Efficient State Estimation for Quantum Systems

László Ruppert

Department of Mathematical Analysis, Budapest University of Technology and Economics, Hungary

Supervisor: Prof. Dénes Petz

2012

Preliminaries

The measurement of a quantum mechanical system is of a probabilistic nature, so even determining a measurable quantity requires statistical methods. This is why state estimation is an important field in quantum information theory [24, 25, 27].

It is well-known that a measurement applied to a quantum system will change the state of it in an irreversible way depending on the measurement outcome. Additionally, D'Ariano and Yuen prove in [15] that it is generally not possible to determine the state of one single quantum system, whatever estimation scheme is used. We use therefore several copies of the same system being in the same state, perform a sequence of measurements, and estimate the unknown state from the outcome statistics. This process is usually called quantum state tomography [13] and can be traced back to the seventies [19, 20]. The problem of state estimation is quite old, however, the interest in a thorough mathematical analysis of quantum state estimation procedures has been flourishing recently [11, 12, 16, 23, 34].

To set up a quantum state estimation two ingredients have to be given: the measurement strategy used to obtain information, and the estimator mapping the measurement data to the state space. Most publications use maximum-likelihood (ML), Bayesian or some other simple method to obtain an estimator from measurement data. For the measurement part the spectrum of approaches is very wide. There are works [10, 18] which perform a single measurement on the compound system from identical copies and obtain optimality in an asymptotic sense. Other authors [28, 29] take measurements independently on states and deal with the properties of the estimate when only a finite number of measurements is available. My thesis takes the latter approach. Furthermore, it presents a new way to incorporate partial information into the state estimation process.

In quantum tomography setups some a priori information about the state can be given in various ways. The most popular subject in this field is state discrimination: in that case we know that the system is in one of several given states, and we would like to determine which one it is [14]. We can have an a priori probability distribution of the true state, too, as another possibility [16]. This thesis considers a setup when we know that the state is in a given subset of the whole state space, i.e., some parameters of the state are given.

The basic ideas of my work can be traced back to the fundamental work of Wooters and Fields in 1989 [35]. They maximized the average information gain of the estimation over the possible true states with respect to the prior distribution, and obtained the optimality of complementary measurements. The heuristic concept of complementarity was born together with quantum theory. A mathematical definition is due to Accardi [9] and Kraus [22]. A recent overview about complementarity can be found in [26]. In our case complementarity means quasiorthogonality of measurements, that is, the traceless parts are orthogonal with respect to the Hilbert-Schmidt inner product.

References [2, 28] mention as a side result the optimality

of the complementary measurement for qubits. This is a much weaker result than the previous one [35], but they optimize a different quantity: instead of maximizing the information gain, they minimize the determinant of the average covariance matrix

$$\det \left\langle \operatorname{Var}\left(\hat{\theta}\right) \right\rangle \to \min. \tag{1}$$

Further investigations of this quantity were carried out in [11], which is the direct premise of my work. They used (1) for proving optimality of complementary measurements in quite general settings, so improved the result of Wooters and Fields. Their approach, however, has its own limitations: they do not consider either the known parameter case, or the single POVM case. But their results suggest that the determinant of the average covariance matrix might be a useful quantity for more complex state estimation scenarios, too.

There are results available for the single POVM case, too, however these approaches are usually different from those using multiple von Neumann measurements. A POVM (Positive Operator Valued Measure) is a set $\{E_i : 1 \le i \le k\}$ of positive operators such that $\sum_i E_i = I$. Let us take a set of projections $P_i, 1 \le i \le k$ such that

$$E_i = \frac{1}{\lambda} P_i$$
 and $\operatorname{Tr} P_i P_j = \mu \quad (i \neq j).$ (2)

The case when we have rank-one projections with $k = n^2$, $\lambda = n$ and $\mu = 1/(n+1)$ is called symmetric informationally complete POVM (SIC-POVM) [36] and is currently a rather popular concept [23, 30, 31]. Zauner showed their existence for $n \leq 5$, there has been some analytic and numerical progress [17, 33], but the existence of a SIC-POVM is still unknown for a general dimension n.

