Stopping criteria and the uniform norm in lattice QCD

Martin Lüscher April 2018

1. Introduction

The numerical solution of the Dirac equation

$$(D\psi)(x) = \eta(x) \tag{1.1}$$

in lattice QCD through an iterative solver requires some stopping criterion to be chosen. Usually the algorithm terminates when the residue of the current approximate solution χ satisfies

$$\|\eta - D\chi\| \leq \epsilon\|\eta\| \tag{1.2}$$

for some $\epsilon > 0$. Here and below, $\|\ldots\|$ stands for the standard L_2 norm.

In master-field simulations [1], where very large lattice are simulated, this criterion may not be appropriate, because it does not guarantee the residue to be uniformly small as one moves through the lattice. The square norm, $\|\eta\|^2$, of the source is typically of order V (the number of lattice points) in these simulations and the magnitude of the residue can, therefore, be of order $V^{1/2}$ in some regions of the lattice. If this happens, the calculated quark forces may be obtained with insufficient accuracy and this may conceivably compromise the correctness of the simulations.

The issue can perhaps be avoided by replacing the L_2 norm in eq. (1.2) by a uniform norm. Whether the uniform accuracy of the computed solutions of the Dirac equation can be enforced in this way is however not completely obvious, since most solver algorithms (Krylov space solvers in particular) are not designed to minimize the uniform norm of the residue.

2. Properties of the uniform norm

The spinor fields considered in this note live on some lattice with V points. Boundary conditions and the shape of the lattice do not matter and need not be specified. The fields have no flavour index so that they have 12 complex components at each lattice point.

2.1 Definition

The uniform (or infinity) norm of any given spinor field $\psi(x)$ is defined by

$$\|\psi\|_\infty = \sup_x \|\psi(x)\|, \tag{2.1}$$

where

$$\|s\|^2 = \sum_{A=1}^{4}\sum_{\alpha=1}^{3} |s_{A\alpha}|^2, \tag{2.2}$$

i.e. $\|s\|$ denotes the L_2 norm of the spinor s. It is straightforward to show that the uniform norm has all the usual properties of a norm. In particular,

$$\|\lambda\psi\|_\infty = |\lambda|\|\psi\|_\infty \quad \text{for all} \quad \lambda \in \mathbb{C}, \tag{2.3}$$

$$\|\psi + \chi\|_\infty \leq \|\psi\|_\infty + \|\chi\|_\infty. \tag{2.4}$$

Moreover, the norm is invariant under translations, hypercubic transformations and gauge transformations of the spinor fields.

2.2 Associated operator norm

Let A be a linear operator acting on spinor fields. The norm defined through

$$\|A\|_\infty = \sup_{\psi\neq 0} \frac{\|A\psi\|_\infty}{\|\psi\|_\infty} \tag{2.5}$$

then has the usual properties too. Moreover, it is a consistent norm,

$$\|AB\|_\infty \leq \|A\|_\infty \|B\|_\infty, \tag{2.6}$$

and satisfies $\|1\|_\infty = 1$. However, one should not expect A and $A^\dagger$ to have the same uniform norm, except in special cases such as the Wilson–Dirac operator.

Another fairly direct consequence of the definition (2.5) is the bound

$$\|A\|_\infty \geq \rho(A), \tag{2.7}$$

$\rho(A)$ being the spectral radius of A. The inequality is obtained by noting that there exists a non-zero spinor field ψ such that $A\psi = \lambda\psi$ and $|\lambda| = \rho(A)$. If this field is inserted on the right of eq. (2.5), the ratio evaluates to $|\lambda|$, which therefore provides a lower bound on $\|A\|_\infty$.

In terms of the position-space kernel,

$$(A\psi)(x) = \sum_y A(x,y)\psi(y), \tag{2.8}$$

a simple upper bound on the uniform norm is given by

$$\|A\|_\infty \leq \sup_x \left\{ \sum_y \|A(x,y)\| \right\}. \tag{2.9}$$

A related exact formula is

$$\|A\|_\infty = \sup_x \left\{ \sup_{\|s\|=1} \sum_y \|A(x,y)^\dagger s\| \right\}, \tag{2.10}$$

where the inner supremum is taken over all y-independent spinors s of norm 1. There is apparently no simple proof of this identity (see appendix A).

