correspond to four quark masses (the mesons consist of mass-degenerate quarks and antiquarks), two particle types (charged or neutral), and 20 octahedral irreducible representations (Λ^{PC}). The 400 operators used (16 local and 384 extended) are detailed in [45]. Diagonal correlators were obtained for all of these operators, encompassing all channels. For operators in representations of dimension greater than one, all the correlators were row-averaged before fitting. The quenched simulation used degenerate twisted mass quarks with quark and link smearing of operators on a $20^3 \times 48$ lattice at $\beta = 6.0, m \sim m_s, m_s/2, m_s/3, m_s/6$ (where m_s is the physical strange quark mass); see [46,47,48] for further details.

For each channel the evolutionary algorithm was run three times: first using all of the data ($N_{config} = 600$ configurations), then one third of it ($N_{config} = 200$), and finally one sixth of it ($N_{config} = 100$). The fitness distribution for the full data set is excellent with χ^2/n_{dof} distributed locally about 1.0, clearly demonstrating the algorithm is robust in its ability to find a good fit, when the latter exists. As the amount of data included drops, however, the certainty with which states are resolved falls and the optimal fit becomes poorer. Fits required a minimum of 600 generations, and ran for up to 1200 generations if improvement still occurred in the best organism. The shown fits are for correlators with smeared operators. Unsmeared correlators (not shown) of the same operators which exhibit a greater number of excited states were also fit for the 600 configuration case with no appreciable difference from the histogram of the smeared one.

As a measure of stability of these fits, bootstrap errors of the fitness, $\sigma_{\chi^2/n_{dof}}$, have been calculated for each fit and their histograms are also shown. Specifically, for each fit, $3 \times N_{config}$ bootstrap configurations of the data were made



Fig. 6. Shown are normalized histograms of χ^2/n_{dof} (thick lines) of fits to 160 meson quantum channels containing between 2 and 16 correlators each. For each channel the evolutionary algorithm was run three times: using all ($N_{config} = 600$ configurations), one third ($N_{config} = 200$), and one sixth ($N_{config} = 100$) of the lattice data. For the full data set, the fitness distribution peaks sharply around 1.0, but as the amount of data included drops, the certainty with which states are resolved falls and the optimal fit becomes poorer. Bootstrap errors of the fitness, $\sigma_{\chi^2/n_{dof}}$, are also shown (thin lines). The stability of the fit is seen to decrease in the same way as the overall χ^2/n_{dof} as the quality of the data declines.

and the functional forms of the best fits were fit to them using a Levenberg-Marquardt routine whose initial values were those of the best fit. For the full 600 configurations one observes the variation in the goodness of the fit is small ($\sigma_{\chi^2/n_{dof}} < 0.3$). Since good fits occur in essentially all of the bootstrap configurations, this increases confidence that the spectrum found is accurate. The



Fig. 7. Shown is the execution time (on a single Intel Xeon 3.06 GHz CPU) per parameter as a function of the number of parameters in the final best fit. The latter includes each of the masses as well as the coefficients on each dataset for the given fit. The number of generations for all fits shown was fixed at 600, by which time all fits were already well converged. Smeared correlators (squares) exhibit a smaller number of fitted parameters than unsmeared ones (circles), which is expected since smearing suppresses contributions from excited states.

same is largely true for 200 configurations as well ($\sigma_{\chi^2/n_{dof}} < 0.6$), but by the time the data set is reduced to only 100 configurations the error in χ^2/n_{dof} is as wide as the value itself, indicating along with the fit histogram, that the amount of data is insufficient for solution of the problem.

Finally, in figure 7 we show the runtime per parameter as a function of the total number of parameters (masses and coefficients in all datasets) in the final fit. Overall, we find that the dominant contribution to runtime comes from

the number of coefficients, which in turn is largely proportional to the number of correlators used for the fit, as might be expected from a naive runtime analysis.

5 Alternatives and Variations

The specific implementation described in the previous section is just one of many possible ways to approach the problem of extracting excited state energies using evolutionary algorithms. In this section we wish to point out some alternatives to our current implementation, many of which we are actively exploring at the moment.

