AVERAGES OF UNLABELED NETWORKS: GEOMETRIC CHARACTERIZATION AND ASYMPTOTIC BEHAVIOR

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It is becoming increasingly common to see large collections of network data objects — that is, data sets in which a network is viewed as a fundamental unit of observation. As a result, there is a pressing need to develop network-based analogues of even many of the most basic tools already standard for scalar and vector data. In this paper, our focus is on averages of unlabeled, undirected networks with edge weights. Specifically, we (i) characterize a certain notion of the space of all such networks, (ii) describe key topological and geometric properties of this space relevant to doing probability and statistics thereupon, and (iii) use these properties to establish the asymptotic behavior of a generalized notion of an empirical mean under sampling from a distribution supported on this space. Our results rely on a combination of tools from geometry, probability theory, and statistical shape analysis. In particular, the lack of vertex labeling necessitates working with a quotient space modding out permutations of labels. This results in a nontrivial geometry for the space of unlabeled networks, which in turn is found to have important implications on the types of probabilistic and statistical results that may be obtained and the techniques needed to obtain them.

1. Introduction. Over the past 15-20 years, as the field of network science has exploded with activity, the majority of attention has been focused upon the analysis of (usually large) individual networks. See [21, 23, 29], for example. While it is unlikely that the analysis of individual networks will become any less important in the near future, it is likely that in the context of the modern era of ‘big data’ there will soon be an equal need for the analysis of (possibly large) collections of (sub)networks, i.e., collections of network data objects.

We are already seeing evidence of this emerging trend. For example, the analysis of massive online social networks like Facebook can be facilitated by local analyses, such as through extraction of ego-networks (e.g., [20]). Similarly, the 1000 Functional Connectomes Project, launched a few years ago in imitation of the data-sharing model long-common in computational

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biology, makes available a large number of fMRI functional connectivity networks for use and study in the context of computational neuroscience (e.g., [11]). It would seem, therefore, that in the near future networks of small to moderate size will themselves become standard, high-level data objects.

Faced with databases in which networks are the fundamental unit of data, it will be necessary to have in place a network-based analogue of the ‘Statistics 101’ tool box, extending standard tools for scalar and vector data to network data objects. The extension of such classical tools to network-based datasets, however, is not immediate, since networks are not inherently Euclidean objects. Rather, formally they are combinatorial objects, defined simply through two sets, of vertices and edges, respectively, possibly with an additional corresponding set of weights. Nevertheless, initial work in this area demonstrates that networks can be associated with certain natural Euclidean subspaces and furthermore demonstrates that through a combination of tools from geometry, probability theory, and statistical shape analysis it should be possible to develop a comprehensive, mathematically rigorous, and computationally feasible framework for producing the desired analogues of classical tools.

For example, in our recent work [19] we have characterized the geometry of the space of all labeled, undirected networks with edge weights, i.e., consisting of graphs \( G = (V, E, W) \), for weights \( w_{ij} = w_{ji} \geq 0 \), where equality with zero holds if and only if \( \{i, j\} \notin E \). This characterization allowed us in turn to establish a central limit theorem for an appropriate notion of a network empirical mean, as well as analogues of classical one- and two-sample hypothesis testing procedures. Other results of this type include additional work on asymptotics for network empirical means [30] and regression modeling with a network response variable, where for the latter there have been both frequentist [13] and Bayesian [18] proposals. Work in this area continues at a quick pace – see, for example, [2] which proposes a classification model based on network-valued inputs and [17] which proposes a nonparametric Bayes model for distributions on populations of networks. Earlier efforts in this space have focused on the specific case of trees. Contributions of this nature include work on central limit theorems in the space of phylogenetic trees [10, 4] and work by Marron and colleagues [32, 3] in the context of so-called object-oriented data analysis with trees.

To the best of our knowledge, all such work to date pertains to the case of labeled networks: that is, to networks in which the vertices \( V \) have unique labels, e.g., \( V = \{1, \ldots, d\} \). In fact, unlabeled networks have received decidedly less attention in the network science literature as a whole but nevertheless
arise in various important settings. The quintessential example of how such networks may arise in practice arguably is that of the study of ego-centric network structure in social network analysis. There, traditionally, individuals (‘egos’) are surveyed for a list of other individuals (‘alters’) with whom they share a certain relationship (e.g., friendship, colleague, etc.) and only common patterns across networks in the structure of the relationships among the individuals within each network are of interest. This leads to analyses that either ignore vertex labels or for which vertex labels are simply not available (e.g., through de-identification). See [27], for example.

In this paper, our focus is on averages of unlabeled, undirected networks with edge weights. Adopting a perspective similar to that in our previous work [19], we (i) characterize a certain notion of the space of all such networks, (ii) describe key topological and geometric properties of this space relevant to doing probability and statistics thereupon, and (iii) use these properties to establish the asymptotic behavior of a generalized notion of an empirical mean under sampling from a distribution supported on this space. In particular, adopting the notion of a Fréchet mean, we establish a corresponding strong law of large numbers and a central limit theorem. In contrast to [19], where the corresponding space of networks was found to form a smooth manifold, here the lack of vertex labeling necessitates working with a quotient space modding out permutations of labels. As a result, we have only an orbifold – a more general geometric structure – which in turn is found to have important implications on the types of probabilistic and statistical results that may be obtained and the techniques needed to obtain them.

