Quantum state estimation

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New algorithm for quantum state estimation based on the maximum likelihood estimation is proposed. Existing techniques for state reconstruction based on the inversion of measured data are shown to be overestimated since they do not guarantee the positive definiteness of the reconstructed density matrix.

State reconstruction belongs to the topical problems of contemporary quantum theory. This sophisticated technique is trying to determine the maximum amount of information about the system–its quantum state. Even if the history of the problem may be traced back to the early days of quantum mechanics, till quantum optics opened the new era of the state reconstruction. Theoretical prediction of Vogel and Risken was closely followed by the experimental realization of the suggested algorithm by Smithey et. al. Since that time many improvements and new techniques have been proposed, to cite without requirements to completeness at least some titles from the existing literature. Even if the method comes from optics, similar methods are currently being used also in atomic physics as quantum endoscopy. Homodyne detection of quadrature operator with varying phase of local oscillator was used as the measurement in the original proposal. The algorithm served for determination of the Wigner function and other quasiprobabilities representing the density matrix. Measurement of rotated quadrature operator may also be used for direct evaluation of the coefficient of density matrix in number state representation and for the analysis of multimode fields. Simultaneous measurement of the pair of quadrature operators using double homodyne or heterodyne detection yields directly the Q–function representing formally the registered data being in general a multidimensional vector with the components belonging to both the discrete and continuous spectrum as shown in above mentioned examples. The key point of the existing reconstruction techniques–inversion of the relation, represents nontrivial problem. Solution may be formally written as an analytical identity

\[ W_\rho(\alpha) = \int d\xi K(\alpha, \xi) w_\rho(\xi), \tag{2} \]

\( W_\rho(\alpha) \) being a representation of density matrix. In order to find the representation \( W(\alpha) \) of a density matrix corresponding to an unknown signal, the existing reconstruction techniques apply the relation \( (1) \) on the actually detected statistics \( w(\xi) \).

Apart from the fact how ingeniously the individual inversions have been done, this treatment is essentially improper for the application in quantum theory. Particularly, it may represent a density matrix only for such measurable probability distributions, which are given exactly by the relation \( (1) \). Deviations between actually detected \( w(\xi) \) and the true statistics \( w_\rho(\xi) \) are not allowed, since they may spoil the positivity of reconstructed density matrix. This algorithm anticipates therefore the absolute precision impossible in quantum theory. There are at least the following imperfections of detected statistics \( w(\xi) \), which should be taken into account: i) Sampling error caused by the limited number of available scanned positions of continuous variable at which the measurement was done. ii) Counting error caused by limited set of available data counted at each position. For example, in Ref. the former one is caused by the division of quadrature \( x_\phi \) into 64 bins and phase into 27 values, whereas the later one by the detection of quadrature \( x_\phi \) at each bin. Other errors such as imperfections of detectors or external noises, may appear in practise as well. In quantum case the algorithm based on inversion provides a result, but does not guarantee the positive definiteness of the reconstructed density matrix. In the example of Ref. the positive definiteness of reconstructed matrix has not been checked explicitly, but can be judged according to the papers. Here the negative part
of photocount distribution indicates the spoiling of positive definiteness. Even if there is a connection between the dimension of Hilbert space where this happens and the number of phases \( n \), a rigorous way how to treat the positive definiteness within reconstruction has not yet been suggested. As pointed out by Jones \cite{Jones19} in his Ref. 12, the failure of similar methods is the rule rather than the exception in the case where the data underdetermine the solution. This happens also in the case of more dense data, even if the region of ill behaviour is shifted to less obvious manifestations. These methods are considered as satisfactory only because some additional information in the form of data smoothing is used and mathematical difficulties are neglected. Instead of inversion of the detected data, a technique motivated by quantum information theory \cite{Maletzky20, Kitsopoulos21} and by phase shift estimation \cite{Guo22}, will be suggested in this Rapid Communication. Previous reconstruction techniques will be embedded into the common scheme based on maximum likelihood estimation.

