Research Article

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On $L^q$ Convergence of the Hamiltonian Monte Carlo

Abstract: We establish $L_q$ convergence for Hamiltonian Monte Carlo algorithms. More specifically, under mild conditions for the associated Hamiltonian motion, we show that the outputs of the algorithms converge (strongly for $2 \leq q < \infty$ and weakly for $1 < q < 2$) to the desired target distribution.

Keywords: Convergence, $L^q$ spaces, Hamiltonian Monte Carlo

1 Introduction

Hamiltonian Monte Carlo or Hybrid Monte Carlo (HMC) algorithm is a method to obtain random samples from a (target) probability distribution on a space $Q$ whose density is known only up to a factor. The target distribution is expressed as $f/\int_Q f$ with function value $f$ known, but the normalizing constant $\int_Q f$ is not known or at least is prohibitively expensive to calculate. It is an algorithm of the Metropolis-Hastings type known for a while [1] for estimating integrals. Convergence in various probability senses can be found in the literature, see, e.g. [2, 3]. In [4], convergence of the densities in $L^2$ Hilbert space was obtained. Meanwhile, utilizing different norms, in addition to providing great flexibility in terms of model selections in the applications of machine learning algorithms, can have significant impact in the behavior of machine learning algorithms, see, e.g. [5]. In this paper, we address the problem of convergence of the algorithm for densities in $L^q$ spaces.

In each HMC iterative step, the input sample point in space $Q$ is lifted to the product space $Q \times \mathbb{P}$ by adding a sample from an auxiliary distribution of choice $g$, where $g > 0$ on $\mathbb{P}$ and $\int_{\mathbb{P}} g = 1$, then the pair is transformed via the Hamiltonian motion generated by the Hamiltonian energy $H(q, p) = -\log(f(q) \cdot g(p))$ and projected back to $Q$ as the input of the next iteration. Details can be found in [4].

Viewing as transformation of distributions, one can present HMC as follows: Given some initial distribution $h(q)$ on $Q$ one produces a joint distribution $(h \cdot g)(q, p) = h(q) \cdot g(p)$ on the phase space $Q \times \mathbb{P}$ (joining them as independent) then the points are moved by the motion, $(q, p) \mapsto (Q, P) = H(q, p)$ producing another distribution $(h \cdot g) \circ H(q, p) = h(Q) \cdot (P)$ in $Q \times \mathbb{P}$, and finally one projects it to a distribution on $Q$ by calculating the marginal $\int_{\mathbb{P}} (h \cdot g) \circ H(q, p) dp$, which is a result of the action of the algorithm in one step. In short

$$\mathcal{T}(h)(q) = \int_{\mathbb{P}} (h \cdot g) \circ H(q, p) dp,$$

and from a rather complicated algorithm we receive a relatively simple, linear operator on some space of integrable functions. The convergence of the algorithm thus corresponds to the convergence of the sequences of iterates of $\mathcal{T}$.

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2 Results

Assume that the motion $H : \mathbb{Q} \times \mathbb{P} \to \mathbb{Q} \times \mathbb{P}$, $H(q, p) = (Q, P)$ satisfies the following invariance properties:

- $(f \cdot g) \circ H = f \cdot g$;
- $\int_{\mathbb{Q} \times \mathbb{P}} A \circ H = \int_{\mathbb{Q} \times \mathbb{P}} A$ for any integrable $A$;
- $Q(q, P) = Q$ for (almost) every $q$;
- $Q$ is the support of $f$.

For $Th = \int_{\mathbb{P}} (h \cdot g) \circ H$ let $T^{n+1} = T^n \circ T$. The adjoint operator $T^\dagger$ is given by the same formula (1) with $H^{-1}$ in place of $H$ and is described below in Section 4, a self-adjoint operator satisfies $T^\dagger = T$.

Let $L^q$ denote the space of functions $h : \mathbb{Q} \to \mathbb{R}$ such that $\|h\|_q^q = \int_{\mathbb{Q}} |h|^{q} / f^{q-1} < \infty$ and the support of $h$ is included in the support of $f$, which we may assume to be equal to $\mathbb{Q}$.

