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Article

Generalized Householder transformations

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Abstract: The Householder transformation, allowing a rewrite of probabilities into expectations of dichotomic observables, is generalized in terms of its spectral decomposition. Dichotomy is modulated by allowing more than one negative eigenvalues, or by abandoning it altogether, yielding generalized operator valued arguments for contextuality. We also discuss a form of state-dependent contextuality by variation of the functional relations of the operators; in particular, by additivity.

Keywords: Householder transformations

1. From probabilities to expectations

A standard way to adapt classical probabilities $p \in [0,1]$ to expectations $E \in [-a,a]$ of two-valued—indeed, $\{-a,a\}$–valued, observables is in terms of affine transformations $E_a(p) = a(2p-1)$, amounting to a doubling of the probability and a shift by minus one, times a. (Often the physical units in terms of which observables are measured are chosen to be such that $a=1$.) This can be motivated by the linearity of classical probabilities which can be defined as the convex polytope of "extreme cases" or truth assignments, symbolized by two-valued measures $v \in \{0,1\}$.

It is an interesting property of quantum mechanics that the dimensionality $n \in \mathbb{N}$ of the associated Hilbert space $\mathbb{C}^n$ is determined by the finest resolution of its contexts or "maximal observables": a context contains an exhaustive (aka maximal or complete) set of mutually exclusive elementary observables. Each one of these elementary observables is identifiable by an elementary proposition, which in turn is formalizable by a one dimensional orthogonal projection operator F that is both self-adjoint as well as idempotent; that is, $\mathsf{F} = \mathsf{F}^\dagger$ and $\mathsf{F}^2 = \mathsf{F}$, respectively. Thereby, $n=2$ associated with dichotomic observables just represents a bound from below for nontrivial predictions. But there are no preferred Leibnizian "dyadic" schemes, such as bases, to represent and encode vectors or pure states in n-dimensional Hilbert spaces: neither the dimensionality suggesting an n–ary encoding nor the scalar product (nor completeness) yields any such preference; albeit arbitrary rotations (unitary transformations) in n dimensions can be obtained (and parmetrized [1]) by the serial composition of rotations (unitary transformations) in two-dimensional subspaces of $\mathbb{C}^n$.

It, therefore, is not too far-fetched to ask what could be the generalizations of the aforementioned affine transformations in arbitrary dimensions. in particular, the quantum mechanical counterparts of classical expectations. These can be given in terms of the so-called Householder transformations (e.g., Ref. [2]) as follows.

Let $|\mathbf{x}\rangle \in \mathbb{C}^n$ be a nonzero vector and $\mathsf{F}_\mathbf{x} = (\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}|$ the respective orthogonal projection operator. The Householder transformation $\mathsf{U}_\mathbf{x}$ is defined by

$$\mathsf{U}_\mathbf{x} = \mathbb{1} - 2\mathsf{F}_\mathbf{x} = \mathbb{1} - 2(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}|. \tag{1}$$

If $|\mathbf{x}\rangle$ is a unit vector, then $\mathsf{U}_\mathbf{x} = \mathbb{1} - 2|\mathbf{x}\rangle\langle\mathbf{x}|$.

The following properties can be asserted by direct proofs:

(i) $\mathsf{U}_\mathbf{x}$ is Hermitian; that is, $\mathsf{U}_\mathbf{x} = \mathsf{U}_\mathbf{x}^\dagger$;

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(ii) $\mathbf{U_x}$ is unitary; that is,

$$\begin{aligned} \mathbf{U_x}\mathbf{U_x}^\dagger = \mathbf{U_x}^\dagger\mathbf{U_x} = \mathbf{U_x}\mathbf{U_x} \\ = \Big(\mathbb{1} - 2(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}|\Big)\Big(\mathbb{1} - 2(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}|\Big) \\ = \mathbb{1} - 4(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}| + 4(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}| = \mathbb{1}. \end{aligned} \tag{2}$$

(iii) Hence $\mathbf{U_x}$ is involutory: $\mathbf{U_x}^{-1} = \mathbf{U_x}$.

(iv) The eigensystem of $\mathbf{U_x}$ has two eigenvalues ± 1:

-1: For the eigenvector $|\mathbf{x}\rangle$ of $\mathbf{U_x}$, with $\mathbf{U_x}|\mathbf{x}\rangle = (\mathbb{1} - 2(\langle \mathbf{x}|\mathbf{x}\rangle)^{-1}|\mathbf{x}\rangle\langle\mathbf{x}|)|\mathbf{x}\rangle = |\mathbf{x}\rangle - 2|\mathbf{x}\rangle = -|\mathbf{x}\rangle$ the associated eigenvalue is -1.