2.3 Uniform norm of random fields

Let $\eta(x)$ be a random field with distribution proportional to $\exp(-\|\eta\|^2)$. Since the field components at different lattice points are statistically independent, it is clear that

$$P(\|\eta\|_\infty \leq r) = p(r)^V \tag{2.11}$$

where V denotes the number of lattice points and

$$p(r) \equiv P(\|\eta(x)\| \leq r) = \frac{2}{11!}\int_0^r \mathrm{d}s\, s^{23} \mathrm{e}^{-s^2} = 1 - \mathrm{e}^{-r^2} \sum_{k=0}^{11} \frac{r^{2k}}{k!}. \tag{2.12}$$

The differential distribution,

$$\frac{\mathrm{d}}{\mathrm{d}r} P(\|\eta\|_\infty \leq r) = \frac{2V}{11!} r^{23} \mathrm{e}^{-r^2} p(r)^{V-1}, \tag{2.13}$$

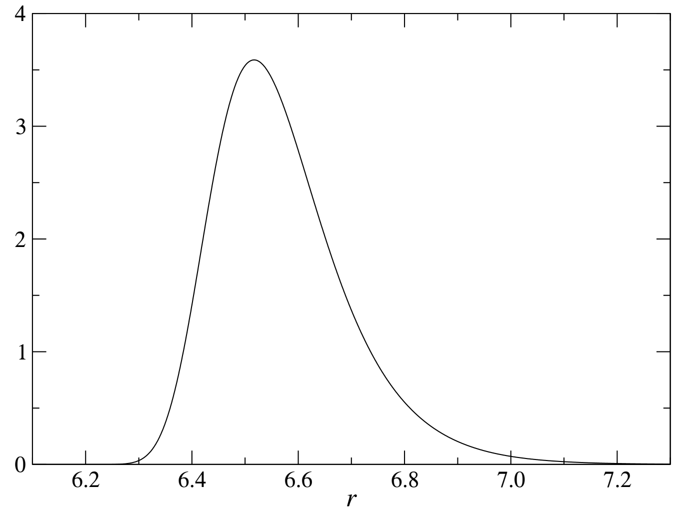

Fig. 1. Differential distribution (2.13) at $V = 10^8$.

then roughly has the shape of a Gaussian (see fig. 1).

As V increases from 10^4 to 10^{12}, the position of the maximum of the distribution grows only very slowly from 5.42 to 7.37. Moreover, the probability for $\|\eta\|_\infty$ to be much larger than these values rapidly gets extremely small. In practice the uniform norm of random fields is thus typically in the range from 5 to 8.

2.4 Bound on the solution of the Dirac equation

If χ is an approximate solution of the Dirac equation (1.1) satisfying

$$\|\eta - D\chi\|_\infty \leq \epsilon \|\eta\|_\infty, \tag{2.14}$$

one can show, in a few lines, that its deviation from the exact solution ψ is bounded by

$$\|\chi - \psi\|_\infty \leq \epsilon \|D^{-1}\|_\infty \|\eta\|_\infty \leq \epsilon \kappa(D)_\infty \|\psi\|_\infty, \tag{2.15}$$

where

$$\kappa(D)_\infty = \|D\|_\infty \|D^{-1}\|_\infty \tag{2.16}$$

is the condition number of the Dirac operator with respect to the uniform norm (see ref. [2], sect. 1.13.2, for example).

From eq. (2.7) and the Hermiticity properties of the Dirac operator it follows that $\kappa(D)_\infty$ is larger than or equal to the condition number $\kappa(D)$ of D with respect to the L_2 norm. On the other hand, the bound (2.15) guarantees that the calculated approximate solution is uniformly accurate.

3. Condition number of the Dirac operator

The uniform norm of operators is, in general, not easy to compute. In this section, some results are reported on the norm of the Wilson–Dirac operator and its inverse. For simplicity, the Pauli term required for O(a)-improvement is omitted and the bare mass m_0 is assumed to be such that $4 + m_0 \geq 0$. The starting point of the calculations is always the formula (2.10) for the uniform norm.