Theorem 1. Assume the invariance properties and assume that the operator $T$ is self-adjoint. For every $h \in L^q(\mathbb{Q})$, $1 < q < \infty$ the sequence $T^n h$ converges weakly in $L^q$ to $f \cdot \int h/ \int f$ and for $2 \leq q < \infty$ it converges also strongly.

Proof. We observe that $T$ is in fact (Lemma 3.2.(6)) an averaging map, thus by the convexity of $x \mapsto x^q$, $q > 1$, the norm of $h$ decreases (Lemma 3.2.(8)) under $T$, sharply unless (by coverage assumption) $h = \alpha f$.

The spaces $L^q$, $1 < q < \infty$ are reflexive, hence bounded sequences have weak accumulation points. Using self-adjointness and the convexity of $x \mapsto x^q$, for $q \geq 2$ (Lemma 3.3) we prove that each accumulation point must be of form $\alpha f$, proving (Corollary 5.1) weak convergence for $q \geq 2$. Meanwhile the proof of the convergence of the norms provides (Corollary 5.2) strong convergence. Weak convergence for $1 < q < 2$ follows (Proposition 5.2) from special properties of the fixed point $f$.

Remark 1.

- The Hamiltonian motion satisfies two first integral invariance assumptions, as both the Hamiltonian and the Lebesque measure are invariant under such a motion.
- The covering property $Q(q, P) = Q$ can be weakened to a statement of an eventual coverage, not necessarily in one step. Some type of irreducibility must be assumed to avoid complete disjoint domains of the motion and hence an obvious non existence of a (unique) limit.

3 The properties of $T$ in $L^q$

We shall be working in the reflexive spaces $L^q(\mathbb{Q})$ and its dual $L^p(\mathbb{Q})$, where $q, p > 1$ are conjugated real numbers $q + p = q \cdot p$. In such spaces for $h \in L^q$ we have standard:

- norm $\|h\|_q^q = \int_{\mathbb{Q}} |h|^q / f^q$,
- bilinear form $\langle \cdot, \cdot \rangle : L^q \times L^p \to \mathbb{R} : (a, b) = \int_{\mathbb{Q}} a \cdot b / f$,
- and conjugacy $* : L^q \to L^p$, $h^* = h : \left( \frac{|h|}{f} \right)^{q-2}$.

We shall assume, unless stated otherwise, that $h \geq 0$. 
Lemma 3.1.

\[
\begin{align*}
a \in L^q, b \in L^p & \implies \langle a, b \rangle \leq |a|_q \cdot |b|_p, \quad (2) \\
h^* \in L^p; \quad ||h||_q^2 &= \langle h, h^* \rangle = ||h^*||_p^2; \quad (h^*)^* = h, \quad (3) \\
f \in L^q; \quad ||f||_q^2 &= \int_Q f; \quad f^* = f, \quad (4) \\
\langle h, f \rangle = \int_Q h, \quad h \in L^q; \quad \langle f, h^* \rangle = \int_Q h^*, \quad h^* \in L^p. \quad (5)
\end{align*}
\]

Proof. (2) is the Hölder inequality for likelihoods \(a/f\) and \(b/f\). (3) follows a straightforward calculation using \(q(p - 1) = p\). We note that \(h \cdot h^* \geq 0\). (4) and (5) follow directly from the definitions.

Lemma 3.2 (Properties of \(T\)). For \(0 \leq h \in L^q\):

\[
\begin{align*}
\mathcal{T}h &= f \cdot \left( \int_P \frac{h}{f} \circ H \cdot g \right), \\
\int_Q \mathcal{T}h &= \int_Q h, \quad (7) \\
||\mathcal{T}h||_q^2 &\leq ||h||_q^2. \quad (8)
\end{align*}
\]

The equality in (8) occurs iff \(h = \alpha \cdot \langle f \rangle \) (a.e.), where \(\alpha = \alpha(h) = \int h/\int f\).