$+1$: The remaining $n-1$ mutually orthogonal eigenvectors span the $n-1$ dimensional subspace orthogonal to $|\mathbf{x}\rangle$. Every vector in that subspace has eigenvalue $+1$. (For $n > 2$ the spectrum is degenerate.)

Stated differently: for all vectors orthogonal to $|\mathbf{x}\rangle$ the Householder transformation $\mathbf{U_x}$ acts as identity; and for $|\mathbf{x}\rangle$ the Householder transformation $\mathbf{U_x}$ acts as a reflection on the one-dimensional subspace spanned by $|\mathbf{x}\rangle$.

(v) Since the determinant of a matrix is the product of its eigenvalues, the determinant of a Householder transformation is -1.

(vi) If $\mathcal{C} = \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle, \ldots, |\mathbf{e}_n\rangle\}$ is an orthonormal basis formalizing a context, then the succession of the respective Householder transformations renders negative unity; that is,

$$\begin{aligned} \mathbf{U}_{\mathbf{e}_1}\mathbf{U}_{\mathbf{e}_2}\cdots\mathbf{U}_{\mathbf{e}_n} = (\mathbb{1} - 2|\mathbf{e}_1\rangle\langle\mathbf{e}_1|)(\mathbb{1} - 2|\mathbf{e}_2\rangle\langle\mathbf{e}_2|)\cdots(\mathbb{1} - 2|\mathbf{e}_n\rangle\langle\mathbf{e}_n|) \\ = \mathbb{1} - 2\underbrace{(|\mathbf{e}_1\rangle\langle\mathbf{e}_1| + |\mathbf{e}_2\rangle\langle\mathbf{e}_2| + \cdots + |\mathbf{e}_n\rangle\langle\mathbf{e}_n|)}_{\mathbb{1}} = -\mathbb{1}. \end{aligned} \tag{3}$$

For the sake of an example, let $|\mathbf{z}\rangle = (1,1)^\intercal$, so that the corresponding Householder transformation can be written in matrix form as

$$\mathbf{U_z} = \mathbb{1} - 2(\langle \mathbf{z}|\mathbf{z}\rangle)^{-1}|\mathbf{z}\rangle\langle\mathbf{z}| \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - 2(2)^{-1}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = -\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Take $|\mathbf{x}\rangle = (2,1)^\intercal$, so that $|\mathbf{y}\rangle = -(1,2)^\intercal$: this "reflected" vector $|\mathbf{y}\rangle$ and the original vector $|\mathbf{x}\rangle$ have the same length or norm. The component of $|\mathbf{y}\rangle$ along $|\mathbf{z}\rangle$ is reversed, whereas its component orthogonal to $|\mathbf{z}\rangle$ remains the same. This situation is depicted in Figure 1.

Because of (iii), if $|\mathbf{x}\rangle \neq |\mathbf{y}\rangle$ are two vectors in $\mathbb{R}^n$ with identical length or norm $\|\mathbf{x}\| = \|\mathbf{y}\|$ then there exists a remarkable "symmetry delivered by" a Householder transformation $\mathbf{U_z}$ such that $\mathbf{U_z}|\mathbf{x}\rangle = |\mathbf{y}\rangle$ and $\mathbf{U_z}\mathbf{U_z}|\mathbf{x}\rangle = \mathbf{U_z}|\mathbf{y}\rangle = |\mathbf{x}\rangle$. For this to hold the vector $|\mathbf{z}\rangle$ needs to be a vector equal to $|\mathbf{x}\rangle - |\mathbf{y}\rangle$: $(\mathbb{1} - 2(\langle \mathbf{z}|\mathbf{z}\rangle)^{-1}|\mathbf{z}\rangle\langle\mathbf{z}|)|\mathbf{x}\rangle = |\mathbf{y}\rangle$ and $|\mathbf{x}\rangle = (\mathbb{1} - 2(\langle \mathbf{z}|\mathbf{z}\rangle)^{-1}|\mathbf{z}\rangle\langle\mathbf{z}|)|\mathbf{y}\rangle$, resulting in $(\langle \mathbf{z}|\mathbf{z}\rangle)^{-1}|\mathbf{z}\rangle\langle\mathbf{z}|(|\mathbf{x}\rangle - |\mathbf{y}\rangle) = |\mathbf{x}\rangle - |\mathbf{y}\rangle$, and thus $|\mathbf{z}\rangle = |\mathbf{x}\rangle - |\mathbf{y}\rangle$. (For $|\mathbf{x}\rangle = |\mathbf{y}\rangle$ identify with $|\mathbf{z}\rangle$ a vector orthogonal to $|\mathbf{x}\rangle = |\mathbf{y}\rangle$.) This is not true for $\mathbb{C}^n$, as for instance, there exists no $|\mathbf{z}\rangle$ which would render $\mathbf{U_z}|\mathbf{x}\rangle = i|\mathbf{x}\rangle$ for nonzero $|\mathbf{x}\rangle$, and an additional unitary transformation is required.

