Gauge invariant extremization on the lattice

A.J. van der Sijs

Theoretical Physics, University of Oxford
1 Keble Road, Oxford OX1 3NP, United Kingdom
[e-mail: vdsijs@dionysos.thphys.ox.ac.uk]

Abstract

Recently, a method was proposed and tested to find saddle points of the action in simulations of non-abelian lattice gauge theory. The idea, called ‘extremization’, is to minimize \( f(\delta S/\delta A_{\mu})^2 \). The method was implemented in an explicitly gauge variant way, however, and gauge dependence showed up in the results.

Here we show how extremization can be formulated in a way that preserves gauge invariance on the lattice. The method applies to any gauge group and any lattice action. The procedure is worked out in detail for the standard plaquette action with gauge groups U(1) and SU(N).

*Supported by SERC grant GR/H01243.
1 Introduction

One of the approaches to understand the non-perturbative nature of non-abelian gauge theories has been to look for topological objects like monopoles and instantons in lattice Monte Carlo simulations. They are local minima of the action and are thought to give important contributions to the path integral. An important question is whether the presence of such objects is related to the string tension. The problem one faces here is that short distance fluctuations obscure the presence of such topological objects in lattice gauge field configurations. Monopoles and instantons are basically semiclassical objects, characterized by their long distance structure.

Several techniques have been developed to extract the relevant long distance information from a lattice gauge field configuration. One of them is the cooling method \[1\], which minimizes the action density of a particular configuration locally in an iterative way, directing it towards a local minimum in configuration space. Apart from local minima, however, saddle points are also solutions to the field equations. The sphaleron is a popular example. It is therefore useful to consider saddle points in lattice field configurations as well.

Recently, Duncan and Mawhinney \[2\] have discussed a method to find saddle point solutions of Yang-Mills theory (or other (lattice) field theories). They applied their method, which they called ‘extremization’, to three-dimensional SU(2) gauge theory and found that configurations after extremization showed lumps in the action density that were highly correlated to lumps found after cooling the same configurations. It was found that the string tension survives moderate extremization but ultimately disappears.

The basic idea of extremization is to minimize the squared gradient of the action, referred to as ‘extremization action’,

\[
\hat{S} = \sum_{x,\mu,a} \left( \frac{\delta S}{\delta A^a_\mu(x)} \right)^2 , \tag{1}
\]

instead of lowering the action itself as in the cooling method. In ref. \[2\] this was implemented for the plaquette action of lattice gauge theory. A conjugate gradient method in terms of the gauge fields \(A^a_\mu(x)\) was used to minimize \(\hat{S}\) and Fourier acceleration was used to speed up the minimization process. The authors stated that \(\hat{S}\) is a gauge variant function, so that lattices differing by a gauge transformation might extremize differently, which is what they observed in their gauge variant minimization procedure.

However, if we take for \(S\) the (continuum) Yang- Mills action

\[
S^{\text{cont}} = \frac{1}{4g^2} \int_V (F^a_{\mu\nu})^2 , \tag{2}
\]

we see that the functional derivative in eq. (1) gives just the gauge covariant equation of motion for \(A^a_\mu(x)\), so that the corresponding extremization action \(\hat{S}\) is the gauge invariant quantity

\[
\hat{S}^{\text{cont}} = \int_V (D^a_\mu F^{a\mu}_\nu)^2 , \tag{3}
\]

disregarding the factor \(1/g^2\) in front of \(S^{\text{cont}}\). This is not surprising, for the extrema of the action, determined by \(\hat{S}\), should be gauge invariant. Since the continuum quantity eq. (3) is gauge invariant, it must be possible to define the lattice analogue in a gauge invariant way as well. It is the purpose of this paper to show how this can be achieved.
In section 2 the gauge invariant extremization action is defined. It is shown that it has the expected behavior in the limit of lattice spacing $a \to 0$ and its structure is visualized in terms of closed Wilson loops. Section 3 contains a discussion of the generality of the method and a few comments about its implementation. Finally, we briefly discuss physical applications.