The nature of our work is in the spirit of statistics on manifolds and statistical shape analysis, which employs the geometry of manifolds or shape spaces for defining Fréchet means and developing large sample theory of their sample counterparts for inference. See [6] for a rather comprehensive treatment on the subject. Our approach to studying the entire family of networks subject to an equivalence relation under a group action, via forming the associated quotient or moduli space, is a common theme in modern geometry, including gauge theory [15], symplectic topology [28], and algebraic geometry [14, 31]. The appearance of orbifolds, often much more complicated than in our case, is quite common. Finally, there is a large literature on graph limits, for which substantial work has been done on analysis of appropriate spaces of networks (e.g., [25]). But the focus therein typically is, by definition, on the case of a single network asymptotically increasing in size. Here, the focus is on asymptotics in many networks, with the dimension fixed.
The organization of this paper is as follows. In Section 2 we present our characterization of the space of unlabeled networks. Results from our investigation of the asymptotic behavior of the Fréchet empirical mean are then provided in Section 3. While a strong law of large numbers is found to emerge under quite general conditions, establishing just when conditions dictated by the current state of the art for central limit theorems on manifolds hold turns out to be a decidedly more subtle exercise. This latter is the focus of Section 4. Some additional discussion of open problems may be found in Section 5. The Appendices discuss implementation issues for the theoretical results in the paper.

2. The space of unlabeled networks. Our ultimate focus in this paper is on a certain well-defined notion of an ‘average’ on elements drawn randomly from a ‘space’ of unlabeled networks and on the statistical behavior of such averages. Accordingly, we need to establish and understand the relevant topology and geometry of this space. We do so by associating labeled networks with vectors and mapping those to unlabeled networks through the use of equivalence classes in an appropriate quotient space. In this section we provide relevant definitions, characterization, and illustrations of this space of unlabeled networks.

2.1. The topological space of unlabeled networks. Let \( G = (V,E) \) be a labeled, undirected graph/network with weighted edges and with \( d \) vertices/nodes. We always think of \( E \) as having \( D := \binom{d}{2} \) elements, where some of the edge weights can be zero. We think of the edge weight between vertices \( i \) and \( j \) as the strength of some unspecified relationship between \( i \) and \( j \).

Let \( \Sigma_d \) be the group of permutations of \( \{1, 2, \ldots, d\} \). A permutation \( \sigma \in \Sigma_d \) of the \( d \) vertex labels technically produces a new graph \( \sigma G \), but with no new information. To define \( \sigma G \) precisely, note that the weight function \( w_G : E \to \mathbb{R}_{\geq 0} \) can be thought of as a symmetric function \( w_G : V \times V \to \mathbb{R}_{\geq 0} \), with \( w_G(i,j) \) the weight of the edge joining vertex \( i \) and vertex \( j \) in \( G \). Therefore the action of \( \Sigma_d \) on \( w_G \) is given by

\[
(\sigma \cdot w_G)(i,j) = w_G(\sigma^{-1}(i), \sigma^{-1}(j)).
\]

(The inverse guarantees that \( (\sigma \tau) \cdot w_G = \sigma \cdot (\tau \cdot w)_G \).) Note that for general \( G \), not all permutations of the entries of \( w_G \) are of the form \( \sigma \cdot w_G \), as \( w_G \) may have \( \lfloor d(d-1)/2 \rfloor! \) distinct permutations and \( \Sigma_d \) has \( d! \) elements.

In summary, \( \sigma G \) is defined to be the graph on \( d \) vertices with weight function \( \sigma \cdot w_G : E \to \mathbb{R}_{\geq 0} \). Let \( \mathcal{G} = \mathcal{G}_d \) be the set of all labeled graphs with
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$d$ vertices. Then the quotient space

$$U_d = \mathcal{G}_d / \Sigma_d$$

is the space of unlabeled graphs, the object we want to study. This means that an unlabeled network $[G] \in U_d$ is an equivalence class

$$[G] := \{ \sigma \cdot G : \sigma \in \Sigma_d \}.$$

As we now explain, $\mathcal{G}_d$ looks like an explicit subset of $\mathbb{R}^D$, and so is easy to picture. In contrast, the quotient space $U_d$ is difficult to picture. Nevertheless, as we describe in the following paragraphs, the topology of $U_d$ may be characterized through standard point-set topology techniques, with the conclusion that everything works as well as possible. Readers who wish can safely skip to the examples in Section 2.2.

Fix an ordering of the vertices $1, \ldots, d$, and take the lexicographic ordering $\{(i, j) : 1 \leq i < j \leq d\}$ on the set of edges. (Thus $(i, j) < (k, \ell)$ if $i < k$ or $i = k$ and $j < \ell$.) Given this ordering, we get an injection

$$\alpha : \mathcal{G}_d \to \mathbb{R}^D, \quad \alpha(G) = (w_1(G), \ldots, w_D(G)),$$

where $w_i(G)$ is the weight of the $i$th edge of $G$. The image of $\alpha$ is the first “octant” $O_D = \{ \vec{x} = (x^1, \ldots, x^D) : x^i \geq 0 \}$. The Euclidean metric on $O_D$ pulls back via $\alpha$ to the obvious metric on $\mathcal{G}_d$: two networks are close iff their edge weights are close. Similarly, the standard topology on $O_D$ (an open ball in $O_D$ is the intersection of an open $\mathbb{R}^D$-Euclidean ball with $O_D$) pulls back to a topology on $\mathcal{G}_D$. (This just means that $A \subset \mathcal{G}_D$ is open iff $\alpha(A)$ is open in $O_D$. This makes $\alpha$ a homeomorphism.) Just as in $\mathbb{R}^D$, the metric and topology are compatible: a sequence of graphs/weight vectors $\vec{x}_i$ in $O_D$ converges to a graph/weight vector $\vec{x}$ in the topology of $O_D$ iff the distance from $\vec{x}_i$ to $\vec{x}$ goes to zero.