This gives rise to the orthonormalizion of a set of k linear independent nonzero vectors $\mathcal{S} = \{|\mathbf{s}_1\rangle, |\mathbf{s}_2\rangle, \ldots, |\mathbf{s}_k\rangle\}$ in $\mathbb{R}^n$ by taking some orthonormal basis $\mathcal{C} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\} \equiv \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle, \ldots, |\mathbf{e}_n\rangle\}$, choosing k vectors thereof—say, the first k vectors of the standard Cartesian coordinate system—and identifying $|\mathbf{s}_i\rangle$ with $|\mathbf{x}_i\rangle$, and (the extra factor $\|\mathbf{s}_i\|$ serves to make the vector of equal length or norm) $|\mathbf{y}_i\rangle$ with $\|\mathbf{s}_i\||\mathbf{e}_i\rangle$, thereby constructing a Householder transformation followed by normalization (through division by $\|\mathbf{s}_i\|$) $\mathbf{U}_{\mathbf{z}_i}$ of $|\mathbf{s}_i\rangle \overset{\mathbf{U}_{\mathbf{z}_i}}{\mapsto} |\mathbf{e}_i\rangle$ with respective $|\mathbf{z}_i\rangle = |\mathbf{s}_i\rangle - \|\mathbf{s}_i\||\mathbf{e}_i\rangle$. This kind of orthonormalization may yield a span "outside" of the subspace spanned by the "original" vectors.

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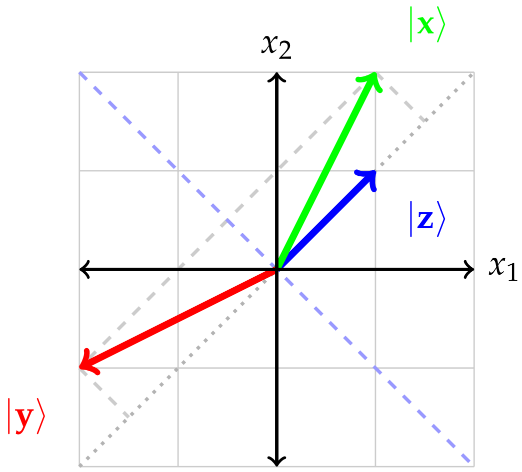

Figure 1. Depiction of the Householder transformation $\mathbf{U_z}$ with $|\mathbf{z}\rangle = \begin{pmatrix}1,1\end{pmatrix}^\intercal$ acting on a vector $|\mathbf{x}\rangle = \begin{pmatrix}2,1\end{pmatrix}^\intercal$. The resulting "reflected" vector $|\mathbf{y}\rangle = \mathbf{U_z}|\mathbf{x}\rangle$ and the original vector $|\mathbf{x}\rangle$ have the same length or norm. Its component along $|\mathbf{z}\rangle$ is reversed, whereas its component orthogonal to $|\mathbf{z}\rangle$ remains the same.

Cabello has used the Householder transformation to argue for what he calls state-independent quantum contextuality [3,4]. Thereby all 2^{16} possible classical value assignments of the elementary propositions $a_1, \cdots, a_{16} \in \{-1, 1\}$ depicted in Figure 2, grouped into the nine contexts $\mathcal{C}_1, \ldots, \mathcal{C}_9$ are enumerated, multiplied in each one of the nine contexts, and these products are added together—that is, every of the 2^{16} valuations yield a number, an integer between -9 and 9.

