

# Statistical Inference in Quantum Computing

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## Introduction

Introduction

## Postulates

States

Evolution

Composite Systems

Measurement

## Statistics

MLE

Statistics in QM

# Motivation

- ▶ Traditional computing: Information sent as bits - 0's and 1's.
- ▶ Quantum computing: Information sent as qubits - these can be 0, 1 or a superposition of 0 and 1
- ▶ Some believe these ideas could lead to very fast computers
- ▶ When measuring system, we have the system in a state with a probability
- ▶ Makes sense therefore to consider questions relating to probabilities and statistics

# State vectors

**Postulate 1:** With every isolated physical system we associate an abstract Hilbert space  $\mathcal{H}$  over the field  $\mathbb{C}$ . The state of the system is exhaustively characterised by a normalised state vector  $|\psi\rangle$ . These state vectors follow the superposition principle.

**Superposition Principle:** If  $|\psi_1\rangle, \dots, |\psi_n\rangle$  are possible state vectors, then any normalised linear combination of these vectors is again a state vector. For example,

$|\psi\rangle = \frac{1}{\sqrt{n}}|\psi_1\rangle + \frac{1}{\sqrt{n}}|\psi_2\rangle + \dots + \frac{1}{\sqrt{n}}|\psi_n\rangle$  is a normalised linear combination of these vectors, and therefore this describes a new state vector.

# Qubits

The simplest quantum system is a *qubit* (QUantum BIT) (also known as the *spin-half* system). A qubit has a two dimensional state space, with orthonormal basis  $\{|0\rangle, |1\rangle\}$ . An arbitrary state vector can therefore be written as

$$|\psi\rangle = a|0\rangle + b|1\rangle,$$

where  $a, b \in \mathbb{C}$  and  $|a|^2 + |b|^2 = 1$ , the normalisation condition. If one imagines that each  $|\psi\rangle$  is an element of  $\mathbb{C}^n$ , one sees that the normalisation condition is equivalent to  $\langle\psi|\psi\rangle = 1$ .

## Density operator

Now let us suppose our finite-dimensional quantum system is prepared in one of a number of states  $\{|\psi_k\rangle\}$ , each with a probability of  $p_k$ , with the probabilities  $p_k$  summing to one. We call  $\{p_k, |\psi_k\rangle\}$  an *ensemble of pure states* and define the following matrix,  $\rho$ , called the *density matrix*, with corresponding operator called the *density operator*.

$$\rho := \sum_k p_k |\psi_k\rangle\langle\psi_k|.$$

A quantum system whose state  $|\psi\rangle$  is known exactly is said to be in a *pure state*. In this case,  $\rho = |\psi\rangle\langle\psi|$ . Otherwise,  $\rho$  is in a *mixed state* and is said to be a *mixture* of the different pure states in the ensemble for  $\rho$ .

# Density Operator vs State Vector

## Theorem

An operator  $\rho$  is the density operator associated to an ensemble  $\{p_k, |\psi_k\rangle\}$  if and only if it satisfies the following conditions:

1.  $\text{tr}(\rho) = 1$
2.  $\rho$  is positive semi-definite

# Alternative Postulate 1

**Postulate 1':** With every isolated physical system we associate an abstract Hilbert space  $\mathcal{H}$  over the field  $\mathbb{C}$ . The system is completely described by its density operator  $\rho$ , which is a positive semi-definite, self-adjoint operator with trace 1 acting on the state space of the system. If the quantum system is in state  $\rho_j$  with probability  $p_j$ , then the density operator associated with the system is

$$\rho = \sum_j p_j \rho_j.$$

## Postulate 2

**Postulate 2:** The evolution of a closed quantum system is described by a unitary transformation. That is, the state  $|\psi_1\rangle$  of the system at time  $t_1$  is related to the state  $|\psi_2\rangle$  of the system at time  $t_2$  by a unitary operator  $U$  which depends only on the times  $t_1$  and  $t_2$ ,

$$|\psi_2\rangle = U|\psi_1\rangle.$$

**Postulate 2':** The time evolution of a closed quantum system is described by the Schrödinger equation,

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle.$$

## Alternative Postulate 2

**Postulate 2''**: The evolution of a closed quantum system is described by a unitary transformation. That is, the state  $\rho_1$  of the system at time  $t_1$  is related to the state  $\rho_2$  of the system at time  $t_2$  by a unitary operator  $U$  which depends only on the times  $t_1$  and  $t_2$ ,

$$\rho_2 = U\rho_1 U^\dagger.$$

## Postulate 3

**Postulate 3:** The state space of a composite physical system is the tensor product of the state spaces of the component physical systems. Moreover, if we have systems numbered 1 through  $n$ , and system number  $k$  is prepared in the state  $\rho_k$ , the joint state of the total system is  $\rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_n$ .

# Entanglement

Suppose we have the following state

$$|\psi\rangle = \frac{|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle}{\sqrt{2}}$$

This state has the property that there are no single qubit states  $|a\rangle$  and  $|b\rangle$  such that  $|\psi\rangle = |a\rangle \otimes |b\rangle$

## Definition

A state of a composite system with the property that it cannot be written as a product of states of its component systems is called an *entangled state*.