Via the bijection $\alpha$, the action of $\Sigma_d$ on $\mathcal{G}_d$ transfers to an action on $O_D$. First, $\sigma \in \Sigma_d$ acts on $\{1, \ldots, D\}$ by $\sigma \cdot i = j$ if $i$ corresponds to the edge $(i_1, i_2)$ and $j$ corresponds to the edge $(\sigma(i_1), \sigma(i_2))$. Then $\sigma$ acts on $O_D$ by $\sigma \cdot \vec{x} = (\sigma^{-1}(1), \ldots, \sigma^{-1}(D))$. Since we’ve arranged the actions to be compatible with $\alpha : \mathcal{G}_d \to O_D$, we get a well defined bijection $\overline{\alpha}$:

$$\mathcal{U}_d = \mathcal{G}_d / \Sigma_d \xrightarrow{\overline{\alpha}} O_D / \Sigma_d, \quad \overline{\alpha}[G] = [\alpha(G)].$$

From now on, we just denote $\overline{\alpha}$ by $\alpha$.

To complete the topological discussion, we note that $\alpha : \mathcal{U}_d \to O_D / \Sigma_d$ is a homeomorphism if we give both sides the quotient topology: for the map $q : \mathcal{G}_d \to \mathcal{U}_d$ taking a graph to its equivalence class, a set $U \subset \mathcal{U}_d$ is open iff $q^{-1}(U)$ is open in $O_D$. The quotient topology on $O_D / \Sigma_d$ is defined similarly.
2.2. Examples of quotient spaces. As a warmup, we first give a simple example of a quotient space resulting from the action of a finite group on a Euclidean space. This particular example is important in providing a relevant non-network analogy to our network-based results. We will revisit it frequently throughout the paper.

Example 2.1. The group $\mathbb{Z}_4 = \{0, 1, 2, 3\}$ acts on the plane $\mathbb{R}^2$ by rotation counterclockwise by 90 degrees: specifically, for $k \in \mathbb{Z}_4$ and $z \in \mathbb{R}^2 = \mathbb{C}$,

$$k \cdot z = e^{ik\pi/2} \cdot z.$$ 

Thus $0 \cdot z = z$, $1 \cdot z = e^{i\pi/2}z$, etc. A point in the quotient space $\mathbb{C}/\mathbb{Z}_4$ is the set $[z_0] = \{e^{ik\pi/2}z_0 : k \in \mathbb{Z}_4\}$. The set $[z_0]$ is called the orbit of $z_0$ under $\mathbb{Z}_4$.

Note that every orbit is a four element set except for the exceptional orbit $[\vec{0}] = \{0\}$. The closed first quadrant $F = \{(x, y) : x \geq 0, y \geq 0\}$ is a fundamental domain for this action; i.e., each orbit $[z_0]$ has a unique representative/element in $F$, except possibly for the orbits of points on the boundary $\partial F = \{(x, y) : x = 0 \text{ or } y = 0\}$ of $F$. Orbits of boundary points like $[(5, 0)]$ have two representatives $(5, 0)$, $(0, 5)$ in $F$, while the origin of course has only one representative.

If we want to picture a set that is bijective to $\mathbb{C}/\mathbb{Z}_4$, we could take e.g. $F'$ to be $F$ minus the positive $y$-axis. This is not so helpful topologically or geometrically, as the points $[(5, 0)]$ and $[(0, 5.01)]$ have close representatives $(5, 0)$, $(5.01, 0)$ in $F$, while their representatives $(5, 0)$ and $(0, 5.01)$ are not close in $F'$. In particular, the sequence $(10^{-k}, 5)$ does not converge in $F'$, but the orbits $[10^{-k}, 5]$ converge to $[0, 5] = [5, 0]$ in $\mathbb{C}/\mathbb{Z}_4$. Thus $F'$ does not give us a good picture of $\mathbb{C}/\mathbb{Z}_4$ topologically.

In summary, it is much better to keep both positive axes in $F$, and to consider $\mathbb{C}/\mathbb{Z}_4$ as (in bijection with) $F$ with the boundary points $(a, 0)$ and $(0, a)$ “glued together.” More precisely, we have a bijection

$$\beta : \mathcal{F} := \frac{F}{(a, 0) \sim (0, a)} \rightarrow \mathbb{C}/\mathbb{Z}_4,$$

where the denominator indicates that the two point set $\{(a, 0), (0, a)\}$ is one point of $\mathcal{F}$, while all other points of $F$ correspond to a single point in $\mathcal{F}$. At the price of this gluing, we now have that $\beta$ is a homeomorphism: points are close in $\mathcal{F}$ iff they are close in $\mathbb{C}/\mathbb{Z}_4$. (Technical remarks: $\mathcal{F}$ gets the quotient topology from the standard topology on $F$ and the obvious surjection $q : F \rightarrow \mathcal{F}$; and “close” refers to the Procrustean distance defined in Section 3.)
Although this seems a little involved, it is quite easy to perform the gluing in \( \mathcal{F} \) in rubber sheet topology: stretching the interior of \( \mathcal{F} \) to allow the gluing of the two axes shows that \( \mathcal{F} \) and hence \( \mathbb{C}/\mathbb{Z}_4 \) is a cone. See Figure 1.