As it turns out 9216 value assignments are rendering the number -7, and none rendering -8 or -9. But these classical value assignments are not admissible [5] in the sense of (iv)—an *ad hoc* assumption—as there does not exist a classical (non-contextual) two-valued $\{0, 1\}$-state on these 18 observables in 9 contexts which would allow a translation into a $\{-1, 1\}$-value assignment such that every context contains exactly one element that is assigned the value "-1" and all other elements of that context are assigned the value "$+1$". For the sake of anedotal demonstration (no proof), Figure 2 contains an "illegal" value assignment that renders the maximal value 7 of the sum of the products of all value assignments within the nine contexts.

Indeed, relative to admissibility, state-independent quantum contextuality is a corollary of the Kochen-Specker theorem for configurations without any two-valued states. Because in this case no (homomorphic) translation E from admissible two-valued $\{0, 1\}$-states p into two-valued $\{-1, 1\}$-observables E with, for instance, affine $E(p) = 2p - 1$, exist.

In the relaxed case admissibility can be violated—in particular, by an *ad hoc* breach of exclusivity, thereby allowing more than one value assignment "1" per context—while at the same time maintaining noncontextuality (at the intertwining observables). State-independent quantum contextuality can only be counterfactually postulated if and only if the quantum Householder transformation-based predictions—equal to the (modulus of) the number of contexts involved—are *not* realizable by classical noncontextual, admissible or inadmissible value assignments. Therefore, the sum of all products of observables within all contexts should not reach its algebraic maximal obtainable value. (As noted earlier this maximal obtainable value is just the number of contexts involved.) That implies that it should not be possible to require the number of noncontextual value assignments "-1" within each given context to be odd. As a result strictly bi-connected (indeed even-number connected) Kochen-Specker configurations involving an odd number of contexts always exhibit state-independent quantum contextuality. The proof is similar to the in-

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direct parity proof of the Kochen-Specker theorem for the configuration introduced by Cabello, Estebaranz-García-Alcaine [6]: for a proof by contradiction suppose the products of observables within all contexts are multiplied. On the one hand, since by assumption, there are odd contexts, each contributing a factor -1, this number—the odd product of products—should be -1. But on the other hand, by bi- or even-connectivity, the product of products contains only squares or even multiples of factors, which return $+1$—a complete contradiction.

Figure 2 contains an instance of classical inadmissible value assignment that cannot reach the algebraic maximal sum, as would be required by the quantum Householder transformation prediction. Further methods to obtain such configurations based on parity proofs are discussed by Waegell, Aravind, Megill, and Pavičić [7–9]. The Greenberger-Horne-Zeilinger operator theorem is based on a similar argument [10,11].

For all other multi-context configurations allowing two-valued states—even with a nonseparable or unital set of two-valued states—the translation from $\{0,1\}$-states into two-valued $\{-1,1\}$-observables there is no state-independent quantum contextuality. For other operator-valued assignments see, for instance, references [4,12].

I shall leave open the question of how convincing and applicable to counterfactual arguments such inadmissible value assignments—even in their operator-valued translations—might be. At the moment, I am inclined to understand such situations and configurations rather in terms of the Kochen-Specker theorem [13], or quantitatively about the associated chromatic number; that is, in terms of how many colors are needed to separate elements in the respective contexts [14].

A quantum realization of the Cabello, Estebaranz-García-Alcaine [3,6] configuration is a faithful orthogonal representation [15–17] that includes 18 unit vectors or associated one-dimensional orthogonal projection operators $\mathbf{F}_i = |a_i\rangle\langle a_i|$, with $1 \leq i \leq 18$ as vector labels of the hypergraph depicted in Figure 2; whereby adjacency of hypergraph vertices is translated into orthogonality of the vectors serving as their labels.

As we have learned in (vi), Equation (3), within each one of the nine contexts the products of these elementary observables is -1. Adding together all nine products of the nine contexts yields the sum -1 for all quantum value assignments. This is in contradiction to the classical predictions which never yield -8 or -9. (Of course, this argument requires counterfactual existence of all quantum observables $\mathbf{F}_i = |a_i\rangle\langle a_i|$, even as only a single one context (from nine contexts $\mathcal{C}_1, \ldots, \mathcal{C}_9$) is operationally accessible.