Many parameters characterizing the quantum state should be estimated in state reconstruction. As pointed out by Helstrom \cite{Helstrom73} this may be done restricting the dimension of Hilbert space, and accepting some residual uncertainty. Similarly, Jones \cite{Jones19} investigated the fundamental limitations of quantum state measurement using Bayesian methodology. On the contrary, the realistic measurements as in the existing techniques will be anticipated here. Assuming the repeated (or multiple) measurement performed on the \( n \) copies of the system, the output of observation may be parametrized by the set of states (projectors) formally denoted as \( |y_1\rangle, \ldots, |y_m\rangle \), repetition of a particular outcome being allowed. Pure states represent here the case of sharp measurement, whereas unsharp measurement involving the finite resolution should be represented by an appropriate POM. Since formal considerations are valid for both these cases, the notation of sharp measurement will be kept in the following for the sake of simplicity. Maximum likelihood estimation ascribes to such a measurement the state \( \hat{\rho} \) maximizing the likelihood functional

\[
\mathcal{L}(\hat{\rho}) = \prod_i^n (y_i | \hat{\rho} | y_i). 
\]

The aim of this contribution is to find this state and to clarify the fluctuations of such a prediction. As the mathematical tool, the inequality between the geometric and arithmetic averages of non-negative numbers \( q_i \) will be used

\[
(\prod_q^n q_i)^{1/n} \leq \frac{1}{n} \sum_q^n q_i.
\]

The equality is achieved if and only if all the numbers \( q_i \) are equal. The variables will be formally replaced by \( q_i = x_i/a_i \), where \( x_i \geq 0 \) are positive and \( a_i > 0 \) are auxiliary positive nonzero numbers. In the following the \( n \)imensional vectors will be denoted by boldface as \( \mathbf{a}, \mathbf{x}, \mathbf{y} \), etc.. Assume now that the numbers \( q_i \) are chosen from the given set of values so that the value \( q_i \) appears \( k_i \) times in the collection of \( n \) data. Hence \( k_i \) represents the frequency, \( f_i = k_i/n \) being the relative frequency \( \sum_i f_i = 1 \). Parametrization revealing explicitly the frequency will be denoted by upper prime in sums and products, indicating that index runs over spectrum of different values. Without loss of generality the variable \( x \) may be interpreted as probability \( \sum_i x_i = 1 \), since the normalization may always be involved in auxiliary variables \( a \). The relation, known as Jensen’s inequality \cite{Jensen14}, then reads

\[
\prod_i \left[ \frac{x_i}{a_i} \right]^{f_i} \leq \sum_i f_i \frac{x_i}{a_i},
\]

(4)

In this form it represents remarkably powerful relation since the equality sign may be achieved for an arbitrary probability \( x = a \). For example, the Gibbs inequality \cite{Gibbs16} follows as a special case choosing the parameters \( a_i = f_i \), since the inequality (4) may be rewritten as

\[
- \sum_i f_i \ln \frac{x_i}{a_i} \leq 0.
\]

These formal manipulations are tightly connected to the maximization of likelihood function. Using the definition

\[
x_i = (y_i | \hat{\rho} | y_i),
\]

(5)

\( a_i \) being a subject of further considerations, the likelihood functional may be simply estimated as

\[
(\mathcal{L}(\hat{\rho}))^{1/n} = \prod_i \left( (y_i | \hat{\rho} | y_i) \right)^{f_i} \leq \prod_j a_j^{f_j} \text{Tr} \{ \hat{\rho} \hat{R}(y, a) \}. \tag{6}
\]

The operator \( \hat{R} \) is given, in general by nonorthogonal, decomposition as

\[
\hat{R}(y, a) = \sum_i \frac{f_i}{a_i} |y_i\rangle \langle y_i|.
\]

(7)

Relation (6) simply follows from the definition (5) and the inequality (4). Further treatment is distinguished by the following specification of auxiliary parameters \( a \):

Reconstructions of wave function

Condition \( a_i = f_i \) tends to considerable simplifications. Since the measurement need not be complete \( \hat{R}(y, a = f) \leq \hat{1} \), the right-hand side of the relation (6) reads

\[
(\mathcal{L}(\hat{\rho}))^{1/n} = \prod_j f_j^{f_j} \text{Tr} \{ \hat{\rho} \sum_i |y_i\rangle \langle y_i| \} \leq \prod_j f_j^{f_j} \tag{8}
\]

