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Vasserstein Distances in Two-State Systems

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We present formulas for the Vasserstein distance between two statistical mechanical states of a two-state system. For example, in a ferromagnetic spin-1/2 Ising model the Vasserstein distance is half the difference in the magnetizations.

KEY WORDS: Rigorous statistical mechanics; Kantorovich distance.

1. INTRODUCTION

In statistical mechanics it is often important to measure quantitatively the similarity of two different (thermodynamic) states of the same system. For example, water at 99°C is in some sense more similar to water at 97°C than to steam at 101°C. This need is often satisfied by the so-called Vasserstein (or Kantorovich) distance,[1,2] which is, for example, precisely the correct distance for use in the important Dobrushin–Shlosman phase uniqueness theorem.[3–5] In general there is no formula for the Vasserstein distance and it must be computed using intricate linear programming techniques.[5] In this paper we produce simple formulas, restricted to two-state systems, relating the Vasserstein distance to the average magnetization (or staggered magnetization).

2. DEFINITIONS

Consider a lattice L and a finite subset of it, the "lattice cell" V. At each site l in L a variable (or spin) takes on one of only two possible

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values, which we call ± 1 (up or down). One configuration of the lattice is chosen as the *reference configuration.* (The most convenient reference configuration is often, but not always, a minimum-energy configuration.) Any configuration of the lattice cell (denoted by i, j, or k) is then specified by the set of spins in V which are overturned from the reference configuration. Thus, we can perform set operations on configurations (e.g., $i \cup j$). The indicator function $I(l)$ flags the status of lattice site l in configuration i: $I(l) = +1$ if the spin at site l is overturned (i.e., if $l \in i$), $I(l) = -1$ otherwise. The *magnetization* (or, more generally, the *staggered magnetization*) of cell configuration i is

$$m(i) = \sum_{l \in V} I(l) \tag{1}$$

The *Hamming distance* $d(i, j)$ between two configurations in V is the number of sites in V at which the two configurations differ, so

$$d(i, j) = \frac{1}{2} \sum_{l \in V} |I(l) - J(l)| \tag{2}$$

This paper will not consider distances between states which differ in temperature, magnetic field, coupling constants, etc. Instead, the two states will differ only by the configuration of boundary spins. (Boundary spins are those which interact with spins in V, but which are not themselves in V. We denote boundary configurations by x or y, and specify them in the usual way by listing the boundary spins overturned from the reference configuration.) The energy of cell configuration i subject to boundary x is $E_x(i)$, and its probability is

$$p_x(i) = \frac{\exp[-E_x(i)/k_B T]}{Z(x; T)} \tag{3}$$

where $Z(x; T)$ is the partition function which normalizes the probabilities. The *average magnetization* (or staggered magnetization) of the cell is

$$M_x = \sum_i m(i)\, p_x(i) \tag{4}$$

where the sum runs over all configurations of V. The *Vasserstein distance* between two states specified by the boundaries x and y is

$$\mathscr{R}_{x,y} \equiv \min \left\{ \sum_{i,j} w(i, j)\, d(i, j) \right\} \tag{5}$$

where the minimization is performed over all joint probability distributions $w(i, j)$ that satisfy

$$\sum_j w(i, j) = p_x(i); \qquad \sum_i w(i, j) = p_y(j); \qquad w(i, j) \geq 0 \tag{6}$$

3. GENERAL RESULTS

We first show that for any two-state system the Vasserstein distance between two states is bounded below by half the difference in their magnetizations. We then show that under certain circumstances it is bounded above by the same amount.

Lemma 1 (Lower bound). The Vasserstein distance between the state with boundary x and the state with boundary y satisfies

$$\mathscr{R}_{x, y} \geq \tfrac{1}{2} |M_x - M_y| \tag{7}$$

Proof. First note that

$$d(i, j) = \frac{1}{2} \sum_{l \in V} |I(l) - J(l)| \geq \frac{1}{2} \left| \sum_{l \in V} [I(l) - J(l)] \right| = \frac{1}{2} |m(i) - m(j)| \tag{8}$$

Now, if $w(i, j)$ is the probability distribution which satisfies (6) and minimizes (5), then

$$\begin{aligned} \mathscr{R}_{x, y} &= \sum_{i, j} w(i, j)\, d(i, j) \\ &\geq \frac{1}{2} \sum_{i, j} w(i, j)\, |m(i) - m(j)| \\ &\geq \frac{1}{2} \left| \sum_{i, j} w(i, j)\, m(i) - \sum_{i, j} w(i, j)\, m(j) \right| \end{aligned} \tag{9}$$

Using relations (6), the last expression becomes

$$\frac{1}{2} \left| \sum_i p_x(i)\, m(i) - \sum_j p_y(j)\, m(j) \right| = \frac{1}{2} |M_x - M_y| \quad \blacksquare \tag{10}$$

The upper bound follows from the following remarkable theorem due to Holley,[6] which can be proven either using the theory of Markov chains[6–8] or through direct combinatoric arguments.[9,10] (In fact, the conclusions of this theorem follow[11] from the weaker hypothesis that the distribution p_y is "less than" the distribution p_x in the precise sense described

by Liggett.[7] This version of the theorem is not, however, needed for this paper.)

