Sensitivity evolution in quantum Hamiltonian estimation

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Abstract: In this paper we investigate the sensitivity evolution in estimating the unknown quantum Hamiltonian parameters. We apply Kullback-Liebler (KL) divergence to quantify the difference of quantum measurements between deviated and authentic parameter values. From explicit formula for the Fisher information matrix (FIM), we can calculate the second order approximation of the KL divergence. For several quantum mechanical systems, we use this analytical method to investigate the sensitivity evolution of estimating the underlying unknown parameters. We find that in all these examples the FIM is divergent, which indicates that it is possible to design an unbiased estimator that yields the unknown parameters precisely.

Keywords: parameter estimation; Fisher information matrix; FIM; sensitivity evolution.

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1 Introduction

In recent years, quantum information processing has made considerably progresses (Nielsen and Chuang, 2001). In many of these applications of quantum technologies, it is a prerequisite condition to know the mathematical model of the physical systems. Because the dynamics of a closed quantum system is dictated by its Hamiltonian, it is of particular interest to identify the real Hamiltonian that conforms to physical theory and experimental data.

For many quantum mechanical systems, people may have *a prior* knowledge about the structure of the Hamiltonian from physical mechanisms and what need to be identified are the unknown parameters within the Hamiltonian. In recent years, many researchers worked on the Hamiltonian parameter estimation and obtained useful results (Burgarth and Yuasa, 2012; Zhang and Sarovar, 2014). For a quantum mechanical system, we can repeatedly prepare the system at the same initial states and then perform the measurements after the system evolves for certain time. Different from the classical systems, the state of a quantum system will collapse after measurement. The result of quantum measurement is a probability distribution and we can repeat the independent measurement for many times to obtain an approximation of this probability distribution. The identification task is to estimate the Hamiltonian parameters from these probability distributions measured at different time instants.

In this paper, we are interested in the sensitivity in estimating the Hamiltonian parameters. In a typical parameter estimation setting, one solves for the unknown system parameters from some given input/output data. For the same input signal, if a small variation about the parameter leads to a relatively large change in the output data, the parameter sensitivity is large and it facilitates better estimation. On the contrary, if variations in the parameters result in little or no change in the output data, it will be very hard to precisely determine the unknown parameter.

Since the results of quantum measurements are probability distributions, we can use Kullback-Liebler (KL) divergence to quantify the difference between the nominal measurement distribution and the perturbed one (Cover and Thomas, 1991). We then expand this divergence to the second order and obtain a quadratic form in terms of perturbations, which naturally introduces the Fisher information matrix (FIM) (Sarovar et al., 2017). For closed quantum system, the FIM can be derived in an analytical manner. The main contribution of this work is to explicitly investigate the parameter estimation sensitivity evolution in quantum Hamiltonian estimation. We investigate several common physical examples and find that in all these examples the FIM are divergent. Because the Cramer-Rao bound (Cover and Thomas, 1991) states that the covariance of an unbiased estimated is lower bounded by the inverse of the FIM divided by the sample number, this implies that it is possible to estimate the parameters precisely.

2 Quantum measurements

In the following, we consider to analyse the sensitivity of identifying the unknown Hamiltonian parameters of a quantum mechanical system. We assume that the dimension of the quantum system is finite and known and the dynamical process can be prepared at some initial states. Further, we assume that the unknown process is governed by unitary evolution, that is, the system has no interaction with its environment.

We express a Hamiltonian that dictates the evolution of a quantum dynamical process as

$$H = \sum_{i=1}^{M} \lambda_i X_i \tag{1}$$

where λ_i are the unknown parameters and X_i are known Hermitian operators. For unitary evolutions, the quantum process is defined on $SU(N)$, the special unitary lie group of unitary matrices with unity determinant. Correspondingly, $iH \in su(N)$, i.e., the Lie algebra consisting of all the $N \times N$ skew-Hermitian matrices. In general, $\{X_n\}$ can be chosen from an orthonormal basis for $su(N)$, where the Hilbert-Schmidt inner product is defined as $\langle X_m, X_n \rangle \equiv \mathrm{tr}(X^{\dagger}_m X_n)$. For example, $\frac{i}{2}\sigma_\alpha^1\sigma_\beta^2$ form a basis for $su(4)$, where σ_α, σ_β can be Pauli matrices σ_x, σ_y, σ_z, or the identity matrix I and superscripts label the qubits. Each element X_k can be considered as an observable for the system since it is Hermitian.