Rehacek, Englert and Kaszlikowski argued that although there are six measurement directions in the standard method, in the qubit case four of them are enough to obtain all possible states [29]. The elements of the POVM were related to the vertices of a regular tetrahedron in Bloch space, which is the well-known example of the SIC-POVM in the qubit case. Scott [32] minimizes the expectation of the squared Hilbert-Schmidt distance to obtain the optimal linear state estimation, proving the optimality of the *n*-dimensional SIC-POVM. I am also interested in the case when some parameters are known, so I generalized Scott's method. As a result I have found examples for the $k < n^2$ case in (2), too.

In my thesis I examine different state estimation scenarios and give the best estimation schemes. I consider the case when we have multiple von Neumann measurements as well as that of a single POVM measurement. I analyze the problem of partial a priori information for qubits and multi-level systems as well. I introduce a new generalization of SIC-POVMs and examine its properties both analytically and numerically.

My main results

1. The quantity: determinant of the average covariance matrix [3, 4]

A density matrix $\rho \in M_n(\mathbb{C})$ has $n^2 - 1$ real parameters. If the parameters $\theta = (\theta_1, \theta_2, \dots, \theta_k)$ are not known, but the others are, we can use this information to estimate $\hat{\theta} = (\hat{\theta}_1, \hat{\theta}_2, \dots, \hat{\theta}_k)$. To obtain optimal state estimation we need an error function $f(\theta, \hat{\theta})$ to minimize. In my work, I mostly (Points 2.-4.) concentrate on minimizing the determinant of the average covariance matrix

$$f(\theta, \hat{\theta}) = \det \left\langle \operatorname{Var} \left(\hat{\theta} \right) \right\rangle \to \min.$$
(3)

This quantity has been used in other works, too, however its full potential has not been explored. A wide range of uses is provided in the thesis: the case of multiple von Neumann measurements, the case of single POVM, even numerical optimization.

2. The multiple von Neumann measurement case [3]

In Section 3.1 we suppose that we have exactly the sufficient number of POVMs with two elements: $\{F_1, I - F_1\}, \{F_2, I - F_2\}, \ldots, \{F_k, I - F_k\}$. If we have a decomposition

$$M_n(\mathbb{C}) = \mathbb{C}I \oplus \mathcal{A} \oplus \mathcal{B},$$

where \mathcal{A} corresponds to the subspace generated by the known, \mathcal{B} to the subspace generated by the unknown parameters, we can summarize the results in the following Theorem:

Theorem 1. If the positive contractions F_1, \ldots, F_k have the same spectrum, then the determinant of the average covariance matrix is minimal if the operators F_1, \ldots, F_k are complementary to each other and to \mathcal{A} .

The main novelty here is the case when some parameters are known. Using this information less measurements are needed, and we also obtain the quasi-orthogonality of measurements to the subspace generated by the known parameters.

3. The single POVM case [3]

In Section 3.2 we cover the case of a single positive operator valued measurement $\{E_1, E_2, \ldots, E_k\}$. In *n* dimensions, analytic results could only be achieved for the case when neither element of the density is assumed to be known.

Theorem 2. If a symmetric informationally complete system exists, the optimal POVM is described by its projections P_i as $E_i = P_i/n \ (1 \le i \le n^2).$

In other words, we proved the optimality of the SIC-POVM, but using the same method and quantity (3) as in the previous, von Neumann case.

We also have a very interesting result in one of the qubit cases:

Theorem 3. The optimal POVM for the unknown Bloch parameters θ_1 and θ_2 can be described by projections P_i , $1 \le i \le 3$:

$$E_i = \frac{2}{3}P_i$$
, $\operatorname{Tr} \sigma_3 P_i = 0$, $\operatorname{Tr} P_i P_j = \frac{1}{4}$ for $i \neq j$.

So if some parameters are known and some unknown the optimal POVM is symmetrical and complementary to the subspace of the known parameters. This theorem is a combination of Theorems 1 and 2. We can think of the optimal measurement as a generalization of SIC-POVMs, hence we named them conditional SIC-POVMs.

