A Bit of Information Theory, and the Data Augmentation Algorithm Converges

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Abstract—The data augmentation (DA) algorithm is a simple and powerful tool in statistical computing. In this note basic information theory is used to prove a nontrivial convergence theorem for the DA algorithm.

Index Terms—Gibbs sampling, information geometry, I-projection, Kullback-Leibler divergence, Markov chain Monte Carlo, Pinsker’s inequality, relative entropy, reverse I-projection, total variation

I. BACKGROUND

In many statistical problems we would like to sample from a probability density \( \pi(x, y) \), e.g., the joint posterior of all parameters and latent variables in a Bayesian model. When \( \pi(x, y) \) is complicated, direct simulation may be impractical; however, if the conditional densities \( \pi_{X|Y}(x|y) \) and \( \pi_{Y|X}(y|x) \) are tractable, the following algorithm is an intuitively appealing alternative. Draw \((X, Y)\) from an initial density \( p^0(x, y) \), and then alternately replace \( X \) by a conditional draw given \( Y \) according to \( \pi_{X|Y}(x|y) \), and \( Y \) by a conditional draw given \( X \) according to \( \pi_{Y|X}(y|x) \); this is a crude description of the data augmentation (DA) algorithm of Tanner and Wong [18] (see also [15], [20] and [22]), a powerful and widely used method in statistical computing.

It is not immediately obvious that iterates of the DA algorithm should approach the target \( \pi(x, y) \). To show convergence, one usually appeals to Markov chain theory (Tierney [19]), which says that (roughly) if a Markov chain is irreducible and aperiodic, and possesses a stationary distribution, then it converges to that distribution. Such results are often stated in terms of the total variation distance, defined for two densities \( p \) and \( q \) as

\[
V(p, q) = \int |p - q|.
\]

Because iterates of the DA algorithm form a Markov chain, they converge in total variation under some regularity conditions.

Total variation, of course, is not the only discrepancy measure. There is actually another discrepancy measure that is natural for the problem, yet rarely explored. Recall that the relative entropy, or Kullback-Leibler divergence, between two densities \( p \) and \( q \) is defined as

\[
D(p|q) = \int p \log(p/q).
\]

It is related to \( V(p, q) \) via the well-known Pinsker’s inequality

\[
D(p|q) \geq \frac{1}{2} V^2(p, q).
\]

so that for a sequence of densities \( p_t, t = 0, 1, \ldots \), \( \lim_{t \to \infty} D(p_t|p_\infty) = 0 \) implies \( \lim_{t \to \infty} V(p_t, p_\infty) = 0 \). Other useful properties of relative entropy can be found in Cover and Thomas [3].

It is the purpose of this note to analyze the DA algorithm in terms of relative entropy and present a short proof of a convergence result (Theorem 2.1) using simple information theoretic techniques.

II. MAIN RESULT

Let \( \mu \times \nu \) be a product measure on a joint measurable space \((\mathcal{X} \times \mathcal{Y}, \mathcal{F} \times \mathcal{G})\). Suppose the target density \( \pi(x, y) \) with respect to \( \mu \times \nu \) satisfies \( \pi(x, y) > 0 \) for all \((x, y) \in \mathcal{X} \times \mathcal{Y}\) (in statistical applications often \( \mathcal{X} \) and \( \mathcal{Y} \) are subsets of Euclidean spaces and each of \( \mu \) and \( \nu \) is either Lebesgue measure or the counting measure). Formally, given an initial density \( p^0(x, y) \), the DA algorithm generates a sequence of densities \( p^t(x, y) \), \( t \geq 0 \), where \( (X^t, Y^t) = \int_{\mathcal{X}} p^t(x, y) \, d\nu(y) \), for example

\[
p^{t+1}(x, y) = \begin{cases} p_t^X(x) \pi_{Y|X}(y|x), & t \text{ odd;} \\ p_t^Y(y) \pi_{X|Y}(x|y), & t \text{ even.} \end{cases}
\]

Theorem 2.1: If \( \pi(x, y) > 0 \) for all \((x, y) \in \mathcal{X} \times \mathcal{Y}\), and \( D(p^0|\pi) < \infty \), then iterates of the DA algorithm converge in relative entropy, i.e.,

\[
\lim_{t \to \infty} D\left(p^t|\pi\right) = 0,
\]

and \( \lim_{t \to \infty} V(p^t, \pi) = 0 \) necessarily.

