Conclusive Exclusion of Quantum States

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In the task of quantum state exclusion we consider a quantum system, prepared in a state chosen from a known set. The aim is to perform a measurement on the system which can conclusively rule that a subset of the possible preparation procedures can not have taken place. We ask what conditions the set of states must obey in order for this to be possible and how well we can complete the task when it is not. Interestingly, the task of quantum state discrimination forms a subclass of this set of problems. Within this paper we formulate the general problem as a Semidefinite Program (SDP), enabling us to derive sufficient and necessary conditions for a measurement to be optimal. Furthermore, we obtain a necessary condition on the set of states for exclusion to be achievable with certainty. This task of conclusively excluding states has recently been considered with respect to the foundations of quantum mechanics in a paper by Pusey, Barrett and Rudolph (PBR). Motivated by this, we use our SDP to derive a bound on how well a class of hidden variable models can perform at a particular task, proving the necessity of a bound given by PBR in the process.

Introduction. Suppose we are given a single-shot device, guaranteed to prepare a system in a quantum state chosen at random from a finite set of k known states. In the quantum state discrimination problem, we would attempt to identify the state that has been prepared. It is a well known result [1] that this can be done with certainty if and only if all of the states in the set of preparations are orthogonal to one another. By allowing inconclusive measurement outcomes [2–4] or accepting some error probability [5], strategies can be devised to tackle the problem of discriminating between non-orthogonal states. For a recent review of quantum state discrimination, see [6]. What however, can we deduce about the prepared state with certainty?

Through state discrimination we effectively attempt to increase our knowledge of the system so that we progress from knowing it is one of k possibilities to knowing it is one particular state. We reduce the size of the set of possible preparations that could have occurred from k to 1. A related, and less ambitious task, would be to exclude m preparations from the set, reducing the size of the set of potential states from k to $k-m$. If we rule out the m states with certainty we say that they have been conclusively excluded. Conclusive exclusion of a single state has previously been considered with respect to quantum state compatibility criteria between three parties [7] and investigating the plausibility of ψ-epistemic theories describing quantum mechanics [8].

As recognized in [8] for the case of single state exclusion, the problem of conclusive exclusion can be formulated in the framework of Semidefinite Programs (SDPs). As well as being efficiently numerically solvable, SDPs also offer a structure that can be exploited to derive statements about the underlying problem they describe [9, 10]. This has already been applied to the problem of state discrimination [11–13]. Given that minimum error state discrimination forms a subclass ($m=k-1$) of the general exclusion framework, it is reasonable to expect that a similar approach will pay dividends here.

State Exclusion SDP. More formally, what does it mean to be able to perform conclusive exclusion? We first consider the case of single state exclusion and then show how it generalizes to m-state exclusion. Let the set of possible preparations on a d dimensional quantum system be $\mathcal{P}=\{\rho_i\}_{i=1}^k$ and let each preparation occur with probability p_i. For brevity of notation we define $\tilde{\rho}_i=p_i\rho_i$. Call the prepared state σ. The aim is to perform a measurement on σ so that, from the outcome, we can state $j\in\{1,\dots,k\}$ such that $\sigma\neq\rho_j$.

Such a measurement will consist of k measurement operators, one for attempting to exclude each element of $\mathcal{P}$. We want a measurement, described by $\mathcal{M}=\{M_i\}_{i=1}^k$, that never leads us to incorrectly produce j such that $\sigma=\rho_j$. We need, $\forall i:\ \mathrm{Tr}\left[\rho_i M_i\right]=0$, or equivalently, since ρ_i and M_i are positive semidefinite matrices and p_i is a positive number: $\alpha=\sum_{i=1}^k \mathrm{Tr}\left[\tilde{\rho}_i M_i\right]=0$. There will be some instances of $\mathcal{P}$ for which an $\mathcal{M}$ can not be found to satisfy this equation. In these cases our goal is to minimize α. The value we achieve is the probability of failure of the strategy, 'If outcome j occurs say $\sigma\neq\rho_j$'.