2 Gauge invariant extremization action

Consider the standard plaquette action for SU(N) lattice gauge theory,

$$S = \beta \sum_{\square} \left( 1 - \frac{1}{2N} (\text{Tr } U_{\square} + \text{Tr } U_{\square}^\dagger) \right)$$  

($\beta = 2N/g^2$)

$$= -\frac{1}{g^2} \sum_{\square} \left( \text{Tr } U_{\square} + \text{Tr } U_{\square}^\dagger \right) + \text{Const.} \quad (5)$$

We will forget about the irrelevant constant. The degrees of freedom in this theory are the link variables $U_{\mu}(x)$ which are matrices in a unitary representation of the gauge group. Therefore it is appropriate to consider the functional derivatives of the action (5) with respect to $U_{\mu}(x)$. Since the link variable $U_{\mu}(x)$ is related to a corresponding continuum gauge field $A_{\mu}(x)$ by the path ordered integral

$$U = U_{\mu}(x) = \mathcal{P} \exp \left[ -ia \int_0^1 A_{\mu}(x + ta\hat{\mu}) \, dt \right] = \overbrace{x + a\hat{\mu}}^{x + a\hat{\mu}}, \quad (6)$$

which can be expanded in $a$ to give

$$U_{\mu}(x) = 1 - iaA_{\mu}(x) + \mathcal{O}(a^2), \quad (7)$$

one expects this derivative to become equivalent to the derivative with respect to $A_{\mu}(x)$ in the limit $a \to 0$. In this way, we shall define a manifestly gauge invariant extremization action on the lattice and show that it reduces to eq. (3) to leading order in the lattice spacing.

We start by rewriting the plaquette action (4) in a form that exhibits the dependence on a particular link $U$ more clearly,

$$S = -\frac{1}{g^2} \sum_{\text{links}} \text{Tr} \left( UF_U + U^\dagger F_U^\dagger \right)$$  

+ terms independent of $U \quad (8)$$

(from now on we will omit factors of $1/g^2$). Here $F_U$ is the sum of the $\gamma = 2(d-1)$ ‘staples’ for the link $U$,

$$F_{U_{\mu}}(x) = \sum_\nu \left( \begin{array}{c} x \\ \nu \end{array} \right)_x + x \left( \begin{array}{c} \nu \\ \mu \end{array} \right) \quad, \quad (9)$$
which upon contraction with $U$ gives the part of the plaquette action depending on $U$. $\gamma$ can be considered as the coordination number for the interactions. A staple is defined as

$$r_r = U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + a\hat{\nu}) U_\nu^\dagger(x).$$

(10)

$F_U$ is sometimes called the ‘force’ (hence the notation $F$) for the link $U$. Note that it is not an element of the SU(N) in general. In the special case of gauge group SU(2) it can always be written as a constant times an SU(2) matrix.

A variation $\delta U$ in the link $U = U_\mu(x)$ gives rise to a change in action $\delta S$ equal to

$$\delta S = -\text{Tr} \left\{ \left( \frac{\delta S}{\delta U} - U^\dagger \frac{\delta S}{\delta U^\dagger} U^\dagger \right) \delta U \right\}$$

(11)

$$= -\text{Tr} \left\{ (UF - (UF)^\dagger) \delta U U^\dagger \right\},$$

(12)

where we have used that

$$0 = \delta(U^\dagger U) = (\delta U^\dagger)U + U^\dagger \delta U,$$

(13)

and it is understood that $F = F_U$. We can visualize $(UF - (UF)^\dagger)$ as

$$\sum \left( \begin{array}{c}
\begin{array}{c}
\square
\end{array}
\end{array} - \begin{array}{c}
\begin{array}{c}
\square
\end{array}
\end{array} \right)$$

(14)

where the sum runs over the $\gamma = 2(d - 1)$ staple directions.

We now define the gauge invariant lattice analogue of the extremization action $\hat{S}$ by

$$\hat{S} = \sum_{\text{links}} \frac{1}{2} \text{Tr} \left\{ (UF - (UF)^\dagger)(UF - (UF)^\dagger) \right\}$$

(15)

$$= \sum_{\text{links}} \frac{1}{2} \text{Tr} \left\{ 2F^\dagger F - FUFU - (FUFU)^\dagger \right\}. $$

(16)

This is a sum over closed Wilson lines of lengths 6 and 8, arising from contractions of the diagrams in eq. (14). Obviously, $\hat{S}$ is gauge invariant.