4. Numerical algorithm [4]

In order to study the concept of conditional SIC-POVMs, I present a numerical algorithm in Section 3.3.1 that optimizes (3). The algorithm works efficiently, with its help I provided many examples in different scenarios, even analytically:

• I show the first non-trivial example of a conditional SIC-POVM

$$E_{1} = \frac{1}{7} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, E_{2} = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^{6} & \varepsilon^{2} \\ \varepsilon & 1 & \varepsilon^{3} \\ \varepsilon^{5} & \varepsilon^{4} & 1 \end{bmatrix},$$
$$E_{3} = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^{2} & \varepsilon^{3} \\ \varepsilon^{5} & 1 & \varepsilon \\ \varepsilon^{4} & \varepsilon^{6} & 1 \end{bmatrix}, E_{4} = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^{4} & \varepsilon^{6} \\ \varepsilon^{3} & 1 & \varepsilon^{2} \\ \varepsilon & \varepsilon^{5} & 1 \end{bmatrix},$$
$$E_{5} = E_{2}^{\mathsf{T}}, E_{6} = E_{3}^{\mathsf{T}}, E_{7} = E_{4}^{\mathsf{T}},$$

- There is a conditional SIC-POVM containing the diagonal matrix units (which can be extended to any dimension, providing a simple example for existence).
- There is an example for conditional SIC-POVMs that contains projections of rank 2.
- There is an example where no conditional SIC-POVM exists.

These results lead us to the accurate definition of conditional SIC-POVMs:

Definition. $\{E_1, E_2, \ldots, E_k\}$ forms a conditional SIC-POVM, if the elements E_i fulfill the conditions in (2) and they are complementary to the subspace of known parameters.

5. Conditional SIC-POVMs [5]

In Section 3.3.2 we obtain the optimality of conditional SIC-POVMs analytically. But instead of using (3) we minimize the square of the Hilbert-Schmidt distance used in [32]. By generalizing their method to the conditional case we obtain

Theorem 4. In the conditional case, the elements of the optimal POVM can be described as multiples of rank-one projections with the following properties $(1 \le i, j \le k)$:

$$E_i = \frac{n}{k} P_i, \quad \text{Tr} \, P_i P_j = \frac{k-n}{n(k-1)} \quad (i \neq j)$$

and $\text{Tr} \, \sigma_l P_i = 0 \quad (\forall l : \sigma_l \in \mathcal{A}).$

Thus, provided a rank-one conditional SIC-POVM exists, it is also optimal. The constants in (2) are

$$\lambda = \frac{k}{n}, \quad \mu = \frac{k-n}{n(k-1)}.$$

Note that they only depend on the dimensionality of the state and on the number of unknown parameters,

When there is no known parameter (i.e., $k = n^2$), we arrive at the case of SIC-POVMs, so these can be considered special conditional SIC-POVMs. The question whether a conditional SIC-POVM exists is obviously at least as difficult as in the case of common SIC-POVMs, however, the answer is not known for the latter case, either.

Related publications

- K.M. Hangos, L. Ruppert: State estimation methods using indirect measurements, Quantum Probability and Related Topics, World Scientific, p. 163-180, 2011
- D. Petz, K.M. Hangos and L. Ruppert, *Quantum state tomography with finite sample size*, in Quantum Bio-Informatics, eds. L. Accardi, W. Freudenberg, M. Ohya, World Scientific, pp. 247–257, 2008.
- [3] D. Petz and L. Ruppert, Efficient quantum tomography needs complementary and symmetric measurements, accepted for publication in Rep. Math. Phys., http://arxiv.org/abs/1011.5210
- [4] D. Petz and L. Ruppert, Optimal quantum state tomography with known parameters, Journal of Physics A: Math. Theor. 45, 085306, 2012.
- [5] D. Petz, L. Ruppert and A. Szántó, Conditional SIC-POVMs, to be published, http://arxiv.org/abs/1202.5741
- [6] L. Ruppert, A. Magyar, K.M. Hangos, Compromising non-demolition and information gaining for qubit state estimation, Quantum Probability and Related Topics, World Scientific, p. 212-224, 2008.
- [7] L. Ruppert, K.M. Hangos: Martingale approach in quantum state estimation using indirect measurements, Proceedings of the 19th International Symposium on Mathematical Theory of Networks and Systems, p. 2049-2054, 2010.
- [8] L. Ruppert, D. Virosztek, K.M. Hangos Optimal parameter estimation of Pauli channels, accepted for publication in Journal of Physics A: Math. Theor.