The condition \( \pi(x, y) > 0 \), \((x, y) \in \mathcal{X} \times \mathcal{Y}\), can be weakened, and the result can be generalized to the Gibbs sampler ([11] [10]); see Yu [21]. Note that the conditions of Theorem 2.1 are already weaker than those of Schervish and Carlin [17], for example (see also Liu et al. [13]), although Theorem 2.1 does not give a qualitative rate of convergence. As a general comment, the approach taken here complements the more traditional \( L_2 \) approach (Amit [1]) that studies the Gibbs sampler in the Hilbert space of square integrable functions.

Section III provides a short, self-contained proof of Theorem 2.1. The main tools (Lemmas 3.1, 3.3) exploit the information geometry of the DA algorithm. Although relative entropy does not define a metric, it behaves like squared Euclidean distance. See Csiszár [4], Csiszár and Shields [6], and Csiszár and Matúš [5] for the notions of I-projection and reverse I-projection that explore such properties in broader contexts.

III. PROOF OF THEOREM 2.1

In this section let \( p^t \) be a sequence of densities generated according to (I) with \( D(p^0|\pi) < \infty \). Lemma 3.1 captures the intuition that each iteration is a projection (more precisely, a reverse I-projection) onto the set of densities with a given conditional. The proof is simple and hence omitted.

Lemma 3.1: For all \( t \geq 0 \),

\[
D\left(p^t|\pi\right) = D\left(p^t|p^{t+1}\right) + D\left(p^{t+1}|\pi\right).
\]
According to Lemma 3.1, $D(p(t)|π)$ can only decrease in $t$ (this holds for Markov chains in general). However, it does not imply $D(p(t)|π) ↓ 0$. To prove the theorem we need further analysis.

**Lemma 3.2.** Let $t ≥ 1$ and $n ≥ 1$. If $n$ is even then

$$D(p(t)|p(t+n)) ≤ D(p(t)|p(t+1)) + D(p(t+1)|p(t+n)),$$

if $n$ is odd then

$$D(p(t)|p(t+n)) = D(p(t)|p(t+1)) + D(p(t+1)|p(t+n)).$$

**(3)**

**Proof:** To prove (2), without loss of generality assume $t$ is odd. Since $n$ is even, $p(t)$ and $p(t+n)$ have the same conditional $p_{X|Y} = p_{X|Y}^*$, whereas $p_{Y}^{(t+n)} = p_{Y}^{(t+n-1)}$ by (1). We have

$$D(p(t)|p(t+n)) = D(p_Y|p_Y^*) = D(p_Y|p_Y^*),$$

the last inequality being a basic property of relative entropy (Cover and Thomas [3]). The proof of (3), omitted, is the same as that of Lemma 3.1.

**Lemma 3.3.** For all $t ≥ 1$ and $n ≥ 0$ we have

$$D(p(t)|p(t+n)) ≤ D(p(t)|π) - D(p(t+n)|π).$$

**(4)**

**Proof:** Let us use induction on $n$. The case $n = 0$ is trivial. Suppose (4) has been verified for all $n' < n$. When $n$ is even, we apply (2), the induction hypothesis, and Lemma 3.1 to obtain

$$D(p(t)|p(t+n)) ≤ D(p(t)|p(t+n-1)) ≤ D(p(t)|π) - D(p(t+n-1)|π),$$

When $n$ is odd, by (3), the induction hypothesis, and then Lemma 3.1 we have

$$D(p(t)|p(t+n)) = D(p(t)|p(t+1)) + D(p(t+1)|p(t+n)) ≤ D(p(t)|p(t+1)) + D(p(t+1)|π).$$

Corollary 3.1: There exists some density $π^*$ such that $\lim_{t→∞} V(p(t), π^*) = 0$.