**Example 2.2.** We work out in detail the case of a network with three vertices. This is a deceptively easy case, as \( 3 = d = D \) implies that every permutation of the \( D \) edge weights comes from a permutation in \( \Sigma_d \). In higher dimensions, the details are more complicated.

We first describe the quotient space \( \mathcal{U}_3 \) of unlabeled graphs directly, and then find a fundamental domain for \( \mathcal{U}_3 \) inside the space of labeled graphs \( \mathcal{O}_3 \). The direct approach is more difficult, which motivates our concentrating on fundamental domains in the rest of the paper.

Note that \( \Sigma_3 \) acts freely on \( \mathcal{O}_3^\neq = \{(x, y, z) \in \mathcal{O}_3 : x \neq y, x \neq z, y \neq z\}; \) i.e., \( \sigma \cdot (x, y, z) = (x, y, z) \) iff \( \sigma = \text{Id} \). The subset
\[
\mathcal{O}_3^{\neq 0} = \{(x, y, z) \in \mathcal{O}_3 : x \neq y, x \neq z, y \neq z; \text{ and } x, y, z \neq 0\}
\]
is an open 3-manifold which is dense in \( \mathcal{O}_3 \) and with a free \( \Sigma_3 \)-action, so we get a smooth 3-manifold structure on the open dense set \( \mathcal{O}_3^{\neq 0}/\Sigma_3 \subset \mathcal{O}_3/\Sigma_3 = \mathcal{U}_3 \).

Now let \( \mathcal{G}_3^0 \) be the subset of \( \mathcal{G}_3 \) consisting of graphs \( G \) with \( w_1(G) = 0 \); i.e., the weight of the edge \( (1, 2) \) (which is lexicographically the first edge) from vertex 1 to vertex 2 is zero. Then \( \alpha(\mathcal{G}_3^0) \) is the subset of the \( yz \)-plane (i.e.
$x = 0$) given by $\mathcal{O}_3^0 = \{(y, z) : y, z \geq 0\}$. The subgroup $\Sigma_3^0 = \{\text{Id}, (23)\} \subset \Sigma_3$ of permutations fixing edge $(2,3)$ fixes $\alpha(G_3^0)$. $\Sigma_3^0$ acts freely on ($\alpha$ of) the set of graphs $\{(y, z) : y, z \geq 0, y \neq z\}$ and fixes the diagonal line $\{y = z\}$. This is because $(2,3) \cdot (y, z) = (z, y)$. Thus the quotient space $\mathcal{O}_3^0 / G_3^0 \mapsto \{(y, z) : y > z \geq 0\}$ is homeomorphic to a closed pie wedge. We think of $\mathcal{O}_3^0 / G_3^0$ as a stratified 2-manifold: it contains an open, dense set which is a 2-manifold, the two edges (minus the origin) which are 1-manifolds, and the origin as a 0-manifold.

Denote the equivalence class of a point in $U_3$ by $[x, y, z]$. Each equivalence class in $\mathcal{O}_3^0 / G_3$ contains six points. In general, the number of elements in an equivalence class $[x, y, z]$ equals $\left|\Sigma_3\right|/\left|\Sigma_3^{[x,y,z]}\right| = 6/\left|\Sigma_3^{[x,y,z]}\right|$, where $\Sigma_3^{[x,y,z]} = \{\sigma \in \Sigma_3 : \sigma \cdot (x, y, z) = (x, y, z)\}$ is the stabilizer subgroup of $(x, y, z)$.

The three coordinate planes $\{(0, y, z) : y, z \geq 0\}$, etc. get glued under the action of $\Sigma_3$. For example, $(12) \cdot (0, 5, 7) = (5, 0, 7)$ and $(13) \cdot (0, 5, 7) = (7, 5, 0)$. Each coordinate plane gets further glued, e.g., $(0, 5, 7)$ gets glued to $(0, 7, 5)$. Thus the three coordinate planes get glued to one pie wedge. This pie wedge is glued onto $\mathcal{O}_3^0 / G_3$ as follows: given $[x_i, y_i, z_i]$ with $x_i \to 0$, we declare the limit point of this sequence to be $[0, y, z]$. We make the similar definition if $y_i \to 0$ or $z_i \to 0$. This is clearly well defined. We make a similar definition if $[x_i, y_i, z_i]$ has $x_i, y_i \to 0$, etc. and if $[x_i, y_i, z_i]$ has $x_i, y_i, z_i \to 0$.

From now on, for expository reasons, we drop the automatic conditions $x \geq 0, y \geq 0, z \geq 0$ from description of subsets of $\mathcal{O}_3$.

Similarly, the three planes $\{(x, y, z) : x = y\}, \{(x = z\}, \{y = z\}$ get glued together (e.g., $(123) \cdot (5, 5, 7) = (7, 5, 5)$). Note that e.g. $|[x, x, z]| = 3$ if $x \neq z$ and $|[x, x, x]| = 1$. For example $(5, 5, 7)$ is glued to $(5, 7, 5), (7, 5, 5)$. These three planes intersect at the line $\{(x, x, x)\}$. Thinking of the three planes as troughs with edge $\{x = y = z\}$, the three troughs are glued together. The two sides of a trough are not glued to each other, but are glued to sides of two other troughs. As above, $[x_i, y_i, z_i]$ has limit point is glued to $[x, x, x]$ if $x_i, y_i \to x$, etc. In particular, if $x_i, y_i \to 0$, this is consistent with the previous gluing.