This represents a state-independent upper bound. The necessary condition for equality sign in (6) is given by the conditions \( (y_i | \hat{\rho} | y_i)/a_i = \text{const} \) for any \( i \), whereas the equality sign appears in relation (6) for complete measurements. These relations together with the normalization of relative frequencies tend to the necessary condition for searched state \( \hat{\rho} \)

\[
(y_i | \hat{\rho} | y_i) = f_i.
\]

(9)

This is nothing else as the experimental counterpart of the relation (5) and hence the starting point of reconstruction based on inversion. The relation (5) may be
simply inverted in the case of orthogonal measurements, which may be considered as complete on the given subspace, tending to the solution

\[ \hat{\rho}_f = \sum_i f_i |y_i\rangle\langle y_i|. \quad (10) \]

Unfortunately, such measurements do not reveal information about full density matrix since the nondiagonal elements are lost, as for example in the case of particle number measurement. Techniques dealing with orthogonal measurements are therefore not suitable for full state reconstruction, which should be based on the usage of nonorthogonal states. On the other hand, in these cases the completeness and the existence of a solution of the equation \( \Box \) cannot be guaranteed. Quantum analogy of Gibbs inequality corresponds to overestimated upper bound and tends to the conditions imposed by reconstruction techniques.

**Maximum likelihood estimation**

The problems with existence of a state achieving the upper bound descends obviously from the fixing of the auxiliary parameters \( \mathbf{a} \). The remedy is to keep them free as a subject of further optimization. For any positively defined operator \( \hat{B} = \sum_i \lambda_i |b_i\rangle\langle b_i| \) and density operator \( \hat{\rho} \) the simple Lemma holds

\[ \text{Tr}(\hat{\rho}\hat{B}) \leq \max_i \lambda_i. \quad (11) \]

The quality sign is achieved for density matrix corresponding to the spectral projector of operator \( \hat{B} \) with maximal eigenvalue. Using this Lemma the estimation of the right hand side of the inequality \( \Box \) than reads

\[ (6) \leq \lambda(\mathbf{y}, \mathbf{a}) \prod_i a_i^{f_i}. \quad (12) \]

where \( \lambda(\mathbf{y}, \mathbf{a}) \) denotes formally the maximal eigenvalue of the operator \( \hat{R}(\mathbf{y}, \mathbf{a}) \) with the corresponding eigenvector \( |\psi(\mathbf{y}, \mathbf{a})\rangle \). Equality signs in the chain of inequalities are achieved simultaneously if and only if

\[ \frac{|\langle y_i | \psi(y, a) \rangle|^2}{a_i} = \text{const}, \quad (13) \]

independently on the index \( i \). Finally, maximum likelihood estimation determines the desired state as \( |\psi(\mathbf{y}, \mathbf{a})\rangle \), where vector \( \mathbf{a} \) is given by the solution of the set of nonlinear equations \( \Box \). The uncertainty of such a quantum state estimation may be, according to the Bayesian formulation \( \Box \), characterized by the likelihood functional \( \Box \). Since the interpretation of the probability distribution on the space of states is rather complicated, the uncertainty of the prediction may be involved in an alternative way. The measured data are fluctuating according to the distribution function \( P(y) \) depending on the true state of the system. Fluctuations of quantum state estimates may be represented by the sum of independent contributions

\[ \hat{\rho}_{MLE} = (|\psi(y)\rangle\langle \psi(y)|)_Y = \int dy P(y)|\psi(y)\rangle\langle \psi(y)|. \quad (14) \]

This density matrix shows how closely the maximum likelihood method allows to estimate an unknown state hidden in the measured statistics \( P(y) \). Unfortunately, the proposed method is rather complicated and examples of reconstructions specified above should be solved separately case by case. Considerable technical difficulties may be caused, for example, by possible degeneracy of operator \( B \) reflecting the structure of performed quantum measurement. This particular questions are beyond the scope of this contribution and represent an advanced program for further re-interpretation of existing reconstruction techniques.

Developed technique may be illustrated on simple but theoretically worth examples. Quantum state reconstruction after the measurement of a Hermitian operator with orthogonal spectrum is the simplest problem. Solution corresponds to the application of Gibbs inequality, since the relation \( \Box \) may be solved in this case. Quantum state is then reconstructed after each measurement by the density matrix \( \Box \). This is a consequence of the possible degeneracy of the operator \( \hat{B} \) mentioned above. The treatment based on the Gibbs inequality is overestimated in general. Provided that \( \Box \) is fulfilled in some special cases, then the solution should coincide with the prediction of maximum likelihood estimation.