Proof. (3): Using the invariance properties we have \(\int_P \frac{h}{f} \circ H \cdot (f \cdot g) \circ H = \int_P \frac{h}{f} \circ H \cdot (f \cdot g)\) and \(f\) does not depend on \(p \in P\).

(7): \(\int_Q \int_P (h \cdot g) \circ H = \int \int_{Q \times P} (h \cdot g) = \left( \int_Q h \right) \left( \int_P g \right)\).

(3): \(||\mathcal{T}h||_q^2 = \int_Q \int_P \frac{h}{f} \circ H \cdot g \cdot f \leq \int_Q \int_P \frac{h}{f} \circ H \cdot g \cdot f = \int \int_{Q \times P} \frac{h}{f} \cdot H \cdot (g \cdot f) \circ H = \int \int_{Q \times P} \frac{h}{f} \cdot g \cdot f\) the last one being equal to \(\left( \int_Q \frac{h}{f} \right) \left( \int_P g \right) = ||h||_q^2\), as \(g \geq 0\) and \(\int_P g = 1\). Given \(q\) the equality occurs only if \(\langle h/f \rangle (H(q,p))\) is a constant for \(g\)-almost all \(p\), but by covering assumption it means that \(h/f\) is a constant on \(f\)-almost all \(Q\). The constant follows from (7).

Remark that inequality (3) is valid also in the boundary cases of \(q = 1\) and \(q = \infty\) (the sup norm). However in case of \(q = 1\) the equality occurs for all positive functions.

The operator \(\mathcal{T}\) is an averaging operator of the (transported) likelihood \(h/f\) with respect to the probability \(g\). The scalar functional is monotone: \(0 \leq a \leq b, \ 0 \leq c \leq d\) implies \(\langle a, c \rangle \leq \langle b, d \rangle\) and \(\mathcal{T}\) is positive, in particular if \(a \leq b\) then \(\mathcal{T}a \leq \mathcal{T}b\). The function \(f\) provides the eigendirection of fixed points and by (3) \(\mathcal{T}\) has its spectrum in the unit disk. The eigenvalue 1 is a unique eigenvalue on the unit circle and it has multiplicity 1. For any \(h \in L^3\) one has the unique decomposition \(h = \alpha f + (h - \alpha f)\) where \(\alpha f\) is a direction of the fixed points and \(h - \alpha f \in \mathcal{N} := \{a \in L^3: f(a) = 0\}\) lies in an invariant subspace. It is not a priori clear under what conditions 1 is isolated in the spectrum, in other terms whether the contraction \(||\mathcal{T}h|| < ||h||\) is uniform on \(N\), which would imply \(\mathcal{T}^nN \to \{0\}\) (point-wise) with exponential speed.

Lemma 3.3. For \(2 \leq q < \infty\) and \(L^q \ni h \geq 0\)

\[(\mathcal{T}^n h)^* \leq T^n (h^*)\]

For \(1 < q \leq 2\) the opposite inequality holds. The equality happens when \(q = 2\) or when \(h\) is aligned with \(f\).
Proof. The comparison acts in $L^p$. It is enough to prove for $n = 1$, as the general case follows by induction and positivity of $\mathcal{T}$. Proof for $n = 1$ follows from the convexity of $x \mapsto x^{q-1}$, positivity of the linear operator $\mathcal{T}$ and its averaging property. Again the inequality is sharp unless $h = \alpha f$.

\section{The adjoint operator $\mathcal{T}^\dagger$}

As $H$ is invertible the inverse map $H^{-1}$ is well defined and it enjoys the same invariance properties as $H$. Define

\[ \mathcal{T}^\dagger h = \int_P (h \cdot g) \circ H^{-1}. \]

It enjoys the same properties as $\mathcal{T}$ enumerated in Lemmata above. It is conjugated to $\mathcal{T}$ with respect to the duality functional $\langle \cdot, \cdot \rangle$, namely

\begin{lemma}
For $h \in L^q$ and $k \in L^p$:
\[ \langle \mathcal{T}h, k \rangle = \langle h, \mathcal{T}^\dagger k \rangle \]
\end{lemma}