Therefore, to obtain the optimal strategy for single state exclusion, our goal is to minimize α over all possible $\mathcal{M}$ subject to $\mathcal{M}$ forming a valid measurement. Such an optimization problem can be formulated as an SDP:

$$\begin{aligned}\underset{\mathcal{M}}{\text{Minimize:}}\ & \alpha=\sum_{i=1}^k \mathrm{Tr}\left[\tilde{\rho}_i M_i\right].\\ \text{Subject to:}\ & \sum_{i=1}^k M_i=\mathbb{I},\\ & M_i\geq 0,\quad \forall i.\end{aligned} \tag{1}$$

Here $\mathbb{I}$ is the d by d identity matrix and $A\geq 0$ implies that A is a positive semidefinite matrix.

Part of the power of the SDP formalism lies in how it is possible to construct a related 'dual' problem to this 'primal' problem given in Eq. (1). Details on the formation of the dual problem to the exclusion SDP can be found in the full version of the paper (submitted separately) and we state it here:

$$\begin{aligned} \underset{N}{\text{Maximize:}} \ & \beta = \mathrm{Tr}\,(N)\,. \\ \text{Subject to:} \ & N \leq \tilde{\rho}_i, \quad \forall i, \\ & N \in \text{Herm}. \end{aligned} \tag{2}$$

For single state exclusion, the problem is essentially to maximize the trace of a Hermitian matrix N subject to $\tilde{\rho}_i - N$ being a positive semidefinite matrix, $\forall\ i$.

What of m-state conclusive exclusion? Define $Y_{(k,m)}$ to be the set of all subsets of the integers $\{1,\ldots,k\}$ of size m. The aim is to perform a measurement on σ such that from the outcome we can state a set, $Y \in Y_{(k,m)}$, such that $\sigma \notin \{\rho_y\}_{y\in Y}$. Such a measurement, denoted $\mathcal{M}_m$, will consist of $\binom{k}{m}$ measurement operators and we require, for each set Y: $\mathrm{Tr}\,[\tilde{\rho}_y M_Y] = 0, \quad \forall y \in Y$. If we define $\hat{\rho}_Y = \sum_{y\in Y} \tilde{\rho}_y$, then this can be reformulated as requiring: $\forall Y \in Y_{(k,m)} : \mathrm{Tr}\,[\hat{\rho}_Y M_Y] = 0$. Hence we can view m-state exclusion as single state exclusion on the set $\mathcal{P}_m = \{\hat{\rho}_Y\}_{Y\in Y_{(k,m)}}$. Furthermore, we can generalize this approach to an arbitrary collection of subsets that are not necessarily of the same size. With this in mind we restrict ourselves to considering single state exclusion in all that follows.

Let us define the optimum solution to the primal problem to be α^* and the solution to the corresponding dual to be β^*. It is a property of all SDPs, known as weak duality, that $\beta^* \leq \alpha^*$. Furthermore, for SDPs satisfying certain conditions, $\alpha^* = \beta^*$ and this is known as strong duality. The exclusion SDP does fulfill these criteria, as shown in the full version of the paper.

Optimal exclusion measurement. We obtain the following characterization of the optimal solutions of the primal and dual SDPs.

Theorem 1. *Let $\mathcal{M}^* = \{M_i^*\}_{i=1}^k$ be an optimal solution to the primal SDP (1) and N^* be an optimal solution to the dual SDP (2). Then, $N^* = \sum_{i=1}^k [\tilde{\rho}_i M_i^*]$.*

The proof of Theorem 1 (and of subsequent results in this work) is given in the full version of the paper. This result provides us with a method for proving a measurement $\mathcal{M} = \{M_i\}_{i=1}^k$ is optimal; show that $N = \sum_{i=1}^k [\tilde{\rho}_i M_i]$ is feasible for the dual problem. We use this technique in the proof of Theorem 3 mentioned later.

Necessary condition for single state conclusive exclusion. We note that for any feasible solution N of the dual SDP (2) we will have $\mathrm{Tr}\,(N) \leq \beta^* = \alpha^*$. In particular if, for a given $\mathcal{P}$, we can construct a feasible N with $\mathrm{Tr}\,(N) > 0$, then we have $\alpha^* > 0$ and hence conclusive exclusion is not possible. We construct one such N and it gives rise to the following necessary condition.

Theorem 2. *Suppose a system is prepared in the state σ using a preparation chosen at random from the set $\mathcal{P} = \{\rho_i\}_{i=1}^k$. Single state conclusive exclusion is possible only if:*

$$\sum_{j\neq l=1}^{k} F(\rho_j, \rho_l) \leq k(k-2), \tag{3}$$

where $F(\rho_j, \rho_l)$ is the fidelity between states ρ_j and ρ_l.

