The geometry of fiber products of probability polytopes

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Quantum contextuality is a central nonclassical feature of quantum theory [1, 2], capturing the impossibility of assigning measurement outcomes independently of context. Beyond its foundational importance, contextuality has been identified as a resource for quantum computation and information processing [3, 4]. In this work [5], we develop new methods for describing extremal contextual simplicial distributions, a core structural problem in the theory. After presenting our results for general simplicial distributions, we focus on applications to one-dimensional contextuality scenarios, i.e. distributions associated to graphs that form a *non-signaling polytope* in a natural way. Examples include cycle scenarios [6]—in particular, the famous CHSH scenario [7]—as well as local marginal polytopes [8].

Simplicial distributions Our approach uses the theory of *simplicial distributions* [9], which provides a topological language in which measurement scenarios are encoded by simplicial sets and probabilistic models appear as compatible families of distributions. A simplicial set X is a combinatorial object built from vertices, edges, triangles, and higher simplices, together with face and degeneracy maps [10]. We view a measurement scenario as a simplicial set X, where an n-simplex $\sigma \in X_n$ represents a *measurement context* consisting of $n + 1$ jointly performable measurements.

Given an outcome simplicial set Y, a *simplicial distribution* on X with outcomes in Y is a simplicial map

$$p\colon X \longrightarrow D(Y),$$

where $D(Y)$ denotes the simplicial set obtained by applying the probability-distribution functor degreewise, i.e. $(D(Y))_n = D(Y_n)$. Equivalently, p assigns to each context $\sigma \in X_n$ a distribution

$$p_\sigma \in D(Y_n),$$

in a way that is compatible with the face and degeneracy maps (marginalization and repetition of outcomes). For m-outcome measurements we typically take $Y = \Delta_{\mathbb{Z}_m}$, whose n-simplices are $(n + 1)$-tuples in $\mathbb{Z}_m^{n+1}$ (with $\mathbb{Z}_m = \{0, 1, \ldots, m - 1\}$), and whose face maps delete coordinates (with degeneracies duplicating coordinates). This encodes outcome assignments for each jointly measurable context.

A simplicial distribution p is called *contextual* if there does not exist a global assignment of outcomes to all measurements that reproduces the distributions prescribed by p on every simplex.

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The set of all simplicial distributions is denoted $\mathsf{sDist}(X,Y)$. It is a *polytope in standard form*. A central object of interest is the set of vertices of these polytopes [11].

Gluing measurement spaces Polytopes in standard form carry a natural preorder relation $\preceq$ that plays an important role in our study. This preorder allows us to define the *vertex support* of a point x in the polytope, denoted by $\mathrm{Vsupp}(x)$, as the set of vertices y such that $y \preceq x$. The convex hull of $\mathrm{Vsupp}(x)$ is precisely the unique face whose relative interior contains x. Our first main result is:

Theorem 0.1. *Let χ be a diagram of polytopes in standard form and let x be a point in the polytope P given by limit of χ. We define a new diagram χ_x of the same shape by replacing each object with the convex hull of the vertex support of the corresponding projection of x. Then*

$$x \text{ is a vertex of } P = \lim \chi \quad \Longleftrightarrow \quad \lim \chi_x = \{x\}.$$

Building on this result, we characterize the vertices of simplicial distribution polytopes in the case where the measurement space is obtained as a colimit of a diagram of simplicial sets. An important special case is a *pushout* (gluing) construction, where a measurement space is formed by gluing simplicial sets along a common subspace:

Corollary 0.2. *Let $X^{(1)}, \ldots, X^{(n)}$ be simplicial sets, and let W be a common simplicial subset of each $X^{(i)}$. Let X be the simplicial set obtained by gluing all $X^{(i)}$ along W:*

$$X = X^{(1)} \cup_W \cdots \cup_W X^{(n)}. \tag{1}$$

A simplicial distribution $p\colon X \to D(Y)$ is a vertex in $\mathsf{sDist}(X,Y)$ if and only if the set

$$\{(q^{(1)}, \ldots, q^{(n)}) \in \prod_{i=1}^{n} \mathsf{Conv}(\mathrm{Vsupp}(p|_{X^{(i)}})) : \; q^{(1)}|_W = \cdots = q^{(n)}|_W\}$$

consists only of $(p|_{X^{(1)}}, \ldots, p|_{X^{(n)}})$.

