An Algorithm for Obtaining Reliable Priors for Constrained-Curve Fits∗†

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We introduce the “Sequential Empirical Bayes Method”, an adaptive constrained-curve fitting procedure for extracting reliable priors. These are then used in standard augmented-chi-square fits on separate data. This better stabilizes fits to lattice QCD overlap-fermion data at very low quark mass where a priori values are not otherwise known. We illustrate the efficacy of the method with data from overlap fermions, on a quenched $16^3 \times28$ lattice with spatial size $La = 3.2$ fm and pion mass as low as $\sim 180$ MeV.

1. Background

Traditionally, Monte Carlo estimates, $\langle G(t) \rangle$, of two-point hadronic correlators have been fit to a theoretical model, such as,

$$G(t; w_i, m_i) = \sum_{i=1}^{\infty} w_i e^{-m_i t}$$

by the maximum-likelihood procedure of minimizing the chi-square.

Fitting with a single-source multi-exponential is usually too unstable, so the default has been the popular single-source single-exponential, wherein one fits only at $t > t_{\text{min}}$ to damp contributions from excited states. One compromises between high statistical for large $t_{\text{min}}$ and high systematic errors for small $t_{\text{min}}$; lattice alchemy provides various recipes for making the compromise and estimating the systematic errors. A multi-source multi-exponential fit is a much better, albeit more expensive, alternative; however, the ambiguity of estimating systematic errors through tuning $t_{\text{min}}$ remains.

“Constrained Curve Fitting” [12] offers the alternative of minimizing an augmented chi-square,

$$\chi^2_{\text{aug}} = \chi^2 + \chi^2_{\text{prior}} ; \quad \chi^2_{\text{prior}} = \sum_i \frac{(\rho_i - \tilde{\rho}_i)^2}{\tilde{\sigma}_i^2}$$

where $\rho$ denotes the collective parameters of the fit (e.g. $\rho = \{w, m\}$). It achieves stability by “guiding the fit” with the use of Bayesian priors, that is, values of the parameters obtained from a priori estimates $\rho = \tilde{\rho} \pm \tilde{\sigma}$. It has improved stability; as data sets are enlarged to include small $t$, many more terms are added in the fit model until convergence is obtained. The $t_{\text{min}}$ systematic error is largely absorbed into the statistical error. The method works well if reliable priors are known; nevertheless, stability of the fit results against choice of prior must be tested, and this reintroduces an element of subjectivity.

However, with our recent data [3], we enter previously unexplored territory, namely, overlap fermions with exact chiral symmetry at unprecedented small quark mass and large spatial size. There is in general no literature from which to obtain estimates to be used as priors and no reliable model for estimates of level spacings.

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2. Overview

We propose an adaptive self-contained constrained curve-fitting procedure, dubbed the “Sequential Empirical Bayes Method” method. We obtain the priors gradually (from the ground state up) as the data set is monotonically enlarged (to include earlier and earlier time slices). The basic “fixed $\Delta t$” algorithm is described below for simplicity. In practice we use a refinement, the more adaptable “variable $\Delta t$” algorithm, results of which are presented in the next section.

1. Choose (i) $t_{\text{min}}$ and $t_{\text{max}}$, the maximum range over which the fits will be done, and (ii) $t_{\text{start}}$, the initial minimum time slice of the fitting range.

2. Loop on various trial values (“scanning”) around central values $w_1$ and $m_1$ obtained from effective mass. For each, use an unconstrained fit on the one-mass-term model (1MTM) to fit over $\{t_{\text{start}}, t_{\text{max}}\}$ to obtain $w_1^{(1)} \pm \sigma_w^{(1)}$ and $m_1^{(1)} \pm \sigma_m^{(1)}$. Choose as input for the next step those values which yield the lowest $\chi^2$.

3. Using these $w_1, \sigma_w, m_1, \sigma_m$, as both priors and initial values, do a constrained-curve fit, using the 1MTM over $\{t_{\text{start}} - 1, t_{\text{max}}\}$, to obtain $w_1^{(2)}, \sigma_w^{(2)}, m_1^{(2)}, \sigma_m^{(2)}$.