3.1 Uniform norm of D

For any given point x, the non-zero elements of the kernel $D(x, y)$ of the Wilson–Dirac operator are

$$
\begin{aligned}
&D(x, x) = 4 + m_0, \\
&D(x, x \pm \hat{\mu}) = -\tfrac{1}{2}(1 \mp \gamma_\mu)\, U(x, \mu).
\end{aligned}
\tag{3.1}
$$

The uniform norm of the operator is thus given by

$$
\begin{aligned}
\|D\|_\infty &= 4 + m_0 + \sup_{\|s\|=1} \left\{ \sum_{\mu=0}^{3} (\|\tfrac{1}{2}(1+\gamma_\mu)s\| + \|\tfrac{1}{2}(1-\gamma_\mu)s\|) \right\} \\
&= 4(1+\sqrt{2}) + m_0.
\end{aligned}
\tag{3.2}
$$

As has to be the case, the uniform norm is larger than the L_2 norm, but the difference is not very large.

3.2 Uniform norm of D^{-1}: general remarks

The quark propagator $S(x, y)$ decays roughly exponentially at large distances $|x - y|$ with a decay rate proportional to M_π. On large lattices and near the chiral limit, the sums in

$$\|D^{-1}\|_\infty = \sup_x \left\{ \sup_{\|s\|=1} \sum_y \|S(x,y)^\dagger s\| \right\} \tag{3.3}$$

are therefore expected to be dominated by the contributions of the points y at large distances from x. Moreover, in the continuum limit the norm should not blow up, since the short-distance singularity of the quark propagator is integrable.

On an infinite lattice, the finiteness of the uniform norm of D^{-1} is guaranteed if

$$D^\dagger D \geq \mu^2 \tag{3.4}$$

for some $\mu > 0$. In fact, following ref. [3] (with the Legendre replaced by Chebyshev polynomials), one can show that the quark propagator decays exponentially in this case, with an exponent proportional to μ. The upper bound for $\|D^{-1}\|_\infty$ obtained in this way however tends to be rather poor and is hence not particularly useful.

3.3 Uniform norm of D^{-1}: the free case

Considering an infinite lattice again, the translation invariance of the free propagator implies

$$\|D^{-1}\|_\infty = \sup_{\|s\|=1} \sum_x \|S(x,0)^\dagger s\|. \tag{3.5}$$

When the bare quark mass m_0 is taken to zero, the leading asymptotic behaviour of the norm coincides with the one in the continuum limit,

$$\|D^{-1}\|_\infty = \sup_{\|s\|=1} \int \mathrm{d}^4x \, \|S(x,0)^\dagger s\| + \ldots, \tag{3.6}$$

$$S(x,0) = (-\gamma_\mu \partial_\mu + m_0) G(x), \tag{3.7}$$

where the ellipsis stands for terms of order 1 as $m_0 \to 0$ and

$$G(x) = \frac{m_0^2}{4\pi^2 z} K_1(z), \qquad z = m_0 |x|, \tag{3.8}$$

denotes the free scalar-field propagator with mass m_0.

A few lines of algebra now show that

$$S(x,0)S(x,0)^{\dagger} = F_0(z) + \gamma_\mu \frac{x_\mu}{|x|} F_1(z), \tag{3.9}$$

$$F_0(z) = \left(\frac{m_0^3}{4\pi^2 z}\right)^2 \left\{K_1(z)^2 + K_2(z)^2\right\}, \tag{3.10}$$

$$F_1(z) = \left(\frac{m_0^3}{4\pi^2 z}\right)^2 2K_1(z)K_2(z). \tag{3.11}$$

Clearly, the positivity of the matrix on the left of eq. (3.9) implies

$$F_0(z) \geq |F_1(z)| \tag{3.12}$$

for all z. For any given spinor s of unit norm, the vector

$$v_\mu = s^{\dagger}\gamma_\mu s \tag{3.13}$$

satisfies $|v| \leq 1$ and the integrand in eq. (3.6) is of the form $\sqrt{a+b}$, where $a \geq |b|$. Moreover, b is odd under reflections at the plane $(v,x) = 0$ so that one may choose to integrate over the half-space $(v,x) \geq 0$ and instead have the integrand

$$\sqrt{a+b} + \sqrt{a-b} \leq 2\sqrt{a}. \tag{3.14}$$

Equality here holds if s is an eigenvector of γ_5, since v and thus b vanish in this case.