Before giving a more detailed survey of the diagrams we shall show that $\hat{S}$ reduces to its continuum counterpart (3) in the limit $a \to 0$. For simplicity, we shall do so for the abelian case. The non-abelian generalization will follow easily. For completeness we mention that for the gauge group U(1) the plaquette action is

$$S_{U(1)} = -\frac{1}{2g^2} \sum_{\Box} (\Box + \Box^*),$$

(17)

and the appropriate definition of $\hat{S}$ is

$$\hat{S}_{U(1)} = \frac{1}{4} \sum_{\text{links}} (UF - (UF)^*)(UF - (UF)^*).$$

(18)
Consider the expression for $UF - (UF)^*$ in eq. (14) with $U = U_\mu(x)$. For each $\nu \neq \mu$ the sum contains a contribution in the positive and one in the negative $\nu$-direction. The term from the positive $\nu$-direction is calculated as follows. First one computes the expansion of the plaquette around its centre,

\begin{equation}
\begin{array}{c}
\text{ plaquette}
\end{array}
\xrightarrow{\mu} = \exp [-ia^2 F_{\mu\nu}(x + \frac{1}{2}a\hat{\mu} + \frac{1}{2}a\hat{\nu}) + \mathcal{O}(a^4)] ,
\end{equation}

so that

\begin{equation}
\begin{pmatrix}
\text{ plaquette}
\xrightarrow{\mu} & \text{ plaquette}
\xrightarrow{\mu}
\end{pmatrix}
= -2i \sin [a^2 F_{\mu\nu}(x + \frac{1}{2}a\hat{\mu} + \frac{1}{2}a\hat{\nu}) + \mathcal{O}(a^4)] .
\end{equation}

If the expansion in eq. (19) were not done around the centre of the plaquette, $\mathcal{O}(a^3)$ terms would be present as well. The contribution from the negative $\nu$-direction is

\begin{equation}
+ 2i \sin [a^2 F_{\mu\nu}(x + \frac{1}{2}a\hat{\mu} - \frac{1}{2}a\hat{\nu}) + \mathcal{O}(a^4)]
\end{equation}

and the sum of eqs. (20) and (21) can be expanded around $x + \frac{1}{2}a\hat{\mu}$ and subsequently summed over $\nu$ to give for $UF - (UF)^*$ in eq. (14):

\begin{equation}
\sum \begin{pmatrix}
\text{ plaquette}
\xrightarrow{\mu} & \text{ plaquette}
\xrightarrow{\mu}
\end{pmatrix}
= -2ia^3 \sum \nu \partial_\nu F_{\mu\nu}(x + \frac{1}{2}a\hat{\mu}) + \mathcal{O}(a^5) .
\end{equation}

Terms of $\mathcal{O}(a^4)$ cancel out. Finally, this result is inserted in eq. (18), giving

\begin{equation}
\hat{S}_U(1) = \int_V a^2 (\partial_\nu F_{\mu\nu})^2 + \mathcal{O}(a^4)
\end{equation}

which is the abelian version of eq. (3) to leading order in $a$, as promised. The extra factor of $a^2$ here is explained by eq. (7) and serves to make $\hat{S}$ dimensionless. This result can be generalized to the non-abelian case immediately, by replacing the derivatives by covariant ones and adjusting the coefficients appropriately.

Now we turn to an overview of the diagrams occurring in $\hat{S}$ (15–16). Each link $U$ in the summation eq. (16) yields $(2\gamma)^2$ closed Wilson loops, with the appropriate signs (recall that $\gamma = 2(d - 1)$). In 2, 3 and 4 dimensions, $4\gamma^2 = 16, 64, 144$ respectively. These huge numbers include a number of trivial and double-counted diagrams as well as hermitian conjugates, however.

The first term in eq. (16) contributes $\gamma^2$ Wilson loops of length 6 in lattice units, each counted twice. These are the diagrams ‘hinging’ around the link $U_\mu(x)$, but independent of it, together with their adjoints, see fig. 1a. Of these, $\gamma$ give the unit matrix, another $\gamma$ are the planar $2 \times 1$ loops, and the remaining $\gamma(\gamma - 2)$ do not lie in a plane. Note that the symmetric length 6 Wilson loops winding around a cube as depicted in fig. 1b
Figure 1:
a. Length 6 Wilson loop contributing to $\hat{S}$.
b. Non-contributing length 6 diagram.
c. Contributing diagram of length 8.
d. ‘Double plaquette’.

are excluded. The other terms in eq. (13) give the length 8 Wilson loops containing the
link $U$ twice (fig. 1c) and their conjugates. These $2\gamma^2$ diagrams include the $\gamma$ ‘double
plaquettes’ shown in fig. 1d with their conjugates. In these double plaquette diagrams,
the loop winds around a plaquette twice before closing on itself.