Proof. Using (8) and invariance $\langle \mathcal{T}h, k \rangle = \int_Q \left( \int_P \frac{h}{T} \circ H \cdot (\frac{g}{T}) \right) k = \int \int_{Q \times P} h \cdot \frac{g}{T} \circ H^{-1} = \int \int_{Q \times P} (K \circ H)^{-1} \cdot (g \circ f) = \int_Q \cdot \left( \int_P K \circ H^{-1} \cdot g \right) = \langle h, \mathcal{T}^\dagger k \rangle.$

The following Lemma provides a sufficient condition for $\mathcal{T}$ to be self-adjoint.

Let $\sigma$ be a measure preserving involution $\sigma : P \to P$, $\sigma \circ \sigma = \text{id}$. We can extend it to $\sigma : Q \times P \to Q \times P$ by $\sigma(q, p) = (q, \sigma(p))$. Assume that $g$ is invariant with respect to $\sigma$: $g \circ \sigma = g$.

\begin{lemma}
If $\sigma \circ H^{-1} \circ \sigma = H$ and $g$ is invariant with respect to $\sigma$ then $\mathcal{T}^\dagger = \mathcal{T}$.
\end{lemma}

Proof. Measure invariance means that $\int_P a \circ \sigma = \int_P a$. Let $(Q, P) = H^{-1}(q, p)$ then $\sigma \circ H^{-1}(q, p) = \sigma(Q, P) = (Q, \sigma(P))$ and $\mathcal{T}h = \int_P (h \cdot g) \circ H = \int_P (h \cdot g) \circ \sigma \circ H^{-1} = \int_P (h \cdot g) \sigma(Q, P) = \int_P (h(Q) \cdot g(\sigma(P))) = \int_P h(Q) g(P) = \int_P h \circ H^{-1} \cdot g \circ H^{-1} = \mathcal{T}^\dagger h.$

As an example take $Q = P = \mathbb{R}$, $\sigma$ to be the symmetry (reflection) of the space $P$ with respect to 0, $\sigma(p) = -p$. An even density $g(p) = g(-p)$ is invariant with respect to $\sigma$. The Hamiltonian motions $H$ and $H^{-1}$ satisfy the condition of the Lemma.

\section{Limits of the sequences $\mathcal{T}^n$ for a self-adjoint operator $\mathcal{T}$}

In this section we assume that $\mathcal{T} = \mathcal{T}^\dagger$. If it is not the case we can use in the algorithm the operator $S = \mathcal{T}^\dagger \circ \mathcal{T}$, as $S^2 = S$.

From $||\mathcal{T}h||_q < ||h||_q$ by induction we obtain $||\mathcal{T}^n h||_q < ||h||_q$ unless $h = \alpha f$, when equality holds. For $h \in L^q$ define

\[ V_q(h) = \inf ||\mathcal{T}^n h||_q^q = \lim ||\mathcal{T}^n h||_q^q. \]

We see that $V_q(h) = V_q(\mathcal{T}^n(h))$. As we are interested in the limit of the sequence $\mathcal{T}^n h$, for a given $h$ we can assume that for an arbitrary $\epsilon > 0$ we have $||h||_q^q < V_q + \epsilon$, taking a high iterate $\mathcal{T}^M h$ instead of $h$ if needed.

By a corollary to Alaoglu Theorem bounded sets in reflexive $L^q$ are weakly (the same as weakly*) compact. Let $h_\infty$ denote any weak accumulation point (limit of a subsequences) of $\mathcal{T}^n h$, say $\mathcal{T}^n h_\rightarrow h_\infty$. We may assume that the subsequence $(m_n)$ has infinite number of even numbers, otherwise take $\mathcal{T}h$ in place of $h$. Then $h_\infty$ is the weak limit of the subsequence indexed by these even numbers. We shall simplify
the notation and use the indices $2m$ for this subsequence. With this notation we have by the definition of weak convergence that $\langle T^{2m}h, b \rangle \to \langle h_\infty, b \rangle$ for every $b \in L^p$.