Detecting vertices We establish a general geometric sufficient condition—stated in terms of affine independence and the intersection pattern of convex hulls—for a simplicial distribution p on a glued measurement space as in (1) to be a vertex. The condition is formulated in terms of the sets

$$A_i = \{\, q|_W : \; q \in \mathrm{Vsupp}(p|_{X^{(i)}}) \,\},$$

i.e. the collection of restrictions to the overlap W of vertices appearing in the vertex support of the local restriction $p|_{X^{(i)}}$.

Theorem 0.3. *If the following conditions hold:*

- *for every $1 \le i \le n$, $|A_i| = |\,\mathrm{Vsupp}(p|_{X^{(i)}})|$, and the set A_i is affinely independent;*
- *the intersection $\cap_{i=1}^{n} \mathsf{Conv} A_i$ consists of a single point;*

then p is a vertex.

Graphical distributions Our particular interest is simplicial distributions on one-dimensional measurement spaces, which can be viewed as distributions on a directed (multi)graph. More precisely, let X be a graph consisting of a vertex set X_0 and an edge set X_1, together with source and target maps $d_1, d_0 \colon X_1 \to X_0$. A *graphical distribution* (equivalently, a simplicial distribution on a one-dimensional measurement space) p on X with outcomes in $\mathbb{Z}_m$ consists of compatible probability matrices

$$p_\sigma = \begin{pmatrix} p_\sigma^{0,0} & \cdots & p_\sigma^{0,m-1} \\ \vdots & \ddots & \vdots \\ p_\sigma^{m-1,0} & \cdots & p_\sigma^{m-1,m-1} \end{pmatrix}, \qquad \sigma \in X_1.$$

We write $\mathrm{Dist}(X, m)$ for the polytope of graphical distributions on X with outcomes in $\mathbb{Z}_m$.

The advantage of the simplicial distribution framework is that it allows us to study non-standard measurement spaces obtained by gluings that cannot be represented as *simplicial complexes*. We investigate the following two measurement spaces as our atomic scenarios:

- the *rose graph* R_n, formed by gluing n 1-circles at a common point;
- the *dipole graph* D_n, formed by gluing n edges along their endpoints.

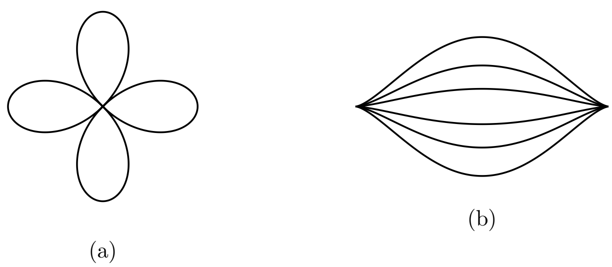

Figure 1: (a) The rose graph R_4. (b) The dipole graph D_6.

We completely characterize the vertices of R_n and D_n using our main Theorem 0.3. Finally, we show how the identification of vertices on dipole and rose graphs can be leveraged to detect vertices on general connected 1-dimensional measurement spaces. This is done by choosing some of the edges and applying the collapsing method (see [12, Section 4.1]). We can always collapse a graph to the rose graph by choosing a spanning tree. In particular, we derive lower bounds on the number of contextual vertices in bipartite scenarios [13], i.e. graphical distributions on the bipartite graph K_{n_1,n_2}.

Proposition 0.4. *Let $\tilde{\kappa}(n, m)$ denote the number of contextual vertices in* $\mathrm{Dist}(R_n, m)$*. There are at least*

$$\sum_{\substack{0<k<n_1 \\ 0<r<n_2}} \binom{n_1}{k} \cdot \binom{n_2}{r} \cdot \tilde{\kappa}(k(n_2 - r) + (n_1 - k)r, m)$$

contextual vertices in $\mathrm{Dist}(K_{n_1,n_2}, m)$.

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