For a quantum system, assume that we can measure an observable O as a function of time. A physically motivated example of such a scenario is where local observables of a collection of spins are measured. We decompose this observable into orthogonal projectors representing individual measurement results:

$$O = \sum_{m=1}^{M} \theta_m P_m \tag{2}$$

where $P_m P_n = P_m \delta_{mn}$.

Denote the initial state of the quantum system as φ_0. When the system evolution is governed by $H(\lambda^0)$, with λ^0 denoting the nominal values of the system parameters, the quantum state at time instant t is given by $e^{-iHt}\varphi_0$. Then if we measure the system with the observable O at time t, the result is a probability distribution

$$p_m(\lambda^0) = \mathrm{tr}\left(P_m e^{-iHt} \varphi_0 \varphi_0^{\dagger} e^{iht}\right) \tag{3}$$

where $m = 1, \ldots, M$.

Assume that we prepare the quantum system for many times and perform a series of independent measurements at different time instants. With sufficiently many measurements, we can obtain approximations of the measurement probability distributions at these time instants. We thus estimate the quantum Hamiltonian parameter from these series of probability distributions.

3 Quantifying parameter estimation sensitivity

In our previous work (Zhang and Sarovar, 2014), we have developed an algorithm to estimate the parameters. However, in that work, we used only the mean values of the probability distributions at different time instants. Since the quantum measurement results are given by a series of probability distributions, dealing with these distributions directly will give us more useful information.

In parameter estimation, we are interested in studying the sensitivity of a particular setup. Given a physical system, we want the input/output data sensitive to the underlying Hamiltonian parameters so that the parameters can be better estimated. Specifically, when a parameter λ is perturbed by a small amount $\Delta\lambda$ around its authentic value λ^0, the measurement probability distribution will change from $p(\lambda^0)$ to $p(\lambda)$ correspondingly. If a small change in the parameter space results in a large change in the measurement probabilities, this means the parameter can be precisely estimated. Note that this is indeed a converse problem of the reliability of analog quantum simulation (AQS) we investigated in Sarovar et al. (2017). In the AQS case, we want the measurement results as insensitive as possible to the underlying parameters so that the parameter uncertainties will not have a significant influence in the final simulation results.

Similar to Sarovar et al. (2017), we use the KL divergence to measure the difference between the measurement probability distributions $p(\lambda)$ and $p(\lambda^0)$:

$$D_{\mathrm{KL}}\left(p_m(\lambda)\|p_m(\lambda^0)\right)=\sum_m p_m(\lambda)\log\frac{p_m(\lambda)}{p_m(\lambda^0)} \tag{4}$$

Assuming that the deviation in parameters from the nominal $\Delta\lambda = \lambda - \lambda^0$ is small, we expand the KL divergence to the second order to obtain

$$D_{\mathrm{KL}}\left(p_m(\lambda)\|p_m(\lambda^0)\right)=\frac{1}{2}\Delta\lambda^T F(\lambda^0)\Delta\lambda+\mathcal{O}\left(\|\Delta\lambda\|^3\right) \tag{5}$$

The first order term vanishes because the sum of a probability distribution is unity. The matrix F is nothing but the FIM for the model and its elements are given by:

$$\begin{aligned}F_{ij}(\lambda^0)&=\left.\frac{\partial^2}{\partial\lambda_j\partial\lambda_i}\right|_{\lambda=\lambda^0} D_{KL}\left(p(\lambda)\|p(\lambda^0)\right)\\&=\sum_{m=1}^{M}p_m(\lambda)\left.\frac{\partial\log p_m(\lambda)}{\partial\lambda_i}\frac{\partial\log p_m(\lambda)}{\partial\lambda_j}\right|_{\lambda=\lambda^0}\\&=\sum_{m=1}^{M}\frac{1}{p_m(\lambda)}\left.\frac{\partial p_m(\lambda)}{\partial\lambda_i}\frac{\partial p_m(\lambda)}{\partial\lambda_j}\right|_{\lambda=\lambda^0}\end{aligned} \tag{6}$$

Note that the FIM is the unique Riemannian metric for the space of probability distributions under some mild conditions (Campbell, 1985) and therefore we can choose any f-divergence and the results are all the same.

Our measurement scheme is to prepare the system and then measure at a specific time instant for many times to get the probability distribution at that time instant. Suppose that at time instant t_k, measuring the observable O results in a probability distribution p_m^k for the measurement results. Combining it with all the probability distributions measured at previous time instants $t = t_1, t_2, \ldots, t_{k-1}$, we obtain the joint probability distribution for the measurement results at these time instants. As time evolves, we get a time series of instant FIMs as well as a cumulative FIM up to certain time instant with respect to λ^0. In the independent measurements with re-preparation case, all the measurements data at different time instants are independent. Therefore, the cumulative FIM based on the measured distribution $p_m^1, p_m^2, \cdots, p_m^k$ is the sum of the FIMs from all the previous instants.