Note how nicely this method provides one with a lattice action reducing to the contin-
umum derivative action eq. (3) in lowest order in the lattice spacing $a$. It is also interesting
to observe that, apart from being gauge invariant, eq. (3) preserves Lorentz-invariance.
This implies that $\hat{S}$ cannot be used as an improvement term for the plaquette action.
The $O(a^6)$ term in the expansion of the plaquette action which is canceled in tree-level
improved actions [3] by adding $2 \times 1$ rectangular Wilson loops, are of the form

$$ \sum_{\mu,\nu} D_\nu F_{\nu\mu} D_\nu F_{\nu\mu} $$

which does not equal $\sum_{\mu} (\sum_{\nu} D_\nu F_{\nu\mu})^2$.

3 Further remarks

It should be clear that the applicability of the procedure described in this paper is not
restricted to the standard plaquette action. For any lattice action $S$, written as a sum
over closed Wilson lines, the quantity

$$ \hat{S} = \frac{1}{2} \sum_U \text{Tr} \left| \frac{\delta S}{\delta U} \right|^2 $$

provides a gauge invariant extremization action. The calculational recipe of $\hat{S}$ can be
visualized as follows. Cut the link $U$ out of the $U$-dependent closed loops occurring in $S$,
and paste the resulting open-ended lines together (with the correct signs) to form closed
loops of $\hat{S}$.

Furthermore, the extremization action eq. (25) can be defined for any gauge group,
including discrete groups such as $\mathbb{Z}_N$, the link variables being group elements. Of course,
it is not possible to define a continuum limit of the extremization action (nor the action
itself) if the gauge group is discrete. This does not limit the use of the extremization
action for lattice gauge theories with discrete groups, however.

We should also make some remarks about implementation of the suggested extremiza-
tion procedure. First of all, in four dimensions the number of diagrams contributing to $\hat{S}$
for each link is large so that calculation and minimization of $\hat{S}$ can be computationally
quite expensive. In two and three dimensions this problem is less severe and the method
may find its applications. Furthermore, minimization of the extremization action $\hat{S}$ is not
straightforward. The dependence of $\hat{S}$ on a particular link $U$ is of the non-linear form

$$\text{Tr} [MUUM + N + \text{hermitian conjugate}], \quad (26)$$

where both $M$ and $N$ are sums over $SU(N)$ matrices (or $U(1)$ numbers). An iterative
procedure is probably required to carry out the local minimization step. Finally, one may
need special algorithms to speed up the long distance modes, as in ref. [2].

We end with a few remarks concerning the application of extremization to physical
problems, in the light of the work of Duncan and Mawhinney [2]. It would be interesting
to see if their results are confirmed when the gauge invariant procedure proposed here is
used to extremize configurations. In any case, gauge dependence in the results should be
absent when the gauge invariant procedure is used.

In the simulation of three-dimensional $SU(2)$ gauge theory in ref. [2] it was found that
during extremization the action itself decreased as well. At first sight, this is somewhat
surprising, as it is hard to see why a quantity should decrease when its derivatives are
minimized. One wonders whether the fact that the functional derivatives in the gauge
variant extremization procedure are not exact lattice derivatives has any influence here.
Similarly, it is surprising that a strong correlation was noticed between lumps in the
action density after cooling a configuration and after extremizing the same configuration.
Finally, it was observed that the string tension disappeared after continued extremization.
These are all interesting problems that merit further investigation.

Acknowledgement

It is a pleasure to thank M. Teper for helpful comments on the manuscript.

References

[1] B. Berg, Phys. Lett. 104B (1981) 475;
   M. Lüscher, Nucl. Phys. B200 (1982) 61;
   J. Hoek, M. Teper and J. Waterhouse, Nucl. Phys. B288 (1987) 589

[2] A. Duncan and R.D. Mawhinney, Nucl. Phys. B (Proc. Suppl.) 26 (1992) 444;
   Phys. Lett. 282B (1992) 423

[3] K. Symanzik, Nucl. Phys. B226 (1983) 187, 205