

# 1 Introduction

TODO:

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

## 2 Classical Fidelity Susceptibility

Classical fidelity between 2 probability distributions  $p$  and  $q$  of bitstrings  $z$  is defined as

$$F_c(p, q) = \sum_z \sqrt{p(z)q(z)}. \quad (1)$$

We are interested in the fidelity between bitstring distributions at different  $s$  (e.g.  $s = s_1$  and  $s = s_2$ ), which we will denote as  $F_c(s_1, s_2)$ .

Fidelity susceptibility is defined as the term  $\chi_{F_c}(s)$  in the Taylor expansion

$$F_c(s, s + \delta s) = 1 - \frac{\delta s^2}{2} \chi_{F_c}(s) + O(\delta s^3). \quad (2)$$

For such Taylor expansion to exist it is sufficient that the probabilities have a Taylor expansion up to  $O(\delta s^3)$ . More generally, probability distribution can depend on a point  $\lambda$  on a manifold  $\Lambda$ , in which case the Taylor expansion (2) would become

$$F_c(\lambda, \lambda + \delta \lambda) = 1 - \frac{\delta \lambda_j \delta \lambda_k}{2} \chi_{F_c}^{jk}(\lambda) + O(\delta \lambda^3). \quad (3)$$

### 2.1 Classical and quantum fidelity susceptibility

Fact 1: For pure states  $\mathbb{E} \chi_{F_c}(s) = \frac{1}{2} \chi_F(s)$  where the expectation is over all orthogonal bases to perform the measurement in.

TODO:proof

Fact 2: For computational basis measurement of a non-degenerate ground state of a real-valued Hamiltonian  $H$ , then  $\chi_{F_c}(s) = \chi_F(s)$  almost everywhere.

TODO:proof

## 3 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  $(\lambda, z)$  s.t.  $P(z|\lambda) = P_{\mathcal{D}_\lambda}(z)$ .
- We are also given (possibly implicitly via coordinate description of  $\Lambda$ ) a naive metric  $g^0$  on  $\Lambda$ .
- We are asked to estimate the Fisher information metric  $g$  on  $\Lambda$  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  $n \rightarrow \infty$ , 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.

## 4 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  $(z, \lambda)$ .
- Sample pairs  $(z_{i+}, \lambda_{i+}), (z_{i-}, \lambda_{i-})$  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

$$\chi_{F_c}^{jk}(\lambda) = \text{smoothen} \left( \lambda_1 \mapsto \text{mean}_{(z, \lambda_1) \in \mathcal{D}_{\text{train}}} M(\lambda_1, 0, z)^j M(\lambda_1, 0, z)^k \right) (\lambda). \quad (4)$$

- Derivation:

$$\begin{aligned} \chi_{F_c}(\lambda) &= \lim_{\delta\lambda \rightarrow 0} \frac{2}{\delta\lambda^2} \left( 1 - \mathbb{E}_{z \sim Q(\bullet)} \frac{\sqrt{P(z|\lambda - \delta\lambda/2)P(z|\lambda + \delta\lambda/2)}}{Q(z)} \right) \\ &\simeq \lim_{\delta\lambda \rightarrow 0} \mathbb{E}_Q \frac{2}{\delta\lambda^2} \frac{2 \sinh^2(l\delta\lambda/4)}{\cosh(l\delta\lambda/2)} \simeq \frac{1}{4} \mathbb{E}_{z|\lambda} M(\lambda, 0, z)^2. \end{aligned}$$