The Reverse Ising Problem

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Introduction and Terminology

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The Ising Model

The vectors h and J encode first and second order energy contributions respectively. Elements of J encode interactions between vertices whereas elements of h encode the individual energy contributions of vertices.

Definition 1.1.1: Ising Graph

An **Ising graph** consists of the following data:

- a finite set G, typically $\{1..n\} \subset \mathbb{N}$ for some n
- a vector $h \in \mathbb{R}^n$ called the **local bias vector**
- a vector $J \in \mathbb{R}^{n(n-1)/2}$ called the **interaction vector**.

We refer to h and J collectively as the **parameters** of G.

We immediately have a couple of additional comments:

- The number $n(n-1)/2$ is exactly the number of elements above the diagonal in a $n \times n$ matrix.
- One typically indexes the elements of J by pairs (i, j) with $i < j$.
- The object G is a vertex set and the vector J records the edge data. If $J_{ij} = 0$ then there is no edge (i, j), and if $J_{ij} \neq 0$ then there is an edge. One can even view G as a directed graph: if $J_{ij} > 0$ then the edge points $i \to j$ and if $J_{ij} < 0$ then $i \leftarrow j$.

One should then picture an Ising graph as a graph with $|G|$ nodes where vertex i is decorated with h_i and edge (i, j) is decorated with J_{ij}.

Though $X = \{-1, 1\}$ in all cases, we keep X arbitrary in order to explore more general graph dynamics in the future and because it's more convenient to write.

Perhaps it would be better to write Σ_G for S_G and σ for states.

Definition 1.1.2: State Space

Let G be an Ising graph and X some set. The **state space** of G, denoted S_G, is the collection of all functions $G \longrightarrow X$:

$$S_G := \mathrm{Hom}(G, X).$$

We refer to the elements of S_G as the *states* of G. It will always be the case that $X = \{-1, 1\}$ in this document unless otherwise specified.

Remark 1.1.3

A function $s : G \longrightarrow X$ just assigns a vertex $i \in G$ to a value ± 1. We can therefore think of s as a "vector" in $X^{|G|}$, where $s_i = s(i)$. For example, the state $s(i) = -1^i$ can be written as the vector $(-1, 1, -1, 1, ..., -1^{|G|})$.

We refer to the value $H(s)$ as the **energy** of the state s.

Definition 1.1.4: Ising Hamiltonian

Let G be an Ising graph. The function $H : S_G \longrightarrow \mathbb{R}$ defined

$$H(s) = \sum_{i \in G} h_i s_i \; + \; \sum_{i<j} J_{ij} s_i s_j$$

is called the **Hamiltonian** of G.

Model 1.1.5: The Ising Model

The probability an Ising graph G is in a state $s \in S_G$ is given by

$$P(s) = \frac{e^{-\beta H(s)}}{Z_\beta}$$

where $\beta \geq 0$ is a parameter called the *inverse temperature* and Z_β is the normalization constant

$$Z_\beta = \sum_{s \in S_G} e^{-\beta H(s)}.$$

In other words, the Ising model says that one is more likely to find an Ising graph in a low energy state than a high energy state. The **Ising Problem** is then to find the lowest energy states of a given Ising graph.

The Reverse Ising Problem

Consider instead the reverse problem: one is given a graph G and some spin (or collection of spins) $s \in S_G$ and wants to find h and J such that the resulting Ising graph is in state s with high probability. Stated another way, one wishes to find h and J which minimize $H(s)$. This is known as the **reverse Ising problem.**

Motivating Example: AND

Why might one care about this? Consider a graph G with three vertices, v_1, v_2, v_3. Let's call v_1 and v_2 "input" vertices and v_3 the "output" vertex. We can write the AND circuit as the following table of states:

s_1	s_2	s_3
1	1	1
1	-1	-1
-1	1	-1
-1	-1	-1

This is the AND truth table with 1 denoting "True" and -1 denoting "False".

The first row is the state $s : G \longrightarrow X$ defined $s(v_1) = s(v_2) = s(v_3) = 1$, the second is the state $s : G \longrightarrow X$ defined $s(v_1) = 1$, $s(v_2) = s(v_3) = -1$, etc.

We would like to build an Ising graph which somehow implements this circuit. What this means is that, if we look at our Ising graph G and observe that the input spins are s_1 and s_2, then we want s_3 to assume the corresponding output value in the above table with high probability. I.e. if our

Ising graph is in a state with $(s_1, s_2) = (1, 1)$ then we want $s_3 = 1$, and so on for the other states.

There are two things we must do to build a robust circuit. First, we need some way to control the input spins – ideally, we should be able to fix the inputs at a certain value while letting the outputs vary. This is a physics problem and is not of our concern. [1] Second, we need to choose h and J such that for each input $s = (s_1, s_2)$, the "correct" output value has a higher probability of occurring than the incorrect output. Since lower energy states occur with higher probability, this is the same as requiring that the following constrains are satisfied:

$$\begin{aligned} H(1,1,1) &< H(1,1,-1) \\ H(1,-1,-1) &< H(1,-1,-1) \\ H(-1,1,-1) &< H(-1,1,-1) \\ H(-1,-1,-1) &< H(-1,-1,1). \end{aligned}$$

One can check that this is indeed possible: **INSERT CORRECT h AND J HERE**.

