HMC, AN EXAMPLE OF FUNCTIONAL ANALYSIS APPLIED TO ALGORITHMS IN DATA MINING. THE CONVERGENCE IN $L^p$

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Abstract. We present a proof of convergence of the Hamiltonian Monte Carlo algorithm in terms of Functional Analysis. We represent the algorithm as an operator on the density functions, and prove the convergence of iterations of this operator in $L^p$, for $1 < p < \infty$, and strong convergence for $2 \leq p < \infty$.

1. Introduction

Functional Analysis for all Functioning Algorithms. We dare not making an acronym of that.

Recent development and usage of Machine Learning (ML) Data Mining (DM) and Artificial Intelligence (AI) resulted in a vast variety of new or refurbished algorithms to deal with large data sets, be it collected or streamed. Such new methods are usually tested on some data sets, however not very often they are thoroughly vetted by theoretical means. Algorithms tend to rely on discrete models, but the nature of data and approximation approaches suggest rather a continuous point of view. In our opinion one should go even further, the right objects of investigation of algorithms should not be the continuous parameters but rather very general features of data such as their probability distributions.

We perceive the algorithms as iterative transformations of the points in some underlying domains. The leading idea is to move from a relatively simple objects such as finite sets or points in finite dimensional Euclidean spaces with quite complicated transformations to simple transformations in richer spaces such as functional spaces of probability distributions.

Hamiltonian Monte Carlo. Or Hybrid Monte Carlo (HMC) algorithm is a method to obtain random samples from a (target) probability distribution $\frac{f}{\int_Q f}$ on the space $Q$ whose density is known only up to a factor, that is to say that $f$ is known, but $\int_Q f$ is not, or at least is very difficult to calculate. It is an algorithms known for a while \cite{1} of the Metropolis-Hastings type used to estimate the integrals. There are known proofs of convergence \cite{2}. Our goal is to provide a clear and understandable reason why HMC algorithm converges to the right limit for densities in the spaces $L^q(Q)$. We refer to our papers \cite{3,4,5} for three approaches to investigation of HMC, analytic (in $L^2$), probabilistic and algorithmic. Here we concentrate on an extension of the analytic one, the convergence in $L^q$.

HMC performs by iterating the following steps. Given an initial distribution $h$ (sample points) in a given space $Q$ double (the dimension of) the space by considering $Q \times P$, with $P \sim Q$. Then spread each point $q \in Q$ to a point $(q,p) \in Q \times P$ by sampling $p \in P$ from a distribution of choice $g$, where $g > 0$ on $P$ and $\int_P g = 1$. Then move each point $(q,p)$ to a new point $(Q,P) = H(q,p)$, where the transformation $H : Q \times P \to Q \times P$ satisfies some special invariance properties. Finally project $(Q,P)$ on $Q$ providing a new sample of points $Q$ in $Q$ with a new distribution $\hat{h}$ which shall be used as the initial sample (or

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probability distribution) for the next step. With the right choice of $H$ the iteration of this procedure will result in an approximate sample from the target distribution.

**Moving to functional spaces.** Thus the success of the algorithm lies in the appropriate choice of the transformation $H$. The Hamiltonian part of the algorithm’s name is due to the Hamiltonian motion $H$. It turns out that if the target distribution has a density proportional to a given function $f$ and the distribution of choice is $g$ then $H$ is a Hamiltonian motion generated by the Hamiltonian energy $\mathcal{H}(q,p) = -\log(f(q) \cdot g(p))$. That is if $(Q,P) = H(q,p)$ is the solution of the time evolution $Q = \partial \mathcal{H}/\partial P$, $P = -\partial \mathcal{H}/\partial Q$ after time $t$ with initial point $(q,p)$ then $H$ has the needed invariance properties for HMC to converge to a distribution proportional to $f$. Effectively it means that one can obtain a normalizing constant $\int_Q f$ or any expected value of a function $\phi$ with respect to the distribution proportional to $f$: $\int (\phi \cdot (f/\int f))$.