2. Generalized operator-valued arguments for mixed states

From now on we shall assume that states are prepared (preselected) to be in a "maximal" mixture $\rho = \frac{1}{n}\mathbb{1}_n$, where n stands for the dimension of the Hilbert space. That is, we abandon state-independence for "maximal ignorance" or "maximally scrambled (pure)states". This cannot be performed from a pure state by merely unitary, one-to-one, means. One has to allow many-to-one processes such as (partial) tracing over constituents of a multipartite state. The advantage of such states is that the expectation value of an operator $\mathbf{A}$ reduces to the weighted sum over its eigenvalues $\lambda_1, \ldots, \lambda_n$; that is, $\langle \mathbf{A} \rangle_\rho = \text{Tr}(\mathbf{A}\rho) = \frac{1}{n}\text{Tr}(\mathbf{A}\mathbb{1}_n) = \frac{1}{n}(\lambda_1 + \ldots + \lambda_n)$.

Then from a purely algebraic point of view, Householder transformations can be characterized in terms of commutativity [18, §79, 84]: the two observables associated with a pure state and the corresponding expectation values are just functional variations of one and the same maximal operator [19, Satz 8] (see also [13, Section 4]). For an illustration consider two operators $\mathbf{P}$ and $\mathbf{E}$ whose respective eigensystems include identical projection operators but different eigenvalues.

To be more precise, according to the spectral theorem, let $\mathcal{C} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\} \equiv \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle, \ldots, |\mathbf{e}_n\rangle\}$ with $n \geq 2$ be an orthormal basis suitable for a spectral decomposition of $\mathbf{P}$ and $\mathbf{E}$, and let $\mathbf{F}_i = |\mathbf{e}_1\rangle\langle \mathbf{e}_1|$ be the associated one-dimensional orthogonal projection

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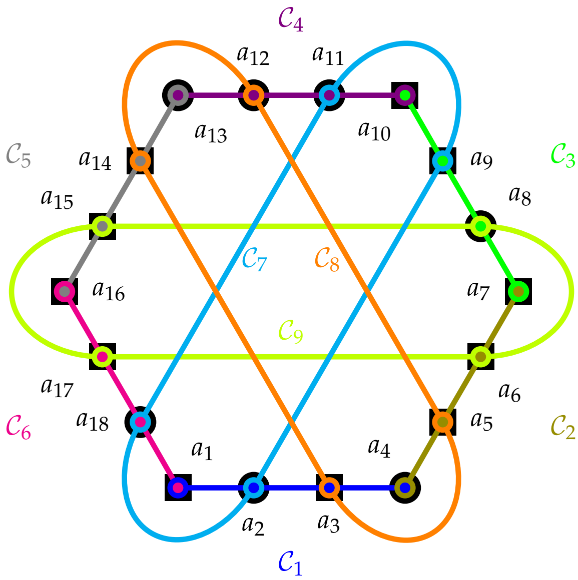

Figure 2. Orthogonality diagram (hypergraph) of a configuration of observables without any two-valued state, used in a parity proof of the Kochen-Specker theorem presented by Cabello, Estebaranz-García-Alcaine [6]. One (from 9216) underlaid value assignments represents squares as "+1" and circles as "-1". A quantum realization is, for example, in terms of 18 orthogonal projection operators associated with the one dimensional subspaces spanned by the vectors from the origin $(0,0,0,0)^\intercal$ to $|a_1\rangle = \left(0,0,1,-1\right)^\intercal$, $|a_2\rangle = \left(1,-1,0,0\right)^\intercal$, $|a_3\rangle = \left(1,1,-1,-1\right)^\intercal$, $|a_4\rangle = \left(1,1,1,1\right)^\intercal$, $|a_5\rangle = \left(1,-1,1,-1\right)^\intercal$, $|a_6\rangle = \left(1,0,-1,0\right)^\intercal$, $|a_7\rangle = \left(0,1,0,-1\right)^\intercal$, $|a_8\rangle = \left(1,0,1,0\right)^\intercal$, $|a_9\rangle = \left(1,1,-1,1\right)^\intercal$, $|a_{10}\rangle = \left(-1,1,1,1\right)^\intercal$, $|a_{11}\rangle = \left(1,1,1,-1\right)^\intercal$, $|a_{12}\rangle = \left(1,0,0,1\right)^\intercal$, $|a_{13}\rangle = \left(0,1,-1,0\right)^\intercal$, $|a_{14}\rangle = \left(0,1,1,0\right)^\intercal$, $|a_{15}\rangle = \left(0,0,0,1\right)^\intercal$, $|a_{16}\rangle = \left(1,0,0,0\right)^\intercal$, $|a_{17}\rangle = \left(0,1,0,0\right)^\intercal$, $|a_{18}\rangle = \left(0,0,1,1\right)^\intercal$, respectively.