We treat the sensitivity of parameter estimation from the spectral analysis of the FIM associated with quantum measurement results. Consider a set of eigenvalues ζ_k and eigenvectors v_k of F, with k indexing the eigenvalues in descending order. Since F is a symmetric matrix, we have

$$F = \sum_{k=1}^{K} \zeta_k \upsilon_k \upsilon_k^\dagger \tag{7}$$

Then the changes in the measurement probability distributions over a time duration by the perturbation in the parameter λ can be approximated to the second order by

$$\sum_{k=1}^{K} \frac{\zeta_k}{2} \left\| \upsilon_k^\dagger \Delta\lambda \right\|^2 \tag{8}$$

This expression quantifies the sensitivity of quantum measurement results to the Hamiltonian parameters around the authentic value λ^0. The magnitude of an eigenvalue indicates its influence on the measurement probability distribution and the eigenvector implies the influential combination of parameters.

One important result in estimation theory is Cramer-Rao bound (Cover and Thomas, 1991):

$$\mathrm{Cov} T_\lambda(X) \geq \frac{1}{N} F^{-1}(\lambda), \tag{9}$$

where T_λ (X) is an unbiased estimator of λ based on the data X and N is the number of samples. The inverse of the FIM thus gives a lower bound on the covariance matrices of all the possible unbiased estimators.

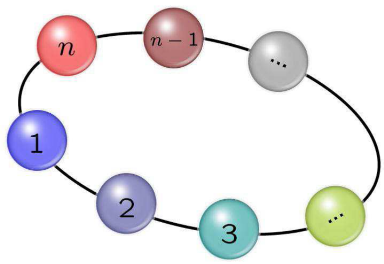
4 Analytical computation of FIM

The cumulative FIM up to the time instant t_k is the sum of all the instant FIMs at previous measured time instants. We now calculate the instant FIM in an analytical manner and then the cumulative FIM can be obtained immediately.

From equation (6), it is critical to calculate the partial derivatives $\frac{\partial p_m(\lambda)}{\partial \lambda_i}$, where $p_m(\lambda)$ is given in equation (3). Then

$$\begin{aligned}\frac{\partial p_m(\lambda)}{\partial \lambda_i} &= \frac{\partial}{\partial \lambda_i}\mathrm{tr}\left(P_m e^{-iHt}\varphi_0\varphi_0^\dagger e^{iHt}\right)\\ &= \mathrm{tr}\left(P_m \frac{\partial e^{-iHt}}{\partial \lambda_i}\varphi_0\varphi_0^\dagger e^{iHt}\right) + \mathrm{tr}\left(P_m e^{-iHt}\varphi_0\varphi_0^\dagger \frac{\partial e^{-iHt}}{\partial \lambda_i}\right)\end{aligned} \tag{10}$$

Figure 1 A periodic Ising ring with transverse field (see online version for colours)



In order to calculate $\frac{\partial e^{-iHt}}{\partial \lambda_i}$, we utilise equation (78) in Najfeld and Havel (1995) to obtain:

$$\frac{\partial e^{-iHt}}{\partial \lambda_k} = -e^{-iHt/2}\int_{-t/2}^{t/2} e^{-iH\tau}H_k e^{iH\tau}d\tau e^{iHt/2} \tag{11}$$

Now we diagonalise the Hamiltonian as

$$H = T\Gamma T^\dagger$$

where T is a unitary matrix of eigenvectors and $\Gamma = \mathrm{diag}\{\gamma_1, \gamma_2, \ldots\}$ is a diagonal matrix of eigenvalues. Substituting this decomposition into equation (11), we get

$$\frac{\partial e^{-iHt}}{\partial \lambda_k} = -Te^{-iHt/2}\int_{-t/2}^{t/2}\left(T^\dagger H_k T\right)\odot\Theta(\tau)d\tau e^{-i\Gamma t/2}T^\dagger$$

where $\odot$ denotes the Hadamard product, i.e., element-wise product and $\Theta_{pq}(\tau) = e^i(\gamma_q - \gamma_p)^\tau$ is the pq-th element of Θ. The τ dependence is entirely in this matrix and therefore we can evaluate this integral to yield:

$$\frac{\partial e^{-iHt}}{\partial \lambda_k} = -Te^{-i\Gamma t/2}\left(\left(T^\dagger H_k T\right)\odot\Phi\right)e^{-i\Gamma t/2}T^\dagger,$$

where Φ is a matrix with elements:

$$\Phi_{pq} = \begin{cases}\frac{\sin\left(\gamma_q - \gamma_p\right)t/2}{\left(\gamma_q - \gamma_p\right)/2}, & \gamma_p \neq \gamma_q;\\ t, & \gamma_p = \gamma_q.\end{cases}$$

Inserting this expression into equation (10) allows us to evaluate the derivatives required to calculate the FIM for thermal states in a manner that is numerically stable.