In terms of the densities of the involved distributions one can present HMC as follows: Given some initial (probability) distribution $h(q)$ on $\mathbb{Q}$ one produces a joint distribution $h \cdot g(q,p) = h(q) \cdot g(p)$ on $\mathbb{Q} \times \mathbb{P}$ then moves the points $(q,p) \mapsto (Q,P) = H(q,p)$ producing another (probability) distribution $(h \cdot g) \circ H(q,p) = h(Q) \cdot (P)$ in $\mathbb{Q} \times \mathbb{P}$ and finally projects the last one onto $\mathbb{Q}$ by calculating the marginal $\int_P (h \cdot g) \circ H(q,p) \, dp$, which is a result of the action of the algorithm in one step. In short

$$T(h)(q) = \int_P (h \cdot g) \circ H(q,p) \, dp$$

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

A few remarks.

- The distribution $g$ may depend on the point $q$, $g(p|q)$ as long as for (almost) all $q$ it satisfies the required conditions.
- It is clear that the Hamiltonian motion $H$ does not depend on the constant factor in front of $f$.
- The motion $H$ in practical implementation is performed by the *leap-frog algorithm* which displays the needed invariance properties. We shall not deal with it in this paper.
- An example of the situation where the target distribution is known up to the normalizing constant is the Bayesian update. In order to establish the distribution of (random) parameters $\theta$ influencing the outcome $D$ of the observations, when we know all the probabilities $P(D|\theta)$ one uses the knowledge of the outcome $D$ to improve the estimate: Given the estimate $\hat{\pi}(\theta)$ before the experiment we calculate $\hat{\pi}(\theta) = P_x(\theta|D) = P_x(\theta,D)/P_x(D) = P(D|\theta) \cdot \hat{\pi}(\theta)/\sum_{\theta'} P(D|\theta') \cdot \hat{\pi}(\theta')$ and take $\hat{\pi}$ as a new estimate. However the sum (integral) in the denominator may be not that easy to calculate. This yields to $\hat{\pi}(\theta) \sim P(D|\theta)\pi(\theta)$ without the normalizing factor.

2. **Results**

Assume that the motion $H : \mathbb{Q} \times \mathbb{P} \to \mathbb{Q} \times \mathbb{P}$ (measurable spaces with measures $dq$ and $dp$) satisfies the following invariance and coverage properties:

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

For $Th = \int_P (h \cdot g) \circ H$ let $T^{n+1} = T^n \circ T$. The adjoint operator $T^\dagger$ is given by the same formula with $H^{-1}$ in place of $H$ and is described below in Section 4. a self-adjoint operator satisfies $T^\dagger = T$. 
Theorem 2.1. Under the above invariance and coverage conditions and when the operator \( T \) is self-adjoint then for every \( h \in L^q(\mathbb{Q}), 1 < q < \infty \) the sequence \( T^n h, h \geq 0 \), converges weakly to \( \int h/\int f \) and for \( 2 \leq q < \infty \) it converges also strongly.

Here \( L^q \) denotes the space of integrable functions \( h : \mathbb{Q} \to \mathbb{R} \) such that \( ||h||^q_q = \int_\mathbb{Q} |h|^q \) is finite and the support of \( h \) is included in the support of \( f \), which we may assume is equal to \( \mathbb{Q} \).

Remark 2.2.
- The Hamiltonian motion satisfies two first integral invariance assumptions, as both the Hamiltonian (energy function equal here \( -\log(f(q) \cdot g(p)) \) and the Lebesgue measure are invariant under such a motion.
- The coverage property \( Q(q, P) = \mathbb{Q} \) 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.
- The support condition takes care of some initialization problems with the division by 0. This can be formally avoided by working in the space of likelihoods, see below.

The proof is not very hard. We observe that \( T \) is in fact \((3.5)\) an averaging map, thus by the convexity of \( x \mapsto x^q, q \geq 1 \), the norm of \( h \) decreases \((3.7)\) under \( T \), sharply unless (by coverage assumption) \( h = \alpha f \). The spaces \( L^q \) for \( 1 < q < \infty \) are reflexive, hence bounded sequences have weak accumulation points. Using self-adjointness and the convexity of \( x \mapsto x^q-1 \), for \( q \geq 2 \) \((1.4)\) we prove that each accumulation point must be of form \( \alpha f \), proving \((Corollary\ 5.2)\) weak convergence for \( q \geq 2 \). Meanwhile the proof of the convergence of the norms provides \((Corollary\ 5.3)\) strong convergence. Weak convergence for \( 1 < q < 2 \) follows \((Proposition\ 5.4)\) from special properties of the fixed point \( f \).