It follows from these remarks that

$$\|D^{-1}\|_\infty = \int \mathrm{d}^4x\, F_0(z)^{1/2} + \ldots = \frac{c}{m_0} + \ldots,$$

$$c = \tfrac{1}{2}\int_0^\infty \mathrm{d}z\, z^2 \left\{K_1(z)^2 + K_2(z)^2\right\}^{1/2} = 2.6016(1). \tag{3.15}$$

In the free theory the uniform norm of D^{-1} thus scales in the same way with the quark mass as the L_2 norm, with a proportionality constant that is not very much larger than 1.

3.4 Uniform norm of D^{-1}: ChPT estimate

As already mentioned subsect. 3.2, the uniform norm of D^{-1} is dominated by the long-distance behaviour of the quark propagator when the quark mass is taken to zero. Chiral perturbation theory may then be used to estimate the norm by replacing

$$S(x,y)S(x,y)^{\dagger} \to \langle S(x,y)S(x,y)^{\dagger}\rangle \tag{3.16}$$

and passing to the continuum limit as in the free case.

As in subsect. 3.3, this leads to the formula

$$\|D^{-1}\|_{\infty}^{\rm ChPT} = \int \mathrm{d}^4x\, F_0(z)^{1/2} + \ldots, \tag{3.17}$$

where

$$F_0(z) = -\tfrac{1}{12}\langle P^{ud}(x)P^{du}(0)\rangle, \tag{3.18}$$

$$P^{rs}(x) = \overline{\psi}_r(x)\gamma_5\psi_s(x), \qquad z = M_\pi|x|, \tag{3.19}$$

is now given by the correlation function of the pion field, M_π being the pion mass and r,s quark-flavour indices.

In the following, F_π denotes the renormalized pion decay constant, G_π the vacuum-to-pion matrix element of the renormalized pseudo-scalar density and m the unrenormalized average up and down quark mass. The renormalized mass

$$m_R = Z_A m/Z_P \tag{3.20}$$

(with Z_A, Z_P the renormalization constants of the axial current and density) then satisfies the PCAC relation

$$2m_R G_\pi = M_\pi^2 F_\pi. \tag{3.21}$$

Moreover, to leading order chiral perturbation theory,

$$Z_P^2\langle P^{ud}(x)P^{du}(0)\rangle = -2\int \frac{\mathrm{d}^4p}{(2\pi)^4}\,\mathrm{e}^{ipx}\,\frac{G_\pi^2}{M_\pi^2+p^2} = -\frac{M_\pi^2 G_\pi^2}{2\pi^2 z}K_1(z), \tag{3.22}$$

and combined with the previous equations this implies

$$\|D^{-1}\|_{\infty}^{\rm ChPT} = 18.058(1) \times \frac{F_\pi}{M_\pi Z_A m} + \ldots \tag{3.23}$$

As $m \to 0$ the uniform norm of D^{-1} thus scales like $m^{-3/2}$, i.e. in a way slightly more singular than in the free theory.

3.5 Synthesis

The discussion in this section shows that the uniform condition number of the Dirac operator can be expected to stay bounded in the infinite-volume limit. It is always larger than the L_2 condition number and it scales somewhat less favourably in the chiral limit. The scaling behaviour in the continuum limit is the same (i.e. proportional to $1/a$).

At physical quark masses and lattice spacing $a = 0.05$ fm, for example, the uniform condition number is estimated to be about 2×10^5 and thus roughly an order of magnitude larger than the L_2 condition number. If the tolerance ϵ in the stopping criterion (2.14) is set to 10^{-14}, the approximate solution χ of the Dirac equation is then rigorously guaranteed to be uniformly accurate up to a relative error of about 5×10^{-8}.