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operators that are mutually orthogonal. Then the spectral sums of P and E can be uniformly written as

$$\begin{aligned}\mathsf{P} &= \sum_{i=1}^{n} \lambda_i \mathsf{F}_i = (+1)\cdot \mathsf{F}_1 + (0)\cdot \underbrace{\left(\sum_{i=2}^{n} \mathsf{F}_i\right)}_{\mathsf{F}_{\{2,\ldots,n\}}} = \mathsf{F}_1,\\ \mathsf{E} &= \sum_{i=1}^{n} \mu_i \mathsf{F}_i = (-1)\cdot \mathsf{F}_1 + (1)\cdot \underbrace{\left(\sum_{i=2}^{n} \mathsf{F}_i\right)}_{\mathsf{F}_{\{2,\ldots,n\}}} = -\mathsf{F}_1 + \mathsf{F}_{\{2,\ldots,n\}}.\end{aligned} \tag{4}$$

From this perspective of the spectral decompositions, a transition from P and E is nothing more than a mapping of the eigenvalues in the spectral sums of (4):

$$\{\lambda_1, \lambda_2, \ldots, \lambda_n\} = \{1, \underbrace{0, \ldots, 0}_{n-1 \text{ times}}\} \mapsto \{\mu_1, \mu_2, \ldots, \mu_n\} = \{-1, \underbrace{1, \ldots, 1}_{n-1 \text{ times}}\}. \tag{5}$$

From this spectral point of view a generalization to mutually disjoint eigenvalues, , for instance, different primes $p_1, \ldots, p_n$, suggests itself; such that, in the orthonormal basis aka context, $\mathcal{C} = \{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n\} \equiv \{|\mathbf{e}_1\rangle, |\mathbf{e}_2\rangle, \ldots, |\mathbf{e}_n\rangle\}$ corresponding to mutually perpendicular orthogonal operators $\mathsf{F}_1, \ldots, \mathsf{F}_n$, the operator associated with the maximal observable has just diagonal entries

$$\mathsf{M} = \sum_{i}^{n} p_i \mathsf{F}_i = \text{diag}(p_1, \ldots, p_n). \tag{6}$$

This generalization has the advantage that, because all eigenvalues are prime, all combinations, and in particular, its product $\Pi = p_1 \cdots p_n$, has a unique prime decomposition. This translates into a unique decomposition into eigenvalues.

The eigenvalues in the spectral sum to the chromatic number of the sphere [20–22] as well as of hypergraphs [14,23]. From the strategy to get noncontextual classical colorings of orthogonality hypergraphs derived from quantum observables, any such graph whose chromatic number n is equal to the dimension n of the associated Hilbert space, there cannot be established any state-independent quantum contextuality: because in this case there exist classical noncontextual observables whose n colors can be one-to-one mapped (relabelled) into the observable values $p_1, \ldots, p_n$.

Another possibility is a choice of the eigenvalues $-1, -1, 1, 1$ or any permutation thereof, yielding a quantum prediction of the sum of the products equal to $9 \cdot (-1 \cdot -1 \cdot 1 \cdot 1) = 9$, which is just the negative of Cabello's prediction [3].

3. Generalized operations

Other methods to derive state-dependent quantum contextuality involving "maximally mixed states" use different operations than multiplication. The most elementary such operation is summation among all eigenvalues within a given maximal observable or context. The resulting violations can be tested in a similar (counterfactual) manner as for the sums of products.

For the sake of an example, we can again use a Kochen-Specker type configuration introduced by Cabello, Estebaranz-García-Alcaine [6] and depicted in Figure 2. If instead of multiplying the eigenvalues within any such context (yielding $-1 \cdot 1 \cdot 1 \cdot 1 = -1$) these eigenvalues are added, we obtain the context sum $-1 + 1 + 1 + 1 = 2$. (This renders an expectation of the context sum divided by four; that is, $\frac{1}{2}$.) The associated function between operators within a given context $\mathcal{C}_j$, $1 \le j \le 9$, is addition:

$$g(\mathsf{F}_{\mathcal{C}_j,1}, \mathsf{F}_{\mathcal{C}_j,2}, \mathsf{F}_{\mathcal{C}_j,3}, \mathsf{F}_{\mathcal{C}_j,4}) = -\mathsf{F}_{\mathcal{C}_j,1} + \mathsf{F}_{\mathcal{C}_j,2} + \mathsf{F}_{\mathcal{C}_j,3} + \mathsf{F}_{\mathcal{C}_j,4} = \mathsf{S}_{\mathcal{C}_j} \tag{7}$$