3. The operator \( T \) in \( L^q \)

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

\[
\begin{align*}
\text{norm} & \quad ||h||_q^q = \int_\mathbb{Q} \left( \frac{h}{f} \right)^q f \\ \text{bilinear form} & \quad \langle \cdot, \cdot \rangle : L^q \times L^p \to \mathbb{R} : \langle a, b \rangle = \int_\mathbb{Q} a \cdot b f^{q-1} \\ \text{and conjugacy} & \quad ^* : L^q \to L^p, h^* = h \cdot \left( \frac{|h|}{f} \right)^{q-2}.
\end{align*}
\]

We shall assume \( h \geq 0 \) unless stated otherwise. Call \( h/f \) a likelihood (up to an irrelevant normalizing constant \( \int f \)) of \( h \) with respect to \( f \). The space of \( L^q = \{ \tilde{h} : \int_\mathbb{Q} |\tilde{h}| f < \infty \} \) of likelihoods \( \tilde{h} = h/f \) is isometric to \( L^q \).

Lemma 3.1.

\[
\begin{align*}
(3.1) & \quad a \in L^q, b \in L^p \implies \langle a, b \rangle \leq ||a||_q \cdot ||b||_p \\
(3.2) & \quad h \in L^q \implies h^* \in L^p; \quad ||h||_q^q = \langle h, h^* \rangle = ||h^*||_p^p; \quad (h^*)^* = h \\
(3.3) & \quad f \in L^q; \quad ||f||_q^q = \int_\mathbb{Q} f; \quad f^* = f \\
(3.4) & \quad \langle h, f \rangle = \int_\mathbb{Q} h, \quad h \in L^q; \quad \langle f, h^* \rangle = \int_\mathbb{Q} h^*, \quad h^* \in L^p.
\end{align*}
\]
Lemma 3.2

for $h \geq 0$ is a straightforward calculation using $q(p-1) = p$.
and $\mathbf{(3.4)}$ follow directly from the definitions.

Operator $\mathcal{T}$.

Lemma 3.2 (Properties of $\mathcal{T}$). For $0 \leq h \in L^\alpha$:

\begin{equation}
\mathcal{T}h = f \cdot \int_P h \circ H \cdot g
\end{equation}

\begin{equation}
\int_Q \mathcal{T}h = \int_Q h
\end{equation}

\begin{equation}
||\mathcal{T}h||_q \leq ||h||_q
\end{equation}

The equality in (3.7) occurs iff $h = \alpha \cdot f$ (a.e.), where $\alpha = \alpha(h) = \int h/ \int f$.

Proof. (3.5): Using the invariance properties we have $\int_P h \circ H \cdot (f \cdot g) \circ H = \int_P h \circ H \cdot (f \cdot g)$ and $f$ does not depend on $p \in P$.

$\mathbf{(3.6)}$: $\int_Q \int_P (h \cdot g) = \left( \int_P h \right) \left( \int_Q g \right)$.

$\mathbf{(3.7)}$: $||\mathcal{T}h||^q_\alpha = \int_Q \left( \int_P \frac{h}{\hat{q}} \circ H \cdot g \right)^q \leq \int_Q \frac{h}{\hat{q}} \circ H \cdot g = \int_Q \frac{h}{\hat{q}} \circ H \cdot (g \circ f) \circ H = \int_Q \frac{h}{\hat{q}} \circ H \cdot (g \circ f)$ the last one being equal to $\left( \int_Q \frac{h}{\hat{q}} \circ H \cdot (f \cdot g) \right) = ||h||^q_\alpha$. For a given $q$ the equality occurs only if $(h/f)(H(q,p))$ is a constant for $(g)$-almost all $p$, but by coverage assumption it means that $h/f$ is a constant on $(\tilde{f})$-almost all $Q$. The constant follows from (3.6).

The operator $\mathcal{T}$ is an averaging operator of the (transported) likelihood $h/f$ with respect to the probability $g$. The scalar bilinear functional is monotone: $0 \leq a \leq b, \quad 0 \leq c \leq d$ 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 (3.7) $\mathcal{T}$ has its spectrum in the unit disk, with 1 being a unique eigenvalue on the unit circle and has multiplicity 1. For any $h \in L^\alpha$ one has the unique decomposition $h = \alpha f + (h - \alpha f)$ where $\alpha f$ is a direction of the fixed points and $h - \alpha f \in N = \{a \in L^\alpha : f a = 0\}$ lies in an invariant subspace. It is not a priori clear under what conditions 1 is isolated in the spectrum, in other words whether the contraction $||\mathcal{T}h|| < ||h||$ is uniform on $N$, which would imply $\mathcal{T}^n N \to \{0\}$ (point-wise) with exponential speed.