Other publications

- [9] L. Accardi, Some trends and problems in quantum probability, in Quantum probability and applications to the quantum theory of irreversible processes, eds. L. Accardi, A. Frigerio and V. Gorini, Lecture Notes in Math. 1055, 1–19. Springer, 1984.
- [10] E. Bagan, M.A. Ballester, R.D. Gill, A. Monras and R. Munoz-Tapia, Optimal full estimation of qubit mixed states, Phys. Rev. A, 73, 032301, 2006.
- [11] T. Baier and D. Petz, Complementarity and state estimation, Rep. Math. Phys., 65, 203–214, 2010.
- [12] M. Cramer, M. B. Plenio, S. T. Flammia, D. Gross, S. D. Bartlett, R. Somma, O. Landon-Cardinal, Y.-K. Liu, D. Poulin, *Efficient quantum state tomography*, Nat. Commun., **1** (9) 149, 2010.
- [13] G. M. D'Ariano, M. G. A. Paris, and M. F. Sacchi, *Quantum tomog-raphy*, Advances in Imaging and Electron Physics, **128**, 205-308, 2003.
- [14] G. M. D'Ariano, M. F. Sacchi, J. Kahn, Minimax quantum state discrimination, Phys. Rev. A, 72, 032310, 2005.
- [15] G.M. D'Ariano and H.P. Yuen, Impossibility of measuring the wave function of a single quantum system, Physical Review Letters, 76, 2832– 2835, 1996.
- [16] R. Demkowicz-Dobrzanski, Beyond quantum Fisher information: optimal phase estimation with arbitrary a priori knowledge, Phys. Rev. A, 83, 061802, 2011.
- [17] S. T. Flammia, On SIC-POVMs in prime dimensions, J. Phys. A: Math. Gen. 39 13483, 2006.
- [18] M. Hayashi and K. Matsumoto, Asymptotic performance of optimal state estimation in quantum two level system, J. Math. Phys. 49, 102101, 2008.

- [19] C. W. Helstrøm, Quantum decision and estimation theory, Academic Press, New York, 1976.
- [20] A. S. Holevo, Probabilistic and statistical aspects of quantum theory, North-Holland, 1982.
- [21] K. Jacobs and D. A. Steck, A straightforward introduction to continuous quantum measurement, Contemporary Physics 47, 279, 2006.
- [22] K. Kraus, Complementary observables and uncertainty relations, Phys. Rev. D (3) 35, 3070–3075, 1987.
- [23] Z. E. D. Medendorp, F. A. Torres-Ruiz, L. K. Shalm, G. N. M. Tabia, C. A. Fuchs, A. M. Steinberg, *Experimental characterization of qutrits* using SIC-POVMs, Phys. Rev. A 83, 051801, 2011.
- [24] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, Cambridge, 2000.
- [25] M. Paris and J. Rehacek, *Quantum State Estimation*, Springer-Verlag, Berlin, 2004.
- [26] D. Petz, Algebraic complementarity in quantum theory, J. Math. Phys. 51, 015215, 2010.
- [27] D. Petz, Quantum Information Theory and Quantum Statistics, Springer-Verlag, Heidelberg, 2008.
- [28] D. Petz, K.M. Hangos, A. Magyar, Point estimation of states of finite quantum systems, J. Phys. A: Math. Theor., 40, 7955-7969, 2007.
- [29] J. Rehacek, B-G. Englert and D. Kaszlikowski, *Minimal qubit tomog-raphy*, Physical Review A, **70**, 052321, 2004.
- [30] M. Renes, R. Blume-Kohout, A. J. Scott and C. M. Caves, Symmetric informationally complete quantum measurements, J. Math. Phys. 45, 2171, 2004.

- [31] M. B. Ruskai, Some connections between frames, mutually unbiased bases, and POVM's in quantum information theory, Acta Appl. Math. 108, 709–719, 2009.
- [32] A. J. Scott, Tight informationally complete quantum measurements, J. Phys. A 39, 13507, 2006.
- [33] A. J. Scott and M. Grassl, SIC-POVMs: A new computer study, J. Math. Phys. 51, 042203, 2010.
- [34] Y. S. Teo, H. Zhu, B.-G. Englert, J. Rehacek, Z. Hradil, *Knowledge and ignorance in incomplete quantum state tomography*, Phys. Rev. Lett. 107, 020404, 2011.
- [35] W.K. Wooters and B.D. Fields, Optimal state determination by mutually unbiased measurements, Annals of Physics, 191, 363–381, 1989.
- [36] G. Zauner, Quantendesigns Grundzüge einer nichtkommutativen Designtheorie, PhD thesis (University of Vienna), 1999.