5 Simulation results

The analytical method to compute the FIM developed in the previous section enables us to investigate parameter estimation problems in several quantum mechanical systems.

First consider an Ising ring with transverse field as shown in Figure 1. The Hamiltonian is given by

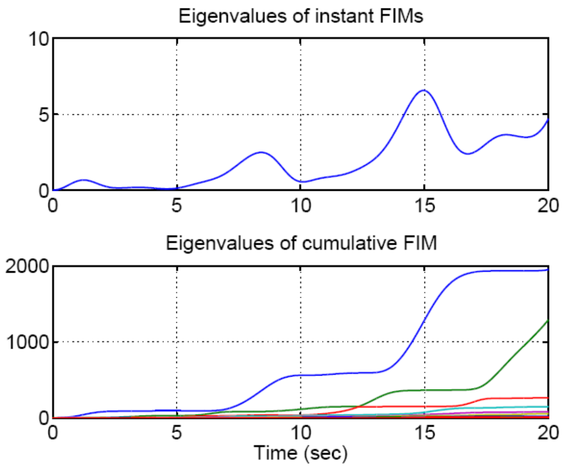
$$H = \sum_{j=1}^{n} B_j \sigma_x^j + \sum_{j=1}^{n} J_j \sigma_z^j \sigma_z^{j+1} \tag{12}$$

where σ_α^j is a Pauli operator with $\alpha \in \{x, y, z\}$ at site j. For the ease of notation, we let $\sigma_z^{n+1} = \sigma_z^1$. The observable to be measured is σ_x^1. It is clear that this observable has only two distinct eigenvalues 1 and −1. The instant FIM can be written as

$$F = [v \quad -v] \begin{bmatrix} \frac{1}{p_1} & \\ & \frac{1}{p_2} \end{bmatrix} \begin{bmatrix} v^T \\ -v^T \end{bmatrix} \tag{13}$$

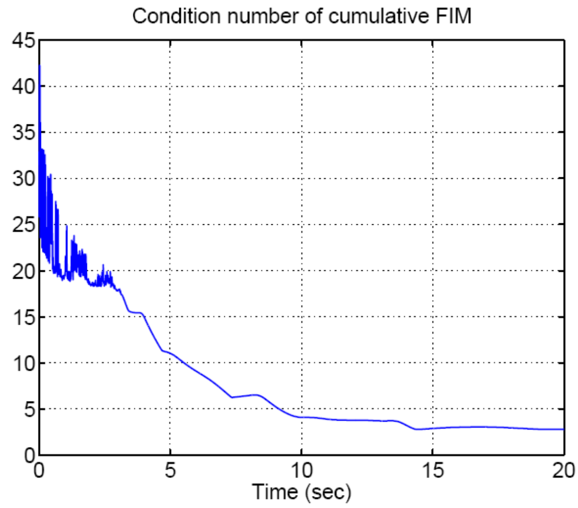
and it has only one non-zero eigenvalue $v^T v/(p_1 p_2)$ with the associated eigenvector v. Furthermore, since the FIM at each time instant is semidefinite positive, the cumulative FIM is also semidefinite positive.

Figure 2 Eigenvalues of the FIM for a periodic Ising ring with transverse field (see online version for colours)



We conduct numerical simulation for a five-qubit ring and show the results in Figure 2. The top plot is the single eigenvalue of the instant FIMs as a function of time and we observe that the eigenvalue fluctuates. In the bottom plot of Figure 2, we show the eigenvalues of the cumulative FIM. It can be observed that the eigenvalues of the cumulative FIM are monotonically increasing as time progresses.

Figure 3 Conditional number of the cumulative FIM (see online version for colours)



We also show the condition number of the cumulative FIM in Figure 3. It becomes stable gradually, which implies that the FIM has full rank and is invertible. From numerical simulations, the cumulative FIM is divergent and thus the right hand side of equation (9) becomes 0. This indicates that the lower bound for the estimator variance can approach 0 and a perfect estimator might be possible.