Note that the probability with which states are prepared, $\{p_i\}_{i=1}^k$, does not impact on whether conclusive exclusion is possible or not.

This is only a necessary condition for single state conclusive exclusion and there exist sets of states, $\mathcal{P}$, that satisfy Eq. (3) for which it is not possible to perform conclusive exclusion. Nevertheless, there exist sets of states on the cusp of satisfying Eq. (3) for which conclusive exclusion is possible. For example, the set of states of the form: $|\psi_i\rangle = \sum_{j\neq i}^k \frac{1}{\sqrt{k-1}} |j\rangle$, for $i = 1$ to k, can be conclusively excluded by the measurement in the orthonormal basis $\{|i\rangle\}_{i=1}^k$ and yet $\sum_{j\neq l=1}^k F\left(|\psi_j\rangle\langle\psi_j|, |\psi_l\rangle\langle\psi_l|\right) = k(k-2)$.

Furthermore, if we consider state discrimination as $(k-1)$-state exclusion, we reproduce the following result:

Corollary 1. *Conclusive state discrimination on the set $\mathcal{P} = \{\rho_i\}_{i=1}^k$ is possible only if $\mathcal{P}$ is an orthogonal set.*

PBR game. As an application of our SDP and its properties we consider a game, motivated by the argument, due to PBR [8], against a class of hidden variable theories. Assume that we have a physical theory, not necessarily that of quantum mechanics, such that, when we prepare a system, we describe it by a state, χ. If our theory were quantum mechanics, then χ would be identified with $|\psi\rangle$, the usual quantum state. Furthermore, suppose that χ does not give a complete description of the system. We assume that such a description exists, although it may always be unknown to us, and denote it λ. As χ is an incomplete description of the system, it will be compatible with many different complete states. We denote these states $\lambda \in \Lambda_\chi$. PBR investigate whether for distinct quantum descriptions, $|\psi_0\rangle$ and $|\psi_1\rangle$, it is possible that $\Lambda_{|\psi_0\rangle} \cap \Lambda_{|\psi_1\rangle} \neq \emptyset$. Models that satisfy this criteria are called ψ-epistemic, see [14] for a full description.

Consider the following game. Alice gives Bob n systems whose preparations are encoded by the string $\vec{x} \in \{0,1\}^n$. The state of system i is χ_{x_i}. Bob's goal is to produce a string $\vec{y} \in \{0,1\}^n$ such that $\vec{x} \neq \vec{y}$.

In the first scenario, where Bob can only observe each system individually and we consider a general theory, we can represent his knowledge of the global system by: $\Omega = \lambda_1 \otimes \ldots \otimes \lambda_n$, where $\lambda_i \in \{\Lambda_0, \Lambda_1, \Lambda_?\}$, representing his three possible observation outcomes. If $\lambda_i \in \Lambda_0$ he is certain the system preparation is described by χ_0, if $\lambda_i \in \Lambda_1$ he is certain the system preparation is described by χ_1 and if $\lambda_i \in \Lambda_?$ he remains uncertain whether the system was prepared in state χ_0 or χ_1 and he may make an error in assigning a preparation to the system. We denote the probability that Bob, after performing his observation, assigns the wrong preparation description to the system, q. Provided $\Lambda_? \neq \emptyset$, $q > 0$.

Bob will win the game if for at least one individual system he assigns the correct preparation description. His strategy is to attempt to identify each value of x_i and choose y_i such that $y_i \neq x_i$. Bob's probability of outputting a winning string is hence: $P^S_{win} = 1 - q^n$.

Now consider the second scenario where the theory is quantum and entangled measurements on the global system are allowed. We can write the global state that Alice gives Bob, labeled by $\vec{x}$, as: $|\Psi_{\vec{x}}\rangle = \bigotimes_{i=1}^n |\psi_{x_i}\rangle$. Bob's task can now be regarded as attempting to perform single state conclusive exclusion on the set of states $\mathcal{P} = \{|\Psi_{\vec{x}}\rangle\langle\Psi_{\vec{x}}|\}_{\vec{x}\in\{0,1\}^n}$; he outputs the string associated to the state he has excluded to have the best possible chance of winning the game.