Appendix A

The proof of eq. (2.10) is somewhat lengthy and has therefore been deferred to this appendix. Since

$$\|A\|_\infty = \sup_{\|\psi\|_\infty=1} \left\{ \sup_x \|(A\psi)(x)\| \right\} = \sup_x \left\{ \sup_{\|\psi\|_\infty=1} \|(A\psi)(x)\| \right\}, \tag{A.1}$$

it suffices to show that

$$\sup_{\|\psi\|_\infty=1} \|(A\psi)(x)\| = \sup_{\|s\|=1} \sum_y \|A(x,y)^\dagger s\| \tag{A.2}$$

for all x.

From now on x is taken to be any fixed lattice point. Without loss the 12×12 matrices $A(x,y)$ may be assumed to be non-zero, since vanishing matrices do not contribute to either side of eq. (A.2) (alternatively the sums over y could be restricted to the points where $A(x,y) \neq 0$).

Lemma A.1. *There exists a spinor field χ such that $\|\chi\|_\infty = 1$ and*

$$\|(A\chi)(x)\|_\infty \geq \|(A\psi)(x)\|_\infty \tag{A.3}$$

for all fields ψ satisfying $\|\psi\|_\infty \leq 1$.

Proof: The existence of a field that maximizes $\|(A\psi)(x)\|$ follows from the fact that the expression is a real-valued continuous function of ψ and that the set of all fields ψ satisfying $\|\psi\|_\infty \leq 1$ is a compact subset of $\mathbb{C}^{12V}$. Clearly, χ must have maximal norm and thus has uniform norm 1. □

In the following, χ denotes one of the maximizing fields, whose existence is guaranteed by lemma A.1. Since A was assumed to be non-zero, the spinor

$$w = (A\chi)(x) \tag{A.4}$$

must be non-zero too.

Lemma A.2. *The field χ is such that*

$$w^\dagger A(x,y) \neq 0, \tag{A.5}$$

for all y.

Proof: If $w^\dagger A(x,y)$ would vanish at some point y, the modified field

$$\psi(z) = \chi(z) + \delta_{zy} s \tag{A.6}$$

would have

$$\|(A\psi)(x)\|^2 = \|w\|^2 + \|A(x,y)s\|^2. \tag{A.7}$$

Setting $s = -\chi(y)$ the maximum property of χ would then imply that $A(x,y)\chi(y) = 0$. Next setting $s = -\chi(y) + r$, where r is an arbitrary spinor of norm 1, one would be led to conclude that $A(x,y) = 0$, contrary to the assumptions made above on these matrices. The inequality (A.5) must therefore hold for all y. □

Lemma A.3. *The field χ satisfies*

$$\chi(y) = \frac{A(x,y)^\dagger w}{\|A(x,y)^\dagger w\|} \tag{A.8}$$

for all y.

Proof: Let y be any fixed lattice point, r a spinor with $\|r\| = 1$ and θ a real variable. The field

$$\psi(z) = \chi(z) + \delta_{zy}\theta r \tag{A.9}$$

then has

$$\|(A\psi)(x)\|^2 = \|w\|^2 + 2\theta\,\mathrm{Re}\,\{w^\dagger A(x,y)r\} + \mathrm{O}(\theta^2). \tag{A.10}$$

If $\|\chi(y)\| < 1$, the spinor $\psi(y)$ has norm less than 1 too if θ is sufficiently small. The maximum property of χ and the fact that r can go in any direction would then imply that $w^\dagger A(x,y) = 0$, which is excluded by lemma A.2. This shows that $\|\chi(y)\| = 1$ for all y.

Next one may consider the field

$$\psi(z) = (1-\delta_{zy})\chi(z) + \delta_{zy}(\cos\theta\chi(y) + \sin\theta r). \tag{A.11}$$

If r is orthogonal to $\psi(y)$, i.e. if $r^\dagger\psi(y) = 0$, this field has $\|\psi\|_\infty = 1$ for all θ and eq. (A.10) holds again. The maximum property then implies that there exists $\lambda \in \mathbb{C}$ such that

$$A(x,y)^\dagger w = \lambda\chi(y). \tag{A.12}$$

Moreover, setting $r = i\psi(y)$ implies $\mathrm{Im}\,\{w^\dagger A(x,y)\psi(y)\} = 0$ and therefore

$$\lambda = \pm\|A(x,y)^\dagger w\|. \tag{A.13}$$

Finally, considering the field

$$\psi(z) = (1-\delta_{zy})\chi(z) + \delta_{zy}\mathrm{e}^{-\theta}\chi(y) \tag{A.14}$$

with $\theta > 0$, the maximum property implies $w^\dagger A(x,y)\chi(y) \geq 0$ and thus excludes the negative sign in eq. (A.13). $\square$