Figure 4 A 1D Ising chain with transverse field (see online version for colours)

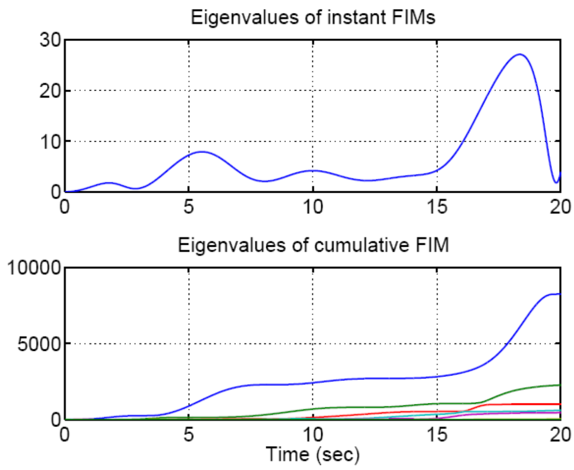
Next consider a 1D Ising chain with transverse field as shown in Figure 4. The Hamiltonian is given by

$$H = \sum_{j=1}^{n} B_j \sigma_x^j + \sum_{j=1}^{n-1} J_j \sigma_z^j \sigma_z^{j+1} \tag{14}$$

and we again measure σ_x^1.

The eigenvalues of the instant and cumulative FIMs are shown in Figure 5. As we can see, changing the boundary condition from periodic to open-end leads to different eigenvalues; however, the general behaviors of the eigenvalues as time evolves are similar: eigenvalues of instant FIMs go up and down whereas eigenvalues of cumulative FIM are monotonically increasing. The eigenvalue of the cumulative FIM is also divergent, which yields the Cramer-Rao bound as 0.

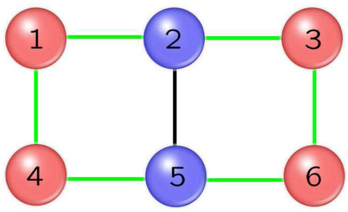
Figure 5 Eigenvalues of the FIM for a 1D Ising chain with transverse field (see online version for colours)



Finally we consider a 2D Ising ladder with transverse field and open-end boundary condition as shown in Figure 6. The Hamiltonian is given by

$$H = \sum_{j=1}^{2n} B_j \sigma_x^j + \sum_{j=1}^{n-1} \left(J_{j1} \sigma_z^j \sigma_z^{j+1} + J_{j2} \sigma_z^{n+j} \sigma_z^{n+j+1} \right) + \sum_{j=1}^{n-1} \left(J_{j3} \sigma_z^j \sigma_z^{n+j} \right) \tag{15}$$

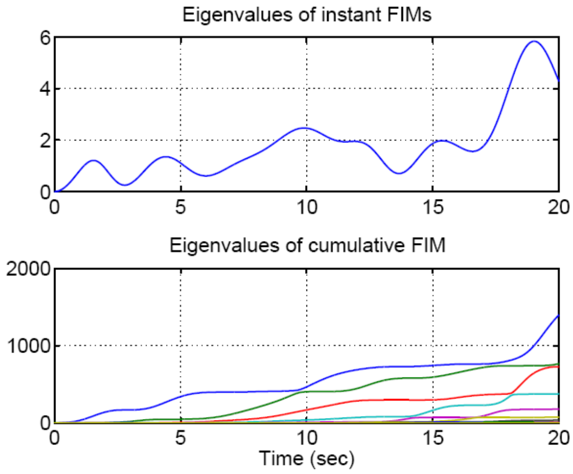
Figure 6 A 2D Ising ladder with transverse field (see online version for colours)



and the observable is again the local operator σ_x^1. The numerical simulation results for a six-qubit ladder are shown in Figure 7.

We observe that the behaviour of the eigenvalues of instant and cumulative FIMs are still similar to the previous two cases. From these numerical examinations, the eigenvalues of the cumulative FIMs are all convergent, which implies the possible existence of an unbiased estimator that can identify the parameters exactly.

Figure 7 Eigenvalues of the FIM for a 2D Ising ladder with transverse field (see online version for colours)



6 Conclusions

In this paper we used the FIM to study the sensitivity evolution of estimating Hamiltonian parameters in quantum mechanical systems. Numerical simulations suggest that the FIM are divergent, which indicates that it is potentially possible to design an unbiased estimator that yields the unknown parameters precisely. Future work includes to study the theoretical problem whether the divergence of the FIM is ubiquitous for all quantum system, as well as to develop unbiased and efficient estimators for Hamiltonian parameter estimation.

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