The final quotient $\mathcal{O}_D / \Sigma_3$ is a stratified 3-manifold:

- The dense 3-dimensional piece is $\mathcal{O}_3^0 / \Sigma_3$, which is topologically a 3-ball.
- With increasingly terse notation, the 2d strata are
  
  (i) $\{[x, y, z] : x = 0, y \neq z; y, z \neq 0\} = \{[x, y, z] : y = 0, x \neq z\} = \{[x, y, z] : z = 0, x \neq y\}$;
  
  (ii) $\{x = y, z > x\} = \{y = z, x > y\} = \{x = z, y > x\}$;
  
  (iii) $\{x = y, 0 < z < x\} = \{y = z, 0 < x < y\}, \{x = z, 0 < y < x\}$.
• The 1d strata are
  (i) \( \{ x = 0, y = z \neq 0 \} = \{ y = 0, x = z \neq 0 \} = \{ z = 0, x = y \neq 0 \} \);
  (ii) \( \{ x = y = 0, z > 0 \} = \{ x = z = 0, y > 0 \} = \{ y = z = 0, x > 0 \} \);
  (iii) \( \{ x = y = z > 0 \} \).

• The 0d stratum is \( \{(0,0,0)\} \).

The point \([0,2,2]\) in the 1d stratum can be perturbed into a 2d stratum point \([\epsilon,2,2]\) or \([0,2,2 + \epsilon]\) or into a 3d stratum point \([\epsilon,2 + \delta,2 + \mu]\). This agrees with the fact that the 1d stratum \( \{ x = 0, y = z \} \) glues both to a trough (a 2d stratum) and to an open wedge in a coordinate plane, and that this 1d stratum also glues to the big cell.

It is easier to picture the quotient space of unlabeled networks by finding a fundamental domain \( F \) inside \( \mathcal{O}_3 \) for the action of \( \Sigma_3 \). As in the previous example, and detailed in Section 4, \( F \) is a closed set such that the quotient map \( q|_F : F \to \mathcal{U}_3 \) is a continuous surjection, a homeomorphism from the interior of \( F \) to a dense set of unlabeled networks, and a finite-to-one map on the boundary \( \partial F \) of \( F \). Thus \( F \) represents \( \mathcal{U}_3 \) bijectively except for some gluings on the boundary. This is illustrated in Figure 2, where \( F = \{(x,y,z) : x \geq y \geq z \geq 0 \} \). Again, the case \( d = 3 \) is deceptively easy, as \( F \) is a bijection even on \( \partial F \).

The situation is more complicated for graphs with 4 (or more) vertices. For \( d = 4 \), if we label the edges as \((1,2), \ldots, (3,4)\), then the weight vectors \((1,1,1,0,0,0)\) and \((1,1,0,1,0,0)\) have the same distributions of ones and zeros, but correspond to binary graphs which are not in the same orbit of \( \Sigma_4 \). In particular, the region \( \{(x_1, \ldots, x_6) : x_1 \geq x_2 \geq \ldots \geq x_6 \} \) is not a fundamental domain for the action of \( \Sigma_4 \).

While a fundamental domain is harder to find in high dimensions (see Section 4), the overall structure of \( \mathcal{U}_d \) for general \( d \) is similar to the \( d = 3 \) case, with just increased notation.

**Theorem 2.3.** The space of unlabeled graphs \( \mathcal{U}_d = \mathcal{G}/\Sigma_d = \mathcal{O}_D/\Sigma_d \) is a stratified space.

**Proof.** We just sketch the proof, since this result is not used below. We don’t need the technical definition of a stratified space, just a general understanding that \( \mathcal{U}_d \) consists of a sequence of \( n \)-dimensional manifolds with boundary, \( n = 1, \ldots, D \), with \( n \)-dimensional strata glued coherently to \((n + 1)\) (or higher) dimensional strata. The big open cell of dimension \( D \) is
As explained in Section 4.1, the infinite solid cone, which is the region \( \{ x \geq y \geq z \geq 0 \} \), is a fundamental domain \( F \) for unlabeled networks with three nodes. With the convention that the bottom side of the triangle has weight \( x \), the left side has weight \( y \), and the right side has weight \( z \), the network with edge weights 1, 2, 3 corresponds to the point \( P \) in the interior of the cone. Other networks shown are color coded to correspond to points on faces or edges of the cone.
Lower strata are characterized by the number of zero entries and the number of equal nonzero entries. More precisely, say the weight vector \( \vec{x} \in \mathcal{O}_D \) has \( k \) zeros and \( s_1 > 1 \) entries equal to \( w_1 \neq 0, \ldots, s_t \) entries equal to \( w_t \neq 0 \), with all \( w_i \) distinct. Then \( [\vec{x}] \in \mathcal{U}_d \) belongs to a stratum of dimension

\[
D - k - \sum_{i=1}^{t} s_i.
\]

A higher dimensional stratum \( S \) has a lower dimensional stratum \( S' \) as part of \( \partial S \) if a sequence of points in \( S \) converges to a point in \( S' \). This can occur either by an entry in this sequence going to zero, or by entries in this sequence going to a common positive limit.