Lemma A.4. *The inequality*

$$\sup_{\|\psi\|_\infty=1} \|(A\psi)(x)\| \leq \sup_{\|s\|=1} \sum_y \|A(x,y)^\dagger s\| \tag{A.15}$$

holds.

Proof: Let χ and w be as above. The results obtained so far imply that

$$w = \sum_y \frac{A(x,y)A(x,y)^\dagger w}{\|A(x,y)^\dagger w\|} \tag{A.16}$$

and thus

$$\|w\|^2 = \sum_y \|A(x,y)^\dagger w\|. \tag{A.17}$$

Setting $s = w/\|w\|$ this leads to

$$\sup_{\|\psi\|_\infty = 1} \|(A\psi)(x)\| = \|w\| = \sum_y \|A(x,y)^\dagger s\|, \qquad \|s\| = 1, \tag{A.18}$$

which proves the lemma. $\square$

In order to show that the opposite inequality

$$\sup_{\|s\|=1} \sum_y \|A(x,y)^\dagger s\| \leq \sup_{\|\psi\|_\infty = 1} \|(A\psi)(x)\| \tag{A.19}$$

holds too, first note that the function

$$f(s) = \sum_y \|A(x,y)^\dagger s\|, \quad \|s\| = 1, \tag{A.20}$$

is continuous. There thus exists a spinor v satisfying $\|v\| = 1$ and

$$f(v) \geq f(s) \quad \text{for all } s. \tag{A.21}$$

In the following v is assumed to have these properties.

Lemma A.5. *The spinor v is such that*

$$A(x,y)^\dagger v \neq 0 \tag{A.22}$$

for all y.

Proof: Let Λ_0 be the set of all points y satisfying $A(x,y)^\dagger v = 0$ and Λ_1 the complementary set of points. If r is any spinor of norm 1 orthogonal to v and θ a real parameter, the expansion

$$f(\cos\theta v + \sin\theta r) =$$

$$f(v) + |\theta| \sum_{y \in \Lambda_0} \|A(x,y)^\dagger r\| + \theta \sum_{y \in \Lambda_1} \frac{\mathrm{Re}\,\{r^\dagger A(x,y) A(x,y)^\dagger v\}}{\|A(x,y)^\dagger v\|} + \mathrm{O}(\theta^2) \tag{A.23}$$

and the maximum property (A.21) imply that $A(x,y)^\dagger r = 0$ for all $y \in \Lambda_0$. Since $A(x,y)^\dagger v$ vanishes at these points too, and since the matrices $A(x,y)$ are not equal to zero, the only possibility is then that Λ_0 is empty. $\square$

Lemma A.6. *The identity*

$$f(v)v = \sum_y \frac{A(x,y)A(x,y)^\dagger v}{\|A(x,y)^\dagger v\|} \tag{A.24}$$

holds.

Proof: Proceeding as in the proof of lemma A.5, one infers from eq. (A.23) and the maximum property (A.21) that

$$\sum_y \frac{A(x,y)A(x,y)^\dagger v}{\|A(x,y)^\dagger v\|} = \lambda v \tag{A.25}$$

for some $\lambda \in \mathbb{C}$. Multiplication of this equation by $v^\dagger$ then shows that $\lambda = f(v)$. $\square$

The inequality (A.19), and thus the proof of eq. (2.10), is now obtained by setting

$$\psi(y) = \frac{A(x,y)^\dagger v}{\|A(x,y)^\dagger v\|} \tag{A.26}$$

and noting that $\|\psi\|_\infty = 1$ and

$$\sup_{\|s\|=1} \sum_y \|A(x,y)^\dagger s\| = f(v) = \|(A\psi)(x)\| \tag{A.27}$$

in view of eq. (A.24).

References

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