Holley's Theorem. Suppose that $p_x(i)$ and $p_y(j)$ are probability distributions over the configurations of a two-state system and that they satisfy

$$p_x(i \cup j)\, p_y(i \cap j) \geqslant p_x(i)\, p_y(j) \tag{11}$$

for all i and j. Then there exists a joint probability distribution $w_0(i, j)$ which satisfies the requirements (6) and for which

$$w_0(i, j) = 0 \qquad \text{whenever} \quad j \not\subseteq i \tag{12}$$

Lemma 2 (Upper bound). If $p_x(i)$ and $p_y(j)$ satisfy (11), then

$$\mathscr{R}_{x,y} \leqslant \tfrac{1}{2}(M_x - M_y) \tag{13}$$

Proof. If $j \subseteq i$, then

$$d(i, j) = \frac{1}{2} \sum_{l \in V} [I(l) - J(l)] = \frac{1}{2} [m(i) - m(j)] \tag{14}$$

In addition, because of (5) and (12),

$$\begin{aligned}
\mathscr{R}_{x,y} &\leqslant \sum_{i,j} w_0(i, j)\, d(i, j) \\
&= \sum_{j \subseteq i} w_0(i, j)\, d(i, j) \\
&= \frac{1}{2} \sum_{j \subseteq i} w_0(i, j)[m(i) - m(j)] \\
&= \frac{1}{2} \left[\sum_{i,j} w_0(i, j)\, m(i) - \sum_{i,j} w_0(i, j)\, m(j) \right] \\
&= \frac{1}{2} \left[\sum_{i} p_x(i)\, m(i) - \sum_{j} p_y(j)\, m(j) \right] \\
&= \frac{1}{2} (M_x - M_y)
\end{aligned} \tag{15}$$

[Note that $M_x \geqslant M_y$ by virtue of Holley's inequality, (11) of ref. 6] ∎

Thus, one need only verify inequality (11) to produce a simple formula for the Vasserstein distance. The use of (3) in (11) converts it from a condition on probabilities to a condition on energies, as follows.

Theorem. If the energies of a two-state system satisfy

$$E_x(i \cup k) - E_x(i) \leqslant E_y(j \cup k) - E_y(j) \tag{16}$$

for all configurations i, j, and k with $j \subseteq i$ and $k \cap i = \varnothing$, then

$$\mathscr{R}_{x,y} = \tfrac{1}{2}(M_x - M_y) \tag{17}$$

Proof. Direct use of (3) in (11) results in

$$E_x(i \cup j) - E_x(i) \leqslant E_y(j) - E_y(i \cap j) \tag{18}$$

for all configurations i and j. But this is the same as (16), where k represents those spins which are in j but not in i, and where j in (16) is the same as $i \cap j$ in (18).

Remark. Equation (16) is simply interpreted. The right-hand side is the energy cost of overturning the spins in k given that the spins in j and in y are already overturned. The left-hand side is again the energy cost of overturning the spins in k, but now given that the spins in i and in x are already overturned.

4. FERROMAGNETIC MODELS

In this section the reference configuration is the one in which all spins point down, so the magnetizations are direct rather than staggered. From the remark interpreting Eq. (16), it is clear that (16) holds for ferromagnetic models whenever $x \supseteq y$: It simply says, "the more spins that are up, the easier it is to overturn down spins." We have proven the following result.

Corollary 1. For ferromagnetic spin-1/2 Ising models and with $x \supseteq y$,

$$\mathscr{R}_{x,y} = \tfrac{1}{2}(M_x - M_y) \tag{19}$$

where M_x is the average (direct) magnetization of the cell with boundary x.

Note the generality of this result: it accomodates any lattice, non-uniform couplings and fields, interactions of any finite range, and multispin interactions. It assumes only that (i) all interactions are ferromagnetic and that (ii) there are only two states per lattice site.

5. ANTIFERROMAGNETIC MODELS

In this section we consider a lattice cell consisting of two sets of spins, A and B, such that interactions between sets are antiferromagnetic, while

interactions within each set are ferromagnetic. An example is the nearest-neighbor antiferromagnetic spin-1/2 Ising model on a bipartite lattice. The reference configuration is one in which all the spins of A point down, while all the spins of B point up, so the magnetizations are staggered rather than direct. Once again, it is clear that the inequality holds whenever $x \supseteq y$, so we have the following result.

Corollary 2. For the models described above, and with $x \supseteq y$,

$$\mathscr{R}_{x,y} = \tfrac{1}{2}(M_x - M_y) \tag{20}$$

where M_x is the average staggered magnetization of the cell with boundary x.

Because the hard-square model is the limit of an Ising antiferromagnet as the repulsive interactions become very strong, this result applies to the hard-square model and in fact constitutes a proof of Radulescu and Styer's[5] conjecture C. Preliminary computer explorations using this result and the Dobrushin–Shlosman theorem[3] confirm the value of the formula: Computation of Vasserstein distances through formula (20) is three orders of magnitude faster than computation through a direct linear programming minimization of (5). This raises the possibility that the Dobrushin–Shlosman theorem may be able to locate phase transitions practically as well as rigorously.

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