The previously described algorithm used a genetic encoding based on real numbers. This offers the advantage of being a straightforward representation, as well as the ability to interject local optimization steps in a natural manner. An alternative would be to use an integer-based representation of real parameters instead; the advantage in this case would be the ability to use bit-based mutation and crossover operations instead of our Gaussian mutations and interpolating crossover. The bit-based operations, besides likely being faster in most cases, are better understood in terms of rigorous theorems regarding global convergence properties (such as from schema theory [26,28]), but do not offer the possibility for easy mixing with local optimization.

Using straight elitism as the selection method has been found to be favorable in the case of problems with a real-number genetic code [18], but introduces a certain risk of premature convergence if the elite should happen to cluster around a local optimum. This risk is significantly reduced by the addition of random survivors and our use of an island-based ecosystem, but other, more sophisticated, selection methods could help to further eliminate any remaining bias. Another disadvantage of elitist selection is that it requires a full sort of the organisms by fitness in each generation, which makes up a fair part of our implementation's computational cost. Other selection methods manage to avoid this requirement, which could lead to further gains in speed. The specific mutation schedule implemented in our algorithm is also to be seen as just one example out of many that are possible. In some cases, it may be more favorable to mutate each parameter separately instead of mutating all parameters at once.

Our evolutionary algorithm depends on a number of parameters, such as the rate for different kinds of mutations, their dependence on χ^2/n_{dof} , and the size of the breeding pool. In the current implementation, these parameters have been set to reasonable values by hand. For a more highly optimized implementation, these parameters should be tuned to values that tend to give the fastest rate of convergence towards the true optimum; in principle, such tuning itself could be done by means of another evolutionary algorithm, although that approach might prove to be fairly expensive computationally.

Evolutionary multi-modal algorithms (see [49] and refs. therein) are able to find not only absolute extrema but relative extrema as well. "Niching" and "diversity preservation" algorithms have been devised that dissuade too many elements of the population from going after the single best solution, thereby finding not only the best solution but other good solutions. This could be useful in the context of fitting since these algorithms can produce the best fit as well as other fits that lie in relative extrema that are perhaps comparable with the best fit. Comparison of such fits would give the researcher a better feel for the uniqueness and likelihood of the functional form of the solution found.

Several improvements might be made for the simultaneous fitting of multiple correlators. Obviously it is of value to cull from the fit any datasets which clearly only contain noise. As well, if fitting a large number of datasets it could be of value to partition the datasets and find viable fits on each subset first. One could then merge these populations into genotypes suitable for the entire dataset by stitching together fits from each subset. This could be done crudely by just putting the masses back to back, or one could implement some algorithm which tried to find common masses at this point between two genotypes being merged in some systematic fashion. Running the algorithm on these new datasets would then optimize these fits globally, presumably by coalescing common masses across the subsets that are statistically equal to improve the final fit.

The local optimization steps used as mutations in our algorithm could be rendered more efficient by employing techniques that exploit the partial linearity of the functional form of equation (1) by separating the linear and non-linear variables [50].

There is also the possibility to combine the variational method with an evolutionary fitting algorithm. To do this, one could diagonalize the correlator matrix as usual with the variational method, and then use the evolutionary algorithm to fit the resulting diagonal correlators. In this way, any remaining mixing between the optimized operators could be detected and quantified, while at the same time reducing the number of correlators to be fit.

An alternative to evolutionary algorithms, which we have not investigated so

far, might be the use of Markov Chain Monte Carlo optimization methods such as simulated annealing [51], which share evolutionary algorithms' ability to accommodate discrete changes in functional form.

6 Conclusions

Evolutionary fitting methods provide an interesting and useful addition to the lattice field theorist's data analysis toolkit. Especially when combined with other well-known and well-tested fitting methods, evolutionary fitting can help to extract information from simulation data without having to impose any external constraints, such as Bayesian priors. Evolutionary methods allow one instead to extract all of this information from the data themselves by harnessing the globally optimizing nature of evolving systems. This is particularly true in the case of discrete parameters such as the number of states to fit, which are hard to determine using more conventional methods.

We have demonstrated a working method for the extraction of excited state masses from lattice QCD correlators using evolutionary fitting. We believe that evolutionary fitting algorithms have significant potential as a data analysis method in lattice QCD, and that further investigation in this direction is warranted.

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