When is the lower bound saturated?

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Let $\{o_i\}$ be an arbitrary assignment of numerical outcomes to a 3-design reference device in quantum theory. Let $O = \sum_i o_i E_i$ be the corresponding operator. The resolution of the identity $A = \sum_{ij} \Phi_{ij} \text{tr}(E_j A)\sigma_i$ tells us that

$$\text{tr}(O^2\rho) = \left(\frac{d}{n}\right) \sum_{ijkl} o_i o_j \Re[\text{tr}(E_i\sigma_j\sigma_k)]\Phi_{kl} P(E_l|\rho). \tag{0.1}$$

An unbiased 3-design has the remarkable property that

$$\begin{aligned}\Re\big[\text{tr}(E_i\sigma_j\sigma_k)\big] = \frac{1}{2}\Bigg[&(d+1)(d+2)\left(\frac{n}{d}\right)\sum_m P(E_i|\sigma_m)P(E_j|\sigma_m)P(E_k|\sigma_m) \\ &- P(E_j|\sigma_k) - P(E_i|\sigma_j) - P(E_i|\sigma_k) - \frac{d}{n}\Bigg].\end{aligned} \tag{0.2}$$

A little algebra later

$$\begin{aligned}\text{tr}(O^2\rho) = \frac{1}{2}\Bigg[&(d+1)(d+2)\sum_k \left(\sum_i P(E_k|\sigma_i)o_i\right)^2 P(E_k|\rho) \\ &- \left(\frac{d}{n}\right)\sum_{ij} o_i P(E_i|\sigma_j) o_j - 2d\langle O|\mu\rangle\langle O|\rho\rangle - d^2\langle O|\mu\rangle^2\Bigg],\end{aligned} \tag{0.3}$$

where $\langle O|\rho\rangle = \sum_i o_i P(E_i|\rho)$, and $\langle O|\mu\rangle = \frac{1}{n}\sum_i o_i$.

We can further simplify this formula if we assume $o \in S = \text{col}(P)$. By the 2-design property,

$\sum_j P(E_i|\sigma_j)\text{tr}(A\sigma_j) = n\text{tr}\left(\frac{1}{n}\sum_j \sigma_j^{\otimes 2}(E_i \otimes A)\right) = \frac{n}{d(d+1)}\text{tr}\big((I+\mathcal{S})(E_i \otimes A)\big) = \frac{1}{d+1}\big(\text{tr}(A) + \text{tr}(A\sigma_i)\big)$

, so that in particular,

$$\sum_j P(E_i|\sigma_j)o_j = \frac{1}{d+1}\big(d\langle O|\mu\rangle + o_i\big) \tag{0.4}$$

$$\left(\sum_j P(E_i|\sigma_j)o_j\right)^2 = \frac{1}{(d+1)^2}\left(d^2\langle O|\mu\rangle^2 + 2d\langle O|\mu\rangle o_i + o_i^2\right) \tag{0.5}$$

$$\sum_{ij} o_i P(E_i|\sigma_j)o_j = \frac{n}{d+1}\big(d\langle O|\mu\rangle^2 + \langle O^2|\mu\rangle\big), \tag{0.6}$$

from which we obtain

$$\mathrm{tr}(O^2\rho) = \frac{1}{2}\left(\frac{d+2}{d+1}\right)\left[\langle O^2|\rho\rangle - \frac{d}{d+2}\big(\langle O^2|\mu\rangle - 2\langle O|\mu\rangle\langle O|\rho\rangle\big)\right], \tag{0.7}$$

relating the second-moments of, on the one hand, a von Neumann measurement of O, and on the other, a reference device measurement of it—which, flipped around, is

$$\langle O^2|\rho\rangle = \frac{d}{d+2}\big(\langle O^2|\mu\rangle - 2\langle O|\mu\rangle\langle O|\rho\rangle\big) + 2\left(\frac{d+1}{d+2}\right)\mathrm{tr}(O^2\rho). \tag{0.8}$$

Thus if we consider the inequality

$$\forall x \in S : \langle O^2|\rho\rangle \geq \frac{d}{d+2}\Big[\langle O^2|\mu\rangle - 2\langle O|\mu\rangle\langle O|\rho\rangle\Big], \tag{0.9}$$

it is saturated iff $\mathrm{tr}(O^2\rho) = 0$. Since O is diagonalizable, this implies that $\mathrm{tr}(O\rho) = 0$. Now how can it be that a quantum mechanical observable has zero variance? Suppose O and ρ can be simultaneously diagonalized, that is, they commute $[O,\rho] = 0$. Then we can write $O = \sum_i \alpha_i \Pi_i$, $\rho = \sum_i \beta_i \Pi_i$ for some common set of projectors $\{\Pi_i\}$. The interpretation is that α_i are the numerical outcomes of the von Neumann measurement, and β_i are the probabilities for each outcome, given the preparation ρ. The variance will be zero if α and β have disjoint support. In fact, then $O\rho = 0$. *Can this happen in any other way?* Thus if ρ is a pure state, O may have at most rank-$(d-1)$, whereas if ρ is full rank, the only observable which gives equality is 0. Thus for example, when ρ is rank-1, $O = I - \rho$ will saturate the lower bound.

Finally, we observe that since the first moment with respect to a von Neumann measurement and the first moment with respect to the reference device agree, saturation of the inequality implies that $\langle O^2|\rho\rangle = \frac{d}{d+2}\langle O^2|\mu\rangle$, or

$$\begin{aligned}&\frac{d}{d+2}\big(\langle O^2|\mu\rangle - 2\langle O|\mu\rangle\langle O|\rho\rangle\big) + 2\left(\frac{d+1}{d+2}\right)\mathrm{tr}(O^2\rho) \\ &= \frac{d}{d+2}\left[\frac{d}{d+2}\big(\langle O^2|\mu\rangle - 2\langle O|\mu\rangle\langle O|\mu\rangle\big) + 2\left(\frac{d+1}{d+2}\right)\mathrm{tr}(O^2\mu)\right],\end{aligned} \tag{0.10}$$

which simplifies to $\langle O^2|\mu\rangle = (d+1)\mathrm{tr}(O^2\mu)$, or $\langle O^2|\rho\rangle = \left(\frac{d+1}{d+2}\right)\mathrm{tr}(O^2)$.