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Fourier accelerated conjugate gradient lattice gauge fixing

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ABSTRACT

We provide details of the first implementation of a non-linear conjugate gradient method for Landau and Coulomb gauge fixing with Fourier acceleration. We find clear improvement over the Fourier accelerated steepest descent method, with the average time taken for the algorithm to converge to a fixed, high accuracy, being reduced by a factor of 2 to 4.

1. Introduction

Conjugate gradient (CG) methods (first used to solve linear equations [1] and later generalised for non-linear, non-quadratic functions [2,3]) are a technique to solve unconstrained local minimisation problems. Numerically these methods can be implemented cheaply because they are iterative and converge in a finite number of steps. They are also often considered computationally faster than the steepest descent method [4]. We illustrate how fixing to the smooth, Landau and Coulomb gauges in the context of lattice field theory can be achieved by using the method of conjugate gradients.

Fixing the gauge is a prescription for removing redundant degrees of freedom of the gauge field in a continuum quantum field theory. Common choices are the Landau $\partial_\mu A_\mu(x) = 0$ and Coulomb $\partial_i A_i(x) = 0$ gauges (where Greek indices run over all dimensions and Roman over the spatial and the A's are the gauge fields of our theory). Fixing the gauge (while not necessary for many lattice measurements) is often required for the direct matching of lattice simulations to continuum perturbation theory.

Measurements of lattice Green's functions in strongly coupled, N_d-dimensional, SU(N_c) theories have to be performed with a fixed gauge and are often computed in Landau gauge. Landau gauge Green's functions are vital for the non-perturbative renormalisation of important physical quantities such as the QCD Kaon bag parameter B_K [5,6] and can also be used for the measurement of the QCD strong coupling α_s [7]. Coulomb gauge fixing is more generally applicable to lattice theorists; it is used in methods such as gauge-fixed wall source quark correlators (also often used in the calculation of B_K), or for computing the static quark potential [8]. Having a fast routine to fix the gauge allows for faster measurements of critical physical quantities.

Lattice "links" transcribe the gauge fields formally by the path-ordered matrix exponential $U_\mu(x) = P[e^{ig_0 \int_x^{x+a} dx_\mu A_\mu(x)}]$ (for lattice site "x", with lattice spacing a and bare coupling g_0), which can be well approximated by,

$$U_\mu\left(x + a\frac{\hat{\mu}}{2}\right) = e^{iag_0 A_\mu\left(x + a\frac{\hat{\mu}}{2}\right)}. \tag{1}$$

The gauge fields are obtained by the logarithm of the links. A common approximation [9] to the logarithm of the map $U = e^{iA}$, $U \in \mathrm{SU}(N_c)$ is what we call the "Hermitian projection" (where $I_{N_c \times N_c}$ is the identity matrix),

$$A = \frac{1}{2i}\left\{\left[U - U^\dagger\right] - \frac{1}{N_c}\mathrm{Tr}\left[U - U^\dagger\right] \cdot I_{N_c \times N_c}\right\}. \tag{2}$$

This definition is not unique, being correct up to terms of $O(A^3)$. Exact logarithm techniques are possible [10,11] but will not be discussed here as they are numerically costly to implement and less commonly used in practice.

2. Gauge fixing on a lattice

We now discuss the case of lattice Landau gauge fixing, as the extension to Coulomb gauge should be simple. After we introduce

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the conjugate gradient procedure we then discuss our implementation for fixing to Coulomb gauge.

There are two common types of gauge fixing routines, the Los Alamos [9] and the Cornell [12], both of which use the method of steepest descent to minimise the functional over the gauge orbits and not the entire gauge manifold (where V is the lattice volume),

$$F(U) = \frac{1}{N_d N_c V} \sum_{x,\mu} \mathrm{Tr} \left[\left(a g_0 A_\mu \left(x + a\frac{\hat{\mu}}{2} \right) \right)^2 \right]. \tag{3}$$

We focus on the Cornell method as it can be Fourier accelerated.[1]

For the Hermitian projection definition (Eq. (2)) of the gauge fields, the following approximation of the functional can be used,

$$F(U) \approx 1 - \frac{2}{N_d N_c V} \sum_{x,\mu} \Re \left(\mathrm{Tr} \left[U_\mu \left(x + a\frac{\hat{\mu}}{2} \right) \right] \right). \tag{4}$$

In general, the method of steepest descent is a technique to find a local minimum of a function. Considering the nth iteration of such a method, the update,

$$x_{n+1} = x_n - \alpha f'(x_n), \tag{5}$$

will step towards a local minimum of the function $f(x)$; provided the parameter α is positive, small and if x_n is close to the solution.