To calculate his probability of winning, P^E_{win}, we need to construct and solve the associated SDP. Without loss of generality, we can take the states $|\psi_0\rangle$ and $|\psi_1\rangle$ to be defined as:

$$\begin{aligned} |\psi_0\rangle &= \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)|1\rangle, \\ |\psi_1\rangle &= \cos\left(\frac{\theta}{2}\right)|0\rangle - \sin\left(\frac{\theta}{2}\right)|1\rangle, \end{aligned} \tag{4}$$

where $0 \leq \theta \leq \pi/2$. The global states, $|\Psi_{\vec{x}}\rangle$, are then given by:

$$|\Psi_{\vec{x}}\rangle = \sum_{\vec{r}} (-1)^{\vec{x}\cdot\vec{r}} \left[\cos\left(\frac{\theta}{2}\right)\right]^{n-|\vec{r}|} \left[\sin\left(\frac{\theta}{2}\right)\right]^{|\vec{r}|} |\vec{r}\rangle, \tag{5}$$

where $\vec{r} \in \{0,1\}^n$ and $|\vec{r}| = \sum_{i=1}^n r_i$.

From [8], we know that single state conclusive exclusion can be performed on this set of states provided θ and n satisfy the condition: $2^{1/n} - 1 \leq \tan\left(\frac{\theta}{2}\right)$. When this relation holds, $P^E_{win} = 1$. What however, happens outside of this range? Whilst strong numerical evidence is given in [8] that it will be the case that $P^E_{win} < 1$, can it be shown analytically? Indeed we show it is true.

Theorem 3. *If* $2^{1/n} - 1 > \tan\left(\frac{\theta}{2}\right)$ *then,*

$$P^E_{win} = 1 - \frac{1}{2^n}\left[\cos\left(\frac{\theta}{2}\right)\right]^{2n}\left(2 - \left[1 + \tan\left(\frac{\theta}{2}\right)\right]^n\right)^2 < 1.$$

The result above can be seen as similar in spirit to Tsirelson's bound [15] in describing how well quantum mechanical strategies can perform at the CHSH game.

What is the relation between P^S_{win} and P^E_{win}? If, in the separable scenario, we take the physical theory as being quantum mechanics and Bob's error probability as arising from the fact that it is impossible to distinguish between non-orthogonal quantum states, we can write $q = \left(\frac{1}{2}\right)(1 - \sin(\theta))$ [5]. With this substitution we find that $P^S_{win} \leq P^E_{win}$, $\forall n$. This is unsurprising as the first scenario is essentially the second but with a restricted set of allowable measurements.

Of more interest however, is if we view q as arising from some hidden variable completion of quantum mechanics. If $\Lambda_? = \emptyset$, then if an observation of each $|\psi_{x_i}\rangle$ were to allow us to deduce λ_{x_i} then $q = 0$ and $P^S_{win} = 1 \geq P^E_{win}$. However, if $\Lambda_? \neq \emptyset$, then we have $q > 0$ and P^S_{win} will have the property that Bob wins with certainty only as $n \to \infty$. On the other hand, $P^E_{win} = 1$ if and only if $2^{1/n} - 1 \leq \tan\left(\frac{\theta}{2}\right)$. Hence, we have defined a game that allows the quantification of the difference between the predictions of general physical theories, including those that attempt to provide a more complete description of quantum mechanics, and those of quantum mechanics.

Conclusion. In this paper we have introduced the task of state exclusion and shown how it can be formulated as an SDP. Using this we have derived conditions for measurements to be optimal and a criteria for the task to be performed conclusively on a given set of states. Furthermore, we have applied our SDP to a game which helps to quantify the differences between quantum mechanics and a class of hidden variable theories.

It is an open question, posed in [7], whether a POVM ever outperforms a projective measurement in conclusive exclusion of a single pure state. Whilst it can be shown from the SDP formalism that this is not the case when conclusive exclusion is not possible to the extent that $\mathrm{Tr}[M_i\rho_i] > 0$, $\forall i$, further work is required to extend it and answer the above question. It would also be interesting to see whether it is possible to find further constraints, similar to Theorem 2, to characterize when conclusive exclusion is possible.

Finally, our SDP, as given in Eq. (1), is just one method for analyzing state exclusion in which we attempt to minimize the average probability of error. Alternative formulations would be unambiguous state exclusion and attempting to minimize the worst case error. We give the primal and dual problems for these SDPs in the full version of the paper and it would be interesting to study the relationships between them and that defined in Eq. (1).

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