By [24], \( \mathbb{R}^D / \Sigma_d \) is PL or Lipschitz homeomorphic to \( \mathbb{R}^{D-1} \times \mathbb{R}_{\geq 0} \), but the proof does not give a cell decomposition of \( \mathbb{R}^D / \Sigma_d \), much less of \( \mathcal{U}_d \).

3. Network averages and their asymptotic behavior. In this section we define the mean of a distribution \( Q \) on the space of networks and investigate the asymptotic behavior of the empirical (or sample) mean network based on an i.i.d sample of networks from \( Q \). Statistical inference can be carried out based on the asymptotic distribution of the empirical mean. We illustrate with an example from hypothesis testing. The results of the previous section, characterizing the topology and geometry of the space of unlabeled networks, are essential for achieving our goals in this section.

3.1. Network averages through Fréchet means. Let \( Q \) be some distribution on a general metric space \((M, \rho)\). One can define the Fréchet function \( f(p) \) on \( M \) as

\[
f(p) = \int_M \rho^2(p, z)Q(dz) \quad (p \in M).
\]

If \( f \) is finite on \( M \) and has a unique minimizer

\[
\mu = \text{argmin}_p f(p),
\]

then \( \mu \) is called the Fréchet mean of \( Q \) (with respect to the metric \( \rho \)). Otherwise, the minimizers of the Fréchet function form a Fréchet mean set \( C_Q \). Given an i.i.d sample \( X_1, \ldots, X_n \sim Q \) on \( M \), the empirical Fréchet mean can be defined by replacing \( Q \) with the empirical distribution \( Q_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i} \), that is,

\[
\mu_n = \text{argmin}_p \frac{1}{n} \sum_{i=1}^{n} \rho^2(p, X_i).
\]
When $M$ is a manifold, one can equip $M$ with a metric space structure through an embedding into some Euclidean space or employing a Riemannian structure of $M$. Respectively, $\rho$ can be taken to be the Euclidean distance $d_E$ after embedding (extrinsic distance) or the geodesic distance (intrinsic distance), giving rise to extrinsic and intrinsic means. Asymptotic theory for extrinsic and intrinsic analysis has been developed in [6],[8], [9], and applied to many manifolds of interest (see e.g., [5], [16]).

Now take $M = \mathcal{U}_d$, the space of unlabeled networks with $d$ nodes, our space of interest, and let $Q$ be a distribution on $\mathcal{U}_d$. Given an i.i.d sample $X_1, \ldots, X_n$ from $Q$, in order to define the Fréchet mean $\mu$ of $Q$ and empirical Fréchet mean $\mu_n$ of $Q_n$, one needs an appropriate choice of distance on $\mathcal{U}_d$. Given the quotient space structure characterized in the previous section, i.e., $\mathcal{U}_d = G_d/\Sigma_d$, a natural choice for the distance $\rho$ is the Procrustean distance $d_P$, where

$$d_P([\vec{x}], [\vec{y}]) := \min_{\sigma_1, \sigma_2 \in \Sigma_d} d_E(\sigma_1 \cdot \vec{x}, \sigma_2 \cdot \vec{y}),$$

for unlabeled networks $[\vec{x}], [\vec{y}] \in \mathcal{U}_d$, with $\vec{x}$ denoting the vectorized representation of a representative network $x$. We recall that $G_d$ is the set of all labeled graphs with $d$ vertices and $\Sigma_d$ is the group of permutations of $\{1, 2, \ldots, d\}$.

In order to carry out statistical inference based on $\mu_n$, defined with respect to the distance (3.4), some natural and fundamental questions related to $\mu$ and $\mu_n$ need to be addressed, which we aim to do in the following subsections. Here are some of the most crucial ones:

1. (Consistency.) What are the consistency properties of the network empirical mean $\mu_n$, i.e., is $\mu_n$ a consistent estimator of the population Fréchet mean $\mu$? Can we establish some notion of a law of large numbers for $\mu_n$?

2. (Uniqueness of Fréchet mean.) This question is concerned with establishing general conditions on $Q$ for uniqueness of the Fréchet mean $\mu$. In general this a challenging task – indeed, the lack of general uniqueness conditions for Fréchet means is still one of the main hurdles for carrying out intrinsic analysis on manifolds [22]. To date the most general results in the literature for generic manifolds [1] force the support of $Q$ to be a small geodesic ball to guarantee uniqueness of the intrinsic Fréchet mean. We address this question for the space of unlabeled networks in Section 4.

3. (CLT.) Once conditions for uniqueness of $\mu$ are provided, the next key question is whether one can derive the limiting distribution for $\mu_n$ for purposes of statistical inference, e.g., proving a central limit type of theorem for $\mu_n$, which in turn might be used for hypothesis testing.
We first illustrate the difficult nature of these problems (in particular for question 2 above) through the example $C = \mathbb{R}^2/\mathbb{Z}_4$ in Section 2, by explicitly constructing a distribution on $C$ that has non-unique Fréchet means.

**Example 3.1 (Example $C = \mathbb{R}^2/\mathbb{Z}_4$ continued).** As in Example 2.1 in Section 2, the quotient $C = \mathbb{R}^2/\mathbb{Z}_4$ is a cone. Working in polar coordinates and taking $F_0 = [0, \infty) \times [-\pi/4, \pi/4)$ to be a fundamental domain, we consider probability distributions of the form $\nu(r, \theta) = \frac{1}{M} R(r) \chi(\theta)$, where $M = \int_{F_0} R(r) \chi(\theta) r d\theta$.