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As there are nine contexts $\mathcal{C}_j$, $1 \le j \le 9$, the sum over all context sums is $2 \cdot 9 = 18$, which is not divisible by four. The respective expectation, given a preselected state $\rho = \frac{1}{4}\mathbb{1}_4$ is

$$\langle \sum_{j=1}^{9} \mathsf{S}_{\mathcal{C}_j} \rangle_\rho = \sum_{j=1}^{9} \langle \mathsf{S}_{\mathcal{C}_j} \rangle_\rho = \sum_{j=1}^{9} \mathrm{Tr}\left(\mathsf{S}_{\mathcal{C}_j}\rho\right) = \frac{1}{4}\sum_{j=1}^{9} \mathrm{Tr}\left(\mathsf{S}_{\mathcal{C}_j}\mathbb{1}_4\right) = \sum_{j=1}^{9} \frac{1}{2} = \frac{9}{2}. \tag{8}$$

A classical computation produces only multiples of four: Since the 18 observables $a_1, \ldots, a_{18}$ are bi-connected—that is, every such observable occurs in exactly two contexts—the sum total of all dichotomic observables is

$$2(a_1 + \cdots + a_{18}) = n, \text{ with } a_1, \ldots, a_{18} \in \{-1, 1\},\ n \in \mathbb{Z}, \tag{9}$$

so that $-36 \le n \le 36$. Suppose there are k potitive observables a_i, and $18 - k$ negative observables a_j. Therefore, all cases are permutations of the following configuration:

$$\underbrace{a_1 + \cdots + a_k}_{k \text{ positive } a_i = 1} + \underbrace{a_{k+1} + \cdots + a_{18}}_{18-k \text{ negative } a_j = -1} = k - (18 - k) = 2(k - 9) = \frac{n}{2}, \tag{10}$$

with $k \in \mathbb{N}$, so that

$$0 \le k = 9 + \frac{n}{4} \le 18, \text{ and } n = -36 + 4k. \tag{11}$$

This results in n arithmetically progressing from -36 in steps of 4, that is

$$k \in \{0, 1, \ldots, 18\}, \text{ with respective } n \in \{-36, -32, \ldots, 0, \ldots, 32, 36\}. \tag{12}$$

In particular, as 18 is not divisible by 4, no sum total of 18 can be classically realized by the configuration of Cabello, Estebaranz-García-Alcaine [6]. Classical expectations from the assumption of equidistribution of the occurrences are obtained by dividing these cases by four.

Indeed, a combinatorial argument shows that there are

$$\#(n(k)) = \#(-36 + 4k) = \binom{18}{k} = \binom{18}{18-k} = \frac{10}{k!(18-k)!} \tag{13}$$

configurations yielding $n = -36 + 4k$, so that the number of occurrences are $\#(\pm 0) = 48620$, $\#(\pm 4) = 43758$, $\#(\pm 8) = 31824$, $\#(\pm 12) = 18564$, $\#(\pm 16) = 8568$, $\#(\pm 20) = 3060$, $\#(\pm 24) = 816$, $\#(\pm 28) = 153$, $\#(\pm 32) = 18$, $\#(\pm 36) = 1$. This classical prediction is in contrast with the quantum prediction 18 which always occurs.

4. Summary

We have discussed Householder transformations as a means to translate arguments involving probabilities into expectations of dichotomic observables. Thereby we have used the spectral decomposition of Householder transformation; more explicitly, we have allowed eigenvalues not restricted to one minus one, and all the others plus one. For instance, dichotomy can be modulated by allowing more than one negative eigenvalues. This yields generalized operator-valued arguments for contextuality. We have also discussed new forms of state-dependent contextuality by variation of the functional manipulation and relation of the operators. In particular, we have considered additivity.

As with original forms of expectation or operator based arguments such as Greenberger-Horne-Zeilinger [10,11] or Householder-based state-independent contextuality [3] those arguments use complementary and thus counterfactual observables. Additionally, additivity arguments use violations of admissibility [5], in particular, exclusivity and completeness.

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