# Operator-valued probability measure

## Definition

Let  $(\Omega, \Sigma)$  be a measurable space. An *operator-valued probability measure* (oprom) (a.k.a generalised measurement, positive operator valued measure)  $\mathcal{M}$  is a collection of self-adjoint matrices  $\mathcal{M}(\Gamma)$  ( $\Gamma \in \Sigma$ ) such that the following hold

1.  $\mathcal{M}(\Omega) = I$
2.  $\mathcal{M}(\Gamma)$  is positive semi-definite for all  $\Gamma \in \Sigma$
3. For a sequence  $(\Gamma_n)_n$  of disjoint elements of  $\Sigma$ ,

$$\mathcal{M}\left(\bigcup_n \Gamma_n\right) = \sum_n \mathcal{M}(\Gamma_n).$$

## Postulate 4

**Postulate 4:** A measurement  $\mathcal{M}$  on a  $d$ -dimensional quantum system taking values from a measurable space  $(\Omega, \Sigma)$  is described by an operator-valued probability measure. If a measurement is performed, then the probability distribution of the outcome  $X$  is given by

$$\mathcal{P}(X \in \Gamma) = \text{tr}(\rho \mathcal{M}(\Gamma)),$$

where  $\Gamma \in \Sigma$ .

### Theorem

The probability distribution described in postulate 4 is a probability measure on the measurable space  $(\Omega, \Sigma)$ .

# Likelihood

## Definition

We define the *likelihood function* for the single variable  $X$  to be

$$L(\theta; x) := f(x; \theta).$$

## Definition

We define the *loglikelihood function* for the single variable  $X$  to be

$$l(\theta; x) := \log(L(\theta; x)).$$

# Score and Information

## Definition

We define the *score*  $V(\theta, X)$  for the single variable  $X$  to be

$$V(\theta, X) := I'(\theta; X).$$

Setting the score to zero gives a stationary point of  $I(\theta; x)$  and this gives us one way of finding an estimate  $\hat{\theta}$  of  $\theta$ .

## Definition

We define the *expected Fisher information*  $I_X(\theta)$  in the random variable  $X$  to be

$$I_X(\theta) := \text{Var}(V(\theta; x)).$$

# Cramér-Rao inequality

## Theorem

Let  $(x_1, \dots, x_n)$  be a sample of  $n$  independent observations of a random variable  $X$  whose probability function at  $x$  is  $f(x, \theta)$ , where  $\theta$  is an unknown parameter. Let  $T(x_1, \dots, x_n)$  be an unbiased estimator of  $\theta$ . Then, subject to a set of regularity conditions about the integrals and differentials of  $f$ ,

$$\text{Var}(T) \geq \frac{1}{nI(\theta)}.$$

# Likelihood

Suppose  $\rho = \rho(\theta)$ , where  $\theta$  is some unknown parameter. Suppose  $\mathcal{M}$  is an oprim taking values from a measurable space  $(\Omega, \Sigma)$  describing a measurement on our quantum system. So, by the fourth postulate, we have

$$\mathcal{P}(X \in \Gamma) = \text{tr}(\rho(\theta)\mathcal{M}(\Gamma)),$$

where  $\Gamma \in \Sigma$ . We will define  $\mu$  by

$$\mu(\Gamma) = \text{tr}(\mathcal{M}(\Gamma))$$

and assume that  $M(\Gamma)$  can be written as

$$M(\Gamma) = \int_{\Gamma} m(x)d\mu(x),$$

where  $m$  is a positive semi-definite, self-adjoint operator

We then have that  $\rho$  has probability density with respect to  $\mu$  given by

$$f(x; \theta) = \text{tr}(\rho(\theta)m(x)).$$

Assuming the relevant integrals and derivatives exist, the expected Fisher information will be

$$I_M(\theta) = \mathbb{E}((V(\theta; X))^2) = \int_{\Omega} (V(\theta; X))^2 f(x; \theta) d\mu(x),$$

where  $I(\theta; X) := \log(f(X; \theta))$  is the loglikelihood and  $V(\theta; X) := \frac{\partial}{\partial \theta}(I(\theta; X))$  is the score function.

# Quantum Analogues

## Definition

We define the *quantum score function* (or *symmetric logarithmic derivative*)  $\lambda$  of  $\rho$  with respect to  $\theta$  to be the self-adjoint operator which is the solution to the equation

$$\dot{\rho} = \frac{\partial \rho(\theta)}{\partial \theta} = \frac{1}{2}(\rho\lambda + \lambda\rho).$$

## Definition

The *expected quantum information number*  $I_Q(\theta)$  (also known as the *Helstrom information number*) is defined by

$$I_Q(\theta) := \text{tr}(\rho\lambda^2).$$

# Big Theorem

## Theorem

$$I_M(\theta) \leq I_Q(\theta)$$

## Theorem

If  $T$  is an unbiased estimator of  $\theta$ , then

$$\text{Var}(T) \geq \frac{1}{I_Q(\theta)}.$$