We can explicitly compute the Fréchet function $f(x)$ with respect to $\nu$. For $x = (r, \theta) \in F_0$, $F_{\theta} = [0, \infty) \times [-\pi/4 + \theta, \pi/4 + \theta]$ is a fundamental domain. For $y \in F_{\theta}$, $dP([x], [y]) = d_E(x, y)$. Then

$$f(x) = \int_{F_{\theta}} ||x - y||^2 \nu(y) dy = \frac{1}{M} \left( c_1 \chi_1 r^2 - 2c_2 \chi_2(\theta) r + c_3 \chi_1 \right),$$

where $c_k = \int_0^\infty r^k R(r) dr$ for $k = 1, 2, 3$, $\chi_1(\theta) = \int_{\theta - \pi/4}^{\theta + \pi/4} \chi(t) dt$ and $\chi_2(\theta) = \int_{\theta - \pi/4}^{\theta + \pi/4} \chi(t) \cos(\theta - t) dt$.

The Fréchet mean occurs when $\partial f/\partial r = \partial f/\partial \theta = 0$, which is difficult to compute in general. Consider the special case

$$(3.5) \quad \nu(r, \theta) = \frac{1}{M} \exp(-(r - \alpha)^2),$$

where $\alpha$ is a fixed constant, $\chi(\theta) \equiv 1$, $M = (\pi^{3/2} / 4)(1 + \text{erf}(\alpha))$; this distribution for $\alpha = 15$ is plotted in Figure 3. The minimum for this $f$ occurs at

$$r_0 = \frac{\sqrt{2} \left( 2\alpha + \sqrt{\pi} e^\alpha \left( 2\alpha^2 + 1 \right) \left( \text{erf}(\alpha) + 1 \right) \right)}{\pi^{3/2} e^{\alpha^2} \alpha (\text{erf}(\alpha) + 1) + \pi},$$

with $\theta$ arbitrary. When $\alpha$ is large, $r_0 \approx \frac{2\sqrt{2}}{\pi} \alpha$. For $\alpha = 15$, $r_0 \approx 13.5348$. This shows that $\nu$ has a circle’s worth of Fréchet means; the $\theta$-independence of $\nu$ implies $\theta$-independence of the Fréchet means. One can see this in Figure 4 where the Fréchet function $f(x)$ is minimal and most blue on a circle of radius approximately 13.53 (corresponding to the red circle on the cone in Figure 3).

### 3.2. A strong law of large numbers.

Before establishing the limiting distribution for $\mu_n$, a natural first step is to explore the consistency properties of $\mu_n$. Drawing on Theorem 3.3 in [6] for general metric spaces, we have the following result.
Figure 3. Plot of the probability distribution $\nu(r, \theta)$ in (3.5), with $\alpha = 15$. The distribution peaks in the red region where $\nu$ is large, and is small in the blue region. The left hand side shows the plot on $\mathbb{R}^2$, and the right hand side shows that plot on the cone.

**Theorem 3.1.** Let $Q$ be a distribution on $\mathcal{U}_d$, let $C_Q$ be the set of means of $Q$ with respect to the Procrustean distance $d_P$, and let $C_{Q_n}$ be the set of empirical means with respect to a sample of unlabeled networks $X_1, \ldots, X_n$. Assume that the Fréchet function is everywhere finite. Then the following holds: (a) the Fréchet mean set $C_Q$ is nonempty and compact; (b) for any $\epsilon > 0$, there exists a positive integer-valued random variable $N = N(\epsilon)$ and a $Q$-null set $\Omega(\epsilon)$ such that

$$C_{Q_n} \subseteq C_Q^\epsilon = \{ p \in M : d_P(p, C_Q) < \epsilon \} \quad \forall \ n \geq N$$

outside of $\Omega(\epsilon)$; (c) if $C_Q$ is a singleton, i.e., the Fréchet mean $\mu$ is unique, then $\mu_n$ is a strongly consistent estimator of $\mu$, or $\mu_n$ converges to $\mu$ almost surely.

**Proof.** We first prove that every closed and bounded subset of $M = \mathcal{U}_d$ is compact.

Let $F$ be a fundamental domain for the action of $\Sigma_d$ on $\mathcal{G}_d$, as defined in Section 4, with the associated projection $q : F \to \mathcal{U}_d$. This map is continuous and a diffeomorphism on the interior of $F$. Take a closed and bounded set $S$ in $\mathcal{U}_d$. Because $q$ is continuous, $q^{-1}(S)$ is closed. We now show that $q^{-1}(S)$ is also bounded. $S$ is contained in a ball centered at some $\vec{z} \in \mathcal{U}_d$ with radius
Fig 4. Plot of the Fréchet function $f(x)$ with $\alpha = 15$ on $\mathbb{R}^2$ and on the cone. The Fréchet mean occurs in the “most blue” region, on a circle of radius approximately 13.53.