4. 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 $H$. It turns out that the operator $\mathcal{T}^\dagger$ defined by $H^{-1}$:

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

is adjoint to $\mathcal{T}$ with respect to the duality functional $\langle \cdot, \cdot \rangle$, namely

Lemma 4.1. For $h \in L^\alpha$ and $k \in L^p$:

$$\langle \mathcal{T}h, k \rangle = \langle h, \mathcal{T}^\dagger k \rangle$$

Proof. Using (3.5) and invariance $\langle Th, k \rangle = \int_Q \left( \int_P \frac{h}{\hat{q}} \circ H \cdot g \right) \cdot k = \int_Q \frac{h}{\hat{q}} \circ H^{-1} \cdot (g \cdot f) \circ H^{-1} = \int_Q \frac{h}{\hat{q}} \circ H^{-1} \cdot (g \cdot f) = \int_Q h \left( \int_P \frac{h}{\hat{q}} \circ H^{-1} \cdot g \right) = \langle h, \mathcal{T}^\dagger k \rangle$. □
Lemma 4.2. For $2 \leq q < \infty$ and $h \in L^q$

\( (T^n h)^* \leq T^n (h^*) \) (4.2)

For $1 < q \leq 2$ the opposite inequality holds. The equality happens when $q = 2$ or when $h$ is aligned with $f$.

Proof. It is enough to prove for $n = 1$. The comparison acts in $L^p$. The Lemma follows from the convexity of $\| \cdot \|_q$, positivity of the linear operator $T$ and its averaging property. Again the inequality is sharp unless $h = af$. By induction and monotonicity of $T$ it follows that $(T^n h)^* \leq T^n (h^*)$.

\[ \square \]

4.1. Case of the self-adjoint operator, when $T = T^\dagger$. Let $\sigma$ be a measure preserving involution $\sigma : \mathcal{P} \to \mathcal{P}$, $\sigma \circ \sigma = \id$. We can extend it to $\sigma : \mathbb{Q} \times \mathcal{P} \to \mathbb{Q} \times \mathcal{P}$ by $\sigma(q, p) = (q, \sigma(p))$. Assume that $g$ is invariant with respect to $\sigma$: $g \circ \sigma = g$.

Lemma 4.3. If $\sigma \circ H^{-1} \circ \sigma = H$ and $g$ is invariant with respect to $\sigma$ then $T^\dagger = T$.

As an example take $\mathbb{Q} = \mathbb{R}$, $\sigma$ to be the symmetry (reflection) of the space $\mathbb{P}$ with respect to the line, $\sigma(p) = -p$. An even $g(p) = g(-p)$ is invariant with respect to $\sigma$. The rotation $H$ around any point on the $Q$ axis and $H^{-1}$ the opposite rotation satisfy the condition of the Lemma. The involution $\sigma(p) = -p$ is applicable the case in the most common choice of $g$: a centralized Gaussian distribution.

Proof. Measure invariance means that $\int f \cdot a \sigma = \int f \cdot a$. Let $(\hat{Q}, \hat{P}) = H^{-1}(q, p)$ then $\sigma \circ H^{-1}(q, p) = (\sigma(Q), \sigma(P))$ and $\tau h = \int (h \cdot g) \circ H = \int (h \cdot g) \circ \sigma \circ H^{-1} \circ \sigma = \int (h \cdot g) \circ \sigma \circ H^{-1}$ which applied to $(q, p)$ yields $\int (h \cdot g) \circ \sigma(\hat{Q}, \hat{P}) = \int h(\hat{Q}) \cdot g(\sigma(\hat{P})) = \int h(\hat{Q}) \cdot g(\hat{P}) = (T^\dagger h)(q)$. \[ \square \]

In what follows we shall assume that

\[ \tau \mathcal{T} = \mathcal{T}^\dagger \] (4.3)

If not we can use $\mathcal{S} = \mathcal{T}^\dagger \circ \mathcal{T}$ such that $\mathcal{S}^\dagger = \mathcal{S}$.