**Proof:** Pinsker’s inequality and (4) imply

$$\frac{1}{2} V^2 (p(t), p(k)) ≤ |D(p(t)|π) - D(p(k)|π)|,$$

for all $t, k ≥ 1$. Because $D(p(t)|π)$ is finite and decreases monotonically in $t$, $\lim_{t→∞} V(p(t), p(k)) = 0$, i.e., $p(t)$ is a Cauchy sequence in $L_1(\mathcal{X} × \mathcal{Y})$. Hence $p(t)$ converges in $L_1(\mathcal{X} × \mathcal{Y})$ to some density $π^*$. (Only the completeness of $L_1(\mathcal{X} × \mathcal{Y})$ is used here. Further properties of $L_π$ spaces can be found in real analysis texts such as Royden [16].)

**Proposition 3.1:** In the setting of Corollary 3.1 $π^* = π$.

**Proof:** Since $p(t), t ≥ 1$, has the conditional $π_{X|Y}$ when $t$ is odd, and $π_{Y|X}$ when $t$ is even, the conditionals of $π^*$ must match those of $π$, i.e.,

$$π^*(x, y) = π_Y^*(y)π_X(π_x|x),$$

almost everywhere. Under the assumption $π(x, y) > 0$, (5) implies

$$π_Y^*(y) = π_X^*(x)π_{Y|X}(π_y|x) = π_X(x)π_Y(π_y|x).$$

Integration over $y$ yields $1 = π_X^*(x)/π_X(x)$, which, together with (5), proves $π^* = π$.

Finally we finish the proof of Theorem 2.1 by showing that the convergence in Corollary 3.1 also holds in relative entropy.

**Lemma 3.4:** $\lim_{t→∞} D(p(t)|π) = 0$.

**Proof:** We already have $D(p(t)|π) ↓ d$, say, with $d ≥ 0$. Taking $n → ∞$ in (4) we get

$$\lim_{n→∞} D(p(t)|p(t+n)) ≤ D(p(t)|π) - d. $$

On the other hand, since

$$D(p(t)|p(t+n)) = \int p(t) \log \left( \frac{p(t)}{p(t+n)} \right) - p(t) + p(t+n),$$

and the integrand is non-negative, by Fatou’s Lemma we have

$$\lim_{n→∞} \inf D(p(t)|p(t+n)) ≥ D(p(t)|π)$$

which forces $d = 0$. The proof is now complete. Note that (6) is a case of the more general lower semi-continuity property of relative entropy (Csiszár [4]).

IV. REMARKS

As pointed out by an anonymous reviewer, the core of Section III consists of two parts: (i) showing $\lim_{t→∞} V(p(t), π^*) = 0$ for some $π^*$, whose conditionals match those of $π$, and (ii) showing that $π^* = π$. Part (i) can be phrased more generally and is related to the results of Csiszár and Shields (6), Theorem 5.1 on alternating I-projections. It is also related to the information theoretic treatment of the EM algorithm (8) [14] of Csiszár and Tusnady [7]. The condition $π(x, y) > 0$, not used in part (i), can be replaced by a weaker assumption, as long as one can show that there exists no density other than $π$ that possesses the two conditionals $π_{X|Y}$ and $π_{Y|X}$.

Lemma 3.1 appears in Yu [21]. Lemmas 3.2 and 3.3 are new. Generalizations of Theorem 2.1 to the Gibbs sampler with more than two components are possible ([21]), but technically more involved, because Lemmas 3.2 and 3.3 are tailored to the two component case. The issue of the rate of convergence, not addressed here, is definitely worth investigating.

The DA algorithm has the following feature. If we let $(X(0), Y(0), X(1), Y(1), \ldots)$ be the iterates generated, i.e., the conditional distribution of $Y(k)|X(k)$, $X(k)|X(k)$ is $π_{Y|X}$ and that of $X(k+1)|Y(k)$ is $π_{X|Y}$, then each of $\{X(k)\}$ and $\{Y(k)\}$...
forms a reversible Markov chain. Fritz [9], Barron [2], and Harremoës and Holst [12] apply information theory to prove convergence theorems for reversible Markov chains. Their results may be adapted to give an alternative (albeit less elementary) derivation of Theorem 2.1.

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