THE REVERSE ISING PROBLEM

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1. Introduction and Terminology

Definition 1.1. Let $\Sigma = \{-1, +1\}$. An **Ising circuit** is a function $f : \Sigma^N \longrightarrow \Sigma^M$ where N and M are finite subsets of $\mathbb{N}$. For convenience we always assume $N = \{1, ..., n\}$ and $M = \{n+1, ..., n+m\}$.

2. Hierarchical Clustering

A choice of "auxililary array" can be thought of as a function $a : \Sigma^N \longrightarrow \Sigma^A$ which assigns an auxiliary state to each input state. The collection of germs of this function partitions Σ^N into subsets of inputs which share the same auxiliary state. To be clear, we're talking about the partition

$$\{a^{-1}(\alpha)\}_{\alpha \in \Sigma^A}$$

of input spin space. If the choice of auxiliary array a makes the Ising circuit feasible, then we say a solves the Ising circuit.

This simple observation motivates a simple question: *can a partition of Σ^N be found such that it matches the partition produced by some feasible auxiliary array using only the logic of the Ising circuit?* Producing such a partition is a clustering problem on input spinspace.

3. Pseudo-boolean optimization and polynomial fitting

A pseudo boolean function (PBF) is any function $f : \{0, 1\} \longrightarrow \mathbb{R}$. It is a well known fact that any such PBF can be uniquely represented by a multilinear polynomial in n variables [pseudo-boolean optimization Boros, Hammer]; that is, a polynomial

$$g(x_1, ..., x_n) = \sum_{S \subset [n]} a_S \prod_{j \in S} x_j$$

with $a_S \in \mathbb{R}$ which equals f pointwise on $\{0, 1\}^n$. To be clear, here S iterates over all subsets of $[n] = \{1, ..., n\}$.

It is another well-known fact that the optimization of any pseudo-boolean function can be reduced in polynomial time to an optimization problem on a quadratic polynomial. The original method for accomplishing this was first written by Rosenberg, and since then a reputable zoo of alternative algorithms have been introduced. Most methods share the same basic idea: reduce degree ≥ 3 monomial terms appearing in the polynomial g by introducing auxiliary variables subject to constraints.

<copy Rosenberg algorithm from Boros, Hammer pg 168>

Theorem 3.1. *Let f be a multilinear polynomial in n variables. There exists an algorithm* Reduce *which produces a multilinear polynomial g in $n + a$ variables such that*

$$\min_{(\mathbf{x}, \mathbf{a}) \in \mathbb{B}^n \times \mathbb{B}^a} g(\mathbf{x}, \mathbf{a}) = \min_{\mathbf{x} \in \mathbb{B}^n} f(\mathbf{x})$$

and if $(\mathbf{x}, \mathbf{a}) = \arg\min_{(\mathbf{x}, \mathbf{a}) \in \mathbb{B}^n \times \mathbb{B}^a} g(\mathbf{x}, \mathbf{a})$ then $\mathbf{x} = \arg\min_{\mathbf{x} \in \mathbb{B}^n} f(\mathbf{x})$.

Boros Hammer Pseudo Boolean Optimization 2002. □

We need a slightly stronger statement however.

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Theorem 3.2. *Let $f : \Sigma^N \longrightarrow \Sigma^M$ be a circuit. Then there exists an Ising circuit with auxiliary spins given by Hamiltonian H which solves f.*

Proof. Fix $G = N \cup M$ and consider the hamming objective function $\mathrm{ham} : \Sigma^N \times \Sigma^M \longrightarrow \mathbb{R}$ defined

$$\mathrm{ham}(s,t) = d(t, f(s))$$

where $d(t, f(s))$ is the Hamming distance between t and the correct output $f(s)$. Then there exists some multilinear polynomial g in $|G|$ variables which recovers ham pointwise. We now apply Rosenberg reduction to g and set H equal to the terminal quadratic polynomial we obtain. All that remains to show is that on any input level s the output which minimizes H is $f(s)$.

Fix an input s and suppose that the minimizer of $g^k(s,\cdot)$ has output coordinates $f(s)$. To obtain g^{k+1} we replace some pair $x_i x_j$ by x_{k+1} and add the expression $M(x_i x_j - 2x_i x_{k+1} - 2x_j x_{k+1} + 3x_{k+1})$. Observe that this expression is zero if $x_i x_j = x_{k+1}$ and is strictly positive otherwise. It follows that $g^k(\mathbf{x}) = g^{k+1}(\mathbf{x}, x_{k+1})$ if $x_{k+1} = x_i x_j$ and $g^k(\mathbf{x}) < g^{k+1}(\mathbf{x}, x_{k+1})$ if $x_{k+1} \neq x_i x_j$. Hence the minimizer of g^{k+1} on input level s also has the correct output coordinates, and inductively, we conclude that H is an Ising Hamiltonian reproducing the circuit f. $\square$