Simple are also the cases of strongly underdetermined data, when the state is estimated after single detection \( n = 1 \). Assume for concretness the standard “measurement of Q-function” corresponding to detection of coherent states \( |y\rangle = e^{\alpha a^\dagger - y^* a}|0\rangle \). If the value \( y \) is detected, the system is with the highest likelihood just in the state \( |y\rangle \). Provided that system was in coherent state \( |\alpha\rangle \), the output fluctuates as \( |\langle \alpha | y \rangle|^2 / \pi \). Estimation after single detection then yields the density matrix of superposition of coherent signal \( \alpha \) and the thermal noise \( \Box \) with mean number of particles equal to \( 1 \),

\[ \hat{\rho}_{MLE} = \frac{1}{\pi} \int d^2 y e^{-|y - \alpha|^2} |y\rangle\langle y|. \]

Difference between the true state and its estimation is negligible in the case of classical fields, but considerable in quantum domain.

Estimating the quantum state after multiple detection of coherent states, the matrix \( \hat{R} \) should be diagonalized. Using the assumption for eigenstates as \( |\psi\rangle = \sum_i V_i|y_i\rangle \), linear equations for desired coefficients \( V_i \) and eigenvalues \( \lambda \) follow as

\[ \frac{f_k}{\lambda_k} \sum_i V_i C_{ki} = \lambda V_k, \quad (15) \]

where \( C_{ki} = C_{ik}^* = \langle y_k | y_i \rangle, C_{ii} = 1 \). This solution determines the coefficients \( \mathbf{a} \) according to the relation \( \Box \).
as $|\sum_k V_k C_{k\ell}|^2/a_k = \text{const}$ for any index $k$. Let us illustrate this strategy on the case of double detection $n = 2$ yielding the values $y_1$ and $y_2$. Parameters are given as $f_1 = f_2 = 1/2$ and without loss of generality $a_1 = 1, a_1/a_2 = x$. The secular equation for maximal eigenvalue $\lambda$ reads $\lambda^2 - (1 + x)\lambda + x - x|C_{12}|^2 = 0$, yielding easily solutions for maximal eigenvalue and its eigenvector. Equations (13) impose single condition as $|C_{12}| = \sqrt{x(\lambda - 1 + |C_{12}|^2)}$. This nonlinear system of equations may be easily solved yielding expected solution as $\lambda = 1 + |C_{12}|, x = 1$. Projector is given by the normalized Schrödinger cat–like state

$$|\varphi\rangle = \frac{1}{\sqrt{2(1 + |C_{12}|)}}(e^{i\arg C_{12}}|y_1\rangle + |y_2\rangle).$$

Density matrix “reconstructing” the coherent state is then given as

$$\rho_{MLE} = \frac{1}{\pi} \int d^2 y_1 d^2 y_2 e^{-|y_1 - a|^2 - |y_2 - a'|^2}|\varphi\rangle\langle\varphi|.$$ Proposed method describes easily the cases, where the data seem to be underdetermined. There is also a strong effort to apply the developed technique to the case of large data sets estimating properly the quantum state in the cases of realistic measurements.

Even if the problem of positive definiteness used for motivation may seem as nit–picking, it has far-reaching consequences. Reconstruction methods based on inversion of detected data are valid only if complete information is available and fail, if the information is limited by quantum theory. The method based on maximum likelihood suggests, how to treat the state reconstruction in this quantum domain. Since quantum state comprises maximum possible information about the system, its proper description is of fundamental interest. For example, the strategy of indirect measurement observing primarily the wave function and deriving all information about desired variable consequently, represents a general scheme for an universal “measurement of everything”. The fee paid for such an observation should be obviously the accuracy of the detection of a particular observable, since the observation of wave function involves the registration of non–commuting variable, too. The fundamental distinction between universal and accurate measurements may easily disappear provided that an improper description of quantum objects is used. Particularly, this is just the case of existing reconstruction techniques, where “negative probabilities” may appear as a consequence of inadequate semiclassical treatment.

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