4. Using these $w_1, \sigma_w, m_1, \sigma_m$, as both priors and initial values, do a half-constrained fit over $\{t_{\text{start}} - 2, t_{\text{max}}\}$ on a 2MTM; the second mass and weight are unconstrained. Loop on various trial values for the latter; choose as input for the next step those values which yield the lowest $\chi^2$.

5. Using these $w_1, \sigma_w, m_1, \sigma_m, w_2, \sigma_w^2, m_2, \sigma_m^2$ as both priors and initial values, do a fully-constrained fit, using the 2MTM over $\{t_{\text{start}} - 3, t_{\text{max}}\}$ to obtain $w_1^{(4)}, \sigma_w^{(4)}, m_1^{(4)}, \sigma_m^{(4)}, w_2^{(4)}, \sigma_w^{(4)}, m_2^{(4)}, \sigma_m^{(4)}$.

6. Repeat the last two steps until all desired mass terms and time slices are included. One thus obtains a complete set of priors.

3. Sample Result

The $\langle A_4 A_4 \rangle$ correlator is dominated by the ground state of the pseudoscalar channel (pion) over all but the few earliest time slices. With the variable $\Delta t$ refinement of the algorithm, rather than deciding a priori on the number of terms in the fit and adding time slices a fixed number at a time, one lets the data decide how many time slices to include with each enlargement of the data by choosing the minimum chi-square over a range of reasonable possibilities. Thus since the pion correlator is dominated by the ground state for many time slices, then many time slices will be automatically added before an attempt is made to fit the first-excited state. We find that the variable $\Delta t$ method works very well for the pion correlators.

![Figure 1. Ground and first-excited state pseudoscalar masses as obtained from the Sequential Empirical Bayes’ Method.](image)

4. Testing the Algorithm

4.1. Partitioning the Configurations

Final results should use the priors on a separate data set, thus preserving the ideal Bayesian case. However, empirically this seems to be unnecessary; the output from the algorithm agrees with the final results. We have implemented the following test: We partition the data into two non-intersecting sets of configurations, $A$ and $B$, with an equal number, $n_A = n_B = 40$ of configurations in each set. Using the set $A$ of configurations, we...
perform our procedure to obtain priors; we next use this fixed set of priors in the canonical way to perform a constrained fit separately on data set $B$, on data set $A$, and on the full set $A \cup B$. We find no appreciable differences beyond expected statistical fluctuations.

4.2. Stability
The Sequential Empirical Bayes’ Method is used to select the priors. Then a standard constrained fit with all of the time slices is made. The number of terms in the fit model is increased until the fit results converge.

4.3. Reconstructing Artificial Data
The method can successfully reconstruct the parameters of artificially-constructed data where the true results are known independently of the fit.

We created a sample of artificial data as a sum of decaying exponentials by adding an independent Gaussian noise to the function at each value of $t$. The fitting procedure was able to reconstruct the means and weights for the ground and excited states; the actual values were within one measured standard deviation of the measured means.

Figure 3. Recovery of masses from artificially-constructed data (masses 0.25, 0.5, 1.0, 1.4, 1.8, and amplitudes 1.20, 1.00, 0.80, 0.60, 0.50).

5. Summary
We have introduced an adaptive self-contained constrained curve-fitting procedure which produces priors to be used in a standard constrained fit on different data. One obtains the priors sequentially as data set is enlarged. The method’s advantages include: it is usable whenever external reliable estimates of the priors are not available; it can be fully automated; it reduces human-induced bias; it decreases the frustrating busy-work of fitting; and it is self-correcting. We have checked that the method can reconstruct artificial data, that it is stable against adding more terms, and against partitioning the data.

For more complete details, see [4] which provides additional examples of applicability and outlines further refinements. The method has been used successfully to make the first lattice identification [3] of the Roper resonance at low quark mass with exact chiral symmetry.

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