**Proposition 5.1.** Assume $\mathcal{T} = \mathcal{T}^1$. Let $h_\infty$ be a weak limit of a subsequence $T^{m_n}(h_0), 0 \leq h_0 \in L^q, \ q \geq 2$. Then $\|h_\infty\|^q_q = V_q(h_0)$.

**Proof.** Denote $V_q(h_0)$ Let $\epsilon > 0$ and $M$ be one of the indices in the weak converging subsequence large enough so that $h = T^M(h_0)$ has the norm $V \leq \|h\|^q_q \leq V + \epsilon$, which is possible by definition as $V_q(h) = V$. Then the sequence $T^{m_n-M}(h) \to h_\infty$ weakly and taking a subsequence and $\mathcal{T}h$ instead of $h$ if needed, we can assume that the sequence $m_n - M$ consists of infinitely many positive even integers $2m$. By Lemma 3.3 and $q/p = q - 1$ we have $V \leq \|T^m(h_0)\|^q_q = \langle T^m(h), (T^m h)^* \rangle \leq \langle T^m(h), T^m(h)^* \rangle = \langle T^{2m}(h), h^* \rangle \to \langle h_\infty, h^* \rangle \leq \|h_\infty\|_q \cdot \|h^*\|_p = \|h_\infty\|_q \cdot (\|h\|_q)^{1/p} = \|h_\infty\|_q \cdot (\|h\|_q)^{q-1} \leq \|h_\infty\|_q \cdot (V + \epsilon)^{1-1/q}$ thus by the arbitrary choice of $\epsilon > 0$ we have $\|h_\infty\|^q_q \geq V$. The opposite direction is standard, we use [2] and (3): $\|h_\infty\|^q_q = \langle h_\infty, (h_\infty)^* \rangle \leftrightarrow \langle T^{2m}(h), (h_\infty)^* \rangle \leq \|T^{2m}(h)\|_q \cdot (\|h_\infty\|_q)^{q/p} \leq \|h\|_q \cdot \|h\|_q^{q-1} \leq (V + \epsilon)^{1/q}\|h_\infty\|_{q}^{q-1}$.

**Corollary 5.1.** For $q \geq 2$ every weak convergent subsequence of $T^n(h_0), h_0 \in L^q$ has a limit of norm $V_q(h_0)$. In consequence $T^n(h_0) \to \alpha f$.

**Proof.** If $T^{m_n}(h_0) \to h_\infty$ then $T^{m_n+1}(h_0) \to T(h_\infty)$ (use the operator $T^1$). As they have the same norm, by Lemma 3.2 (3) they are equal $h_\infty = \alpha f$. Therefore every weakly convergent subsequence converges to the same limit, and as every subsequence has a weakly convergent subsequence the whole sequence converges.

**Corollary 5.2.** For $q \geq 2$ for each $h_0$ the sequence $T^n(h_0)$ converges strongly to $\alpha f$, where $\alpha = \int_Q h_0 / \int_Q f$.

**Proof.** Due to the strong convexity of the ball in $L^q$ weak convergent sequence with the convergence of the norms to the norm of the limit convergences strongly.

**Proposition 5.2.** For any $1 < q < \infty$ and $h \in L^q$ the sequence $T^n(h)$ converges weakly to $\alpha(h)f$, where $\alpha(h) = \int_Q h / \int_Q f$.

**Proof.** The case $q \geq 2$ follows from Corollary 5.1. Let $1 < q \leq 2$, then $p \geq 2$ and for any $a \in L^p$ we have $T^m a \to \alpha(a) f$, where $\alpha(a) = \int a / \int f$. Let $h \in L^q$ with $q \leq 2$ and $a \in L^p$. We have $\langle T^n h, a \rangle = \langle h, T^n a \rangle \to \langle h, \alpha(a) f \rangle = \alpha(a) \int h \cdot a / \int f = \langle \alpha(h) f, a \rangle$. Which means $T^n h \to \alpha(h)f$.

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