1 Introduction

TODO:

Such a family can arise, e.g., from measurements of a low-temperature Gibbs ensemble of Hamiltonians parametrized by a parameter λ.

2 Problem setup

- In this work we consider a family of distributions of bitstrings $\{\mathcal{D}_\lambda\}_{\lambda\in\Lambda}$, each of length n.
- We are given a finite sample $\mathcal{D}_{\text{train}}$ of size N of pairs (λ, z) s.t. $P(z|\lambda) = P_{\mathcal{D}_\lambda}(z)$.
- We are also given (possibly implicitly via coordinate description of Λ) a naive metric g^0 on Λ.
- We are asked to estimate the Fisher information metric g on Λ corresponding to distributions $\mathcal{D}_\lambda$.
- Locations with high g/g^0 are then considered to be conjectured locations of possible phase transitions.

We focus on the task of identifying phase transitions in that family. Rigorously speaking, phase transitions are only defined in the limit $n \to \infty$, while we are dealing with finite size systems. A solution to that is to look at Fisher information metric: high distances according to Fisher information metric for points close according to naive metric likely correspond to phase transitions.

3 Bitstring-ChiFc method

In this work we propose the following method:

- Collect training dataset $\mathcal{D}_{\chi_{F_c}\text{-train}}$ of the form $(\lambda_0, \delta\lambda, z, y)$, where z is sampled from $p(\bullet, \lambda = \lambda_z)$, $p_+ = p(\lambda_z = \lambda_0 + \delta\lambda/2 | \lambda_z = \lambda_0 \pm \delta\lambda/2)$, and $\mathbb{E}(y|\lambda_0, \delta\lambda, z) = p_+$. In practice $y \in \{0, 1\}$. Do it in the following way:
    - Consider $\mathcal{D}_{\text{train}}$ consisting of pairs (z, λ).
    - Sample pairs (z_{i+}, λ_{i+}), (z_{i-}, λ_{i-}) from $\mathcal{D}_{\text{train}}$.
    - Compute $\lambda_i = (\lambda_{i+} + \lambda_{i-})/2$, $\delta\lambda_i = \lambda_{i+} - \lambda_{i-}$.
    - Add tuples $(\lambda_i, \delta\lambda_i, z_{i+}, 1)$ and $(\lambda_i, \delta\lambda_i, z_{i-}, 0)$ to the dataset $\mathcal{D}_{\chi_{F_c}\text{-train}}$.
- Train a model M, which given $(\lambda_0, \delta\lambda, z)$ will predict $l = M(\lambda_0, \delta\lambda, z)$ s.t. $p_+ = (1 + e^{-l\cdot\delta\lambda})^{-1}$. Do this by minimizing cross-entropy loss on the dataset $\mathcal{D}_{\chi_{F_c}\text{-train}}$.
- Estimate
$$\chi^{jk}_{F_c}(\lambda) = \text{smoothen}\left(\lambda_1 \mapsto \text{mean}_{(z,\lambda_1)\in\mathcal{D}_{\text{train}}} M(\lambda_1, 0, z)^j M(\lambda_1, 0, z)^k\right)(\lambda). \tag{1}$$
- Derivation:
$$\chi_{F_c}(\lambda) = \lim_{\delta\lambda\to 0} \frac{2}{\delta\lambda^2}\left(1 - \mathbb{E}_{z\sim Q(\bullet)} \frac{\sqrt{P(z|\lambda - \delta\lambda/2)P(z|\lambda + \delta\lambda/2)}}{Q(z)}\right)$$
$$\simeq \lim_{\delta\lambda\to 0} \mathbb{E}_Q \frac{2}{\delta\lambda^2} \frac{2\sinh^2(l\delta\lambda/4)}{\cosh(l\delta\lambda/2)} \simeq \frac{1}{4}\mathbb{E}_{z|\lambda} M(\lambda, 0, z)^2.$$