In direct analogy to the general procedure of Eq. (5) we first approximate the derivative of a gauge field by,

$$a\Delta_\mu A_\mu(x) = \sum_\mu \left(A_\mu \left(x + a\frac{\hat{\mu}}{2} \right) - A_\mu \left(x - a\frac{\hat{\mu}}{2} \right) \right). \tag{6}$$

The nth iteration of the lattice steepest descent Landau gauge fixing procedure updates the links via the gauge transformation,

$$\begin{aligned} g(x) &= e^{-i\alpha a\Delta_\mu a g_0 A_\mu^{(n)}(x)}, \\ U_\mu^{(n+1)} \left(x + a\frac{\hat{\mu}}{2} \right) &= g(x) U_\mu^{(n)} \left(x + a\frac{\hat{\mu}}{2} \right) g(x + a\hat{\mu})^\dagger. \end{aligned} \tag{7}$$

This procedure successively reduces $a\Delta_\mu a g_0 A_\mu^{(n)}(x)$ towards zero, whilst retaining the gauge invariance of the action. A local minimum of the functional of Eq. (3) occurs when $a\Delta_\mu a g_0 A_\mu^{(n)}(x) = 0$ [12].

The parameter α is again a small tuning parameter, which could be tuned at each step but is best fixed to a near-optimal constant value. We found setting α to 0.08 and 0.1 for Landau and Coulomb gauge respectively to be best for the ensembles considered in this work.

The exponential in Eq. (7) could be computed exactly using the technique of [14], but expansion to the term linear in α and reunitarisation is sufficient and numerically faster.

It is common to stop the gauge fixing routine once the quantity,

$$\Theta^{(n)} = \frac{1}{N_c V} \sum_x \mathrm{Tr} \left[\left(a\Delta_\mu a g_0 A_\mu^{(n)}(x) \right)^2 \right], \tag{8}$$

reaches some small value (often $\Theta^{(n)} \approx 10^{-14}$).

2.1. Fourier acceleration

The steepest descent method of fixing to Landau gauge as outlined above was shown in [12] to suffer from critical slowing down, meaning that the number of iterations required to converge to a fixed accuracy grows drastically with the volume of the problem. Their method to ameliorate this was to apply a re-scaling in momentum space of the eigenvalues of the (Abelian) Laplacian Δ^2,

$$g(x) = e^{-i\alpha \tilde{F} \frac{p^2_{\mathrm{Max}}}{Vp^2} F a\Delta_\mu a g_0 A_\mu^{(n)}(x)}, \tag{9}$$

where F and $\tilde{F}$ are forward and backward fast Fourier transforms (FFTs) respectively, and the factor of $\frac{1}{V}$ is for the FFT normalisation. In practice, it is best if the quantities $\frac{p^2_{\mathrm{Max}}}{Vp^2}$ are precomputed as a look up table. The discrete momenta p^2 have the usual lattice definition,

$$p^2 = 2 \left(N_d - \sum_\mu \cos \left(\frac{2\pi n_\mu}{L_\mu} \right) \right), \tag{10}$$

with Fourier modes $n_\mu = \left(\frac{-L_\mu}{2}, \ldots, -1, 0, 1, \ldots, \frac{L_\mu}{2} - 1 \right)$. L_μ is the length of the lattice in the μ direction. Special care should be taken at the zero mode, where we set the value of p^2 to 1 [12]. The quantity $p^2_{\mathrm{Max}} = 4N_d$ is the maximum value of the lattice momentum.

In our implementation of Fourier acceleration, the shared-memory parallel version of the library FFTW [15] was used. The Fourier accelerated steepest descent method will be denoted as FASD later on in this paper.

3. The conjugate gradient method

An outline of the general approach for the non-linear (Polyak–Ribieré [3])[2] conjugate gradient method is shown in Algorithm 1.

Algorithm 1 General non-linear CG

```
Compute the gradient direction f'(x_0)
Perform a line search for α_0 s.t min(f(x_0 − α_0 f'(x_0)))
Perform the update x_1 = x_0 − α_0 f'(x_0)
Set s_0 = −f'(x_0)
n = 1
while |f'(x_n)|^2 > Tolerance do
    Compute the gradient f'(x_n)
    Compute β_n = max[0, f'(x_n)^T (f'(x_n) − f'(x_{n−1})) / (f'(x_{n−1})^T f'(x_{n−1}))]
    Compute conjugate direction s_n = −f'(x_n) + β_n s_{n−1}
    Perform a line search for α_n s.t min(f(x_n + α_n s_n))
    Update x_{n+1} = x_n + α_n s_n
    n = n + 1
end while
```

The translation of this approach to lattice Landau gauge fixing follows almost directly, and we call it the Fourier Accelerated Conjugate Gradient (FACG) method, and outline it in Algorithm 2. This algorithm should not be confused with the CGFA algorithm of [16], which uses the CG algorithm to invert the Laplacian instead of performing FFTs.

The approach begins with an FASD step as in Eq. (9), storing the result of the Fourier accelerated derivative in the conjugate direction $s_n(x)$. Once the algorithm has reached a sufficient minimum we are finished, otherwise we repeat the procedure generating conjugate directions weighted by the factor β_n.

We choose to use a line search to approximately determine the optimal tuning parameter α_n at each iteration. To do so we evaluate the gauge fixing functional (Eq. (4)) for possible fixed probe values

[1] Over-relaxation techniques in combination with the Los Alamos method similarly reduce the iteration count of a steepest descent routine [13], such techniques are not compatible with the method presented here.

[2] We find that the Polyak–Ribieré definition of β_n reduces the iteration count in comparison to the Fletcher–Reeves.