[1] It is nonetheless possible, for instance, one could choose the components of h corresponding to inputs in such a way as to drastically favor a certain value for the input spins.

Ising Circuits

Definition 1.2.1: Pre-Ising Circuit

A **pre-Ising circuit** (G, N, M, f) is a set of vertices G with a decomposition $G = N \cup M$ satisfying $N \cap M = \varnothing$ and a function $f : S_N \longrightarrow S_M$.

Comments:

- We call N the collection of **input vertices** and M the collection of **output vertices**.
- We call S_N the **input state/spin space** and S_M the **output state/spin space**.
- The function f is the **logic** of the circuit and it is not required to satisfy any additional requirements. We consider the output state $f(s)$ to the correct output corresponding to the input state s.

Notice that $Hom(N, X) \times Hom(M, X)$ is canonically isomorphic to $Hom(G, X)$ in the category Set, which is another nicety of the way we've set everything up.

Definition 1.2.2: Ising Circuit

An **Ising circuit** consists of the data (G, N, M, h, J, f) such that

(i) (G, h, J) is an Ising graph

(ii) (G, N, M, f) is a pre-Ising circuit

(iii) For each pair $(s, t) \in S_N \times S_M = S_G$ we have that $H(s, t) \geq H(s, f(s))$ with equality if and only if $f(s) = t$.

If you stop to think about condition (iii), you'll conclude that it really couldn't be anything else. What other way is there to make an Ising graph and an abstract circuit compatible?

Conditions (i) and (ii) in the above definition are self explanatory. Condition (iii) merely requires that the circuit structure of G is compatible with the Ising graph structure of G. It asks that the output t which minimizes $H(s, t)$ is the correct one; in other words, the correct output corresponding to an input s is the one which occurs with highest probability. We have an immediate question:

Question 1.2.3

Can every pre-Ising circuit G be realized as an Ising circuit for an appropriate choice of h and J? (This is known as *solving* a pre-Ising circuit.)

In order to solve a pre-Ising circuit, we need to find h and J such that condition (iii) is satisfied. This means we need to satisfy all constraints of the form

$$H(s, f(s)) < H(s, t)$$

simultaneously for all possible input states $s \in S_N$ and output states $t \neq f(s)$. We can arrange these constraint equations in a convenient way through *input levels*.

Input Levels

Definition 1.2.4: Input Level

Let $\mathbf{s} \in S_N$ be an input spin. Then $L_{\mathbf{s}} = \{\mathbf{s}\} \times S_M$ is called the **input level** at $\mathbf{s}$.

We say that a choice of h and J **solves** an input level $L_{\mathbf{s}}$ if all constraints of the form

$$H(\mathbf{s}, t) > H(\mathbf{s}, f(\mathbf{s}))$$

are satisfied for $t \neq f(\mathbf{s})$, i.e. if $(\mathbf{s}, f(\mathbf{s}))$ *strictly* minimizes the Hamiltonian for the input level:

$$(\mathbf{s}, t) = \min_{\mathbf{u} \in L_{\mathbf{s}}} H(\mathbf{u}) \implies t = f(s).$$

There are $M - 1$ constraint equations for each input level and N distinct input levels, so to solve a pre-Ising circuit one must find h and J which simultaneously satisfy $N(M - 1)$ constraints.

A non-example: XOR

I'll fill this in at some point, seems tedious now though.

The Reverse Ising Problem

Virtual States and Random Parameters

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Consider a pre-Ising circuit G. Define a new set

$$E = \{(i,j) \mid i \leq j, i, j \in G\}.$$

This is the set of all possible edges we could form between vertices in G if we allow self-connections. The cardinality of E is $|G| \cdot (|G|+1)/2$, or written another way $|G| + |G| \cdot (|G|-1)/2$. From this it is clear that the state space S_E has one spin for every vertex and pair of vertices in G.

Now consider the map

$$\varphi : S_G \longrightarrow S_E,\ \varphi(s)(i,j) = \begin{cases} s(i) & \text{if } i = j \\ s(i)s(j) & \text{if } i = j \end{cases} \tag{2.1}$$

The map φ takes states of G and produces states on E. If we identify G with its image in E under the diagonal embedding $i \longmapsto (i,i)$ we see that $\varphi(s)|_G = s$, meaning that the state $\varphi(s)$ recovers s when restricted to G. However, it also contains the second order interactions between spins of s. If we think of states instead as vectors in $X^{|G|}$ and $X^{|E|}$, then we can write φ in a more enlightening way:

$$\varphi(s_1, ..., s_G) = (s_1, ..., s_G, s_1 s_2, s_1 s_3, ..., s_1 s_G, s_2 s_G, ..., s_{G-1} s_G).$$

From this description, it is clear that φ simply concatenates all possible products between spins in s to s itself.

Notice that, for some choice of h, J, the Hamiltonian of G can now be written as the dot product

$$H(s) = (h, J) \cdot \varphi(s)$$

where (h, J) is the element in $\mathbb{R}^{|E|}$ given by concatenating h and J. For this reason, we call E the **virtual state space** of G. It contains states which correspond to states of G, but it also contains far more.

References