5. Limits of the sequences $T^n$ of self-adjoint operator

From $\|\mathcal{T} h\|_q < \|h\|_q$ by induction we obtain $\|\mathcal{T}^n h\| < \|h\|$ unless $h = 0$, when equality holds. For $h \in L^q$ let

\[ V_q(h) = \inf \|\mathcal{T}^n h\|_q = \lim \|\mathcal{T}^n h\|_q^q. \] (5.1)

By definition $V_q(h) = V_q(T^n(h))$. As we are interested in the limit of the sequence $T^n h$, 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 $T^M h$ 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 $\mathcal{T}^m h \to h_\infty$.

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

Proof. As $V = V_q(h_0) = V(T^M(h_0))$, for any $\epsilon > 0$ there is an index $M$ in the set of indices $m_\alpha$ large enough so that $h = T^M(h_0)$ has the norm $V \leq \|h\|^q \leq V + \epsilon$. We may assume that $(m_\alpha - M)$ has infinite number of even numbers, otherwise we take $M + 1$ instead of $M$. Simplifying the notation we have $\mathcal{T}^m h \to h_\infty$ on a subsequence of $m$'s. With this we have $(\mathcal{T}^{2m} h, b) \to (h_\infty, b)$ for every $b \in L^p$. By (4.2) and $q/p = q - 1$ we have $V \leq \|\mathcal{T}^m(h)\|_q^q = (\mathcal{T}^m h)^* \leq (\mathcal{T}^m h)^* \leq (\mathcal{T}^m(h), \mathcal{T}^m(h^*)) = (\mathcal{T}^{2m}(h), h^*) \to (h_\infty, h^*) \leq \|h_\infty\|_q \cdot \|h^\ast\|_p = \|h_\infty\|_q \cdot \|h^\ast\|_q^{1/p} = \|h_\infty\|_q \cdot \|h^\ast\|_q^{1/p} = \|h_\infty\|_q \cdot \|h^\ast\|_q^{1/p}$ thus by the arbitrary choice of $\epsilon > 0$ we have $\|h_\infty\|_q^q \geq V$. The opposite direction is standard, we
use (3.1) and (3.2): $\|h_\infty\|_q^p = (h_\infty, (h_\infty)^\ast) \leftrightarrow \langle T^{2m}(h), (h_\infty)^\ast \rangle \leq \|T^{2m}(h)\|_q \cdot \|(h_\infty)^\ast\|_p \leq \|h\|_q \cdot \|h_\infty\|_q^{q/p} \leq (V + \epsilon)^{1/q} \|h_\infty\|_q^{q-1}$. □

Corollary 5.2. For $q \geq 2$ every weak convergent subsequence of $T^n(h_0)$, $h_0 \in L^q$ has a limit $h_\infty$ of norm $\|h_\infty\|_q = V_q(h_0)$. In consequence $T^n(h_0) \rightharpoonup \alpha f$.

Proof. If $T^m(h_0) \rightharpoonup h_\infty$ then $T^{m+1}(h_0) \rightharpoonup T(h_\infty)$ (use the operator $T^\dagger$). As they have the same norm, by Lemma 3.2, (3.7) they are equal $h_\infty = T h_\infty = \alpha f$. Therefore every weakly convergent subsequence converges to the same limit, and as every subsequence has a weakly convergent subsequence, the whole sequence converges. □

Corollary 5.3. 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 implies strong convergence. □

Proposition 5.4. For any $1 < q < \infty$ and $h \in L^q$ the sequence $T^n(h)$ converges weakly to $\alpha(h)f$, where $\alpha(h) = \int_Q h / \int_Q f$. In particular $\langle T^n h, a \rangle \rightarrow \int h \cdot a / \int f$.

Proof. The case $q \geq 2$ follows from Corollary 5.2. Let $1 < q \leq 2$, then $p \geq 2$ and for any $a \in L^p$ we have $T^n a \rightharpoonup \alpha(a)f$, where $\alpha(a) = \int a / \int f$. Let $h \in L^q$ with $q \leq 2$ and $a \in L^p$. We have $\langle T^n h, a \rangle = \langle h, T^n a \rangle \rightarrow \langle h, \alpha(a)f \rangle = \alpha(a) \langle h, f \rangle = \alpha(a) \int h \cdot a / \int f = \langle \alpha(h)f, a \rangle$. Which means $T^n h \rightharpoonup \alpha(h)f$. □

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