$r$, so $d_P([\tilde{z}], [\tilde{x}]) < r$ for $[\tilde{x}] \in S$. Now say that the largest entry in $[\tilde{z}]$ (in any ordering of the entries of $\tilde{z}$) is $C$. If the largest entry in $\tilde{x}$ (in any ordering) is greater than $C + r$, then $d_P([\tilde{z}], [\tilde{x}]) > (C + r) - C$, a contradiction. (This holds because under any permutation $\sigma$ of the entries of $\tilde{x}$, one entry in $d_E(\tilde{z}, \sigma \cdot \tilde{x})$ is greater than $(C + r) - C$.) Thus for any choice of $\tilde{x} \in S$, $\|\tilde{x}\| \leq \sqrt{D}(C + r)$. Thus $q^{-1}(S)$ is contained in the ball of radius $\sqrt{D}(C + r)$ centered at the origin, and thus is bounded.

Since $F$ is a closed subset of $\mathbb{R}^D$, the closed and bounded set $q^{-1}(S)$ is compact. Since $q$ is continuous, $S$ is compact.

Then by Theorem 3.3 in [6], (a) and (b) follow.

Part (c) follows from [33] under the uniqueness of Fréchet mean.

\[ \square \]

3.3. A central limit theorem. The goal of this section is to derive a central limit theorem for the empirical Fréchet mean, as an important precursor for statistical inference. One of the key challenges is to establish geometric conditions on distributions on $U_d$ which ensure the uniqueness of the population Fréchet mean. We discuss and address the uniqueness issue in detail in Section 4. Here, our central limit theorem assumes that the uniqueness conditions of Section 4 are met.

Let $q : \mathcal{O}_D \to U_d$ be the projection from the space of labeled networks to the space of unlabeled networks.

**Theorem 3.2.** Assume $Q$ has support on a compact set $K \subset \mathcal{O}_D$ defined in Theorem 4.1, so that the pushdown measure $Q' = q_*Q$ supported on $K' = q(K)$ has a unique Fréchet mean $\mu$. Let $\mu_n$ be the empirical Fréchet mean
of an i.i.d sample \( X_1, \ldots, X_n \sim Q \) with respect to the distance (3.4). Let \( \phi = q^{-1} \). Then we have

\[
\sqrt{n} (\phi(\mu_n) - \phi(\mu)) \xrightarrow{L} N(0, \Sigma),
\]

where \( \Sigma = \Lambda^{-1} C \Lambda^{-1} \) with the Hessian matrix

\[
\Lambda = \left( \mathbb{E}[D_{r,s}\|\phi(\mu) - \phi(X_1)\|] \right)_{r,s=1,\ldots,D},
\]

and \( C \) is the covariance matrix of \( \{D_r\|\phi(\mu) - \phi(X_1)\|\}_{r=1,\ldots,D} \).

Here \( D_r \) denotes the partial derivative with respect to the \( r \)th direction, \( D_{r,s} \) denotes second partial derivatives, and \( \xrightarrow{L} \) means convergence in law or distribution.

**Proof.** Let \( U \) be a small open neighborhood of \( \mu \) inside \( K \), so \( S = \phi^{-1}(U) \) is an open subset of \( \mathbb{R}^D \). Note that \( \phi : U \to S \) is a homeomorphism. By Theorem 4.1, the projection map \( q \) is a Euclidean isometry. Therefore, for any vectorized network \( \vec{x} \in S \) and \( [\vec{z}] \in U \), one has

\[
d^2_P([\vec{x}], [\vec{z}]) = d^2_P(\phi^{-1}(\vec{x}), [\vec{z}]) = \|\vec{x} - \vec{z}\|^2,
\]

where \( \vec{z} = \phi([\vec{z}]) \). Thus \( d^2_P(\phi^{-1}(\vec{x}), [\vec{z}]) \) is twice differentiable in \( \vec{x} \) for any \( [\vec{z}] \in U \). Tracing through the definition of the smooth structure on \( U \) induced from the standard structure on \( \mathbb{R}^D \), we see that \( d^2_P([\vec{x}], [\vec{z}]) \) is twice differentiable in \( [\vec{x}] \). Also note that by the consistency of \( \mu_n \) (see Theorem 3.1), one has \( P(\mu_n \in U) \to 1 \) as \( n \to \infty \). One can also verify the conditions (A5) and (A6) on the Hessian matrices of Theorem 2.2 in [7], and our Theorem follows.

As an immediate consequence of this central limit theorem, we can define natural analogues of classical hypothesis tests. For example, consider the construction of a statistical test for two or more independent samples using the same framework. Assume that we have \( k \) independent sets of networks on \( d \) vertices, and consider the problem of testing whether or not these sets have in fact been drawn from the same population. Formally, we have independent samples \( X_{ij} \sim Q_j \), for \( i = 1, \ldots, n_j \) and \( j = 1, \ldots, k \). Each of these \( k \) populations has an unknown mean, denoted \( \mu^{(j)} \). Then, as a direct corollary to Theorem 3.2, we have the following asymptotic result.

**Corollary 3.2.** Assume that the distributions \( Q_1, \ldots, Q_k \) satisfy the conditions of Theorem 3.2. Moreover, also assume that \( n_j/n \to p_j \) for every
sample, with $n := \sum_j n_j$, and $0 < p_j < 1$. Then, under $H_0 : \phi(\mu^{(1)}) = \ldots = \phi(\mu^{(k)})$, we have

$$T_k := \sum_{j=1}^k n_j (\phi(\mu_{j,n_j}) - \phi(\mu_n))^t \hat{\Xi}^{-1} (\phi(\mu_{j,n_j}) - \phi(\mu_n)) \to \chi^2_{(k-1)D},$$

where $\mu_{j,n_j}$ denotes the empirical mean of the $j$th sample, $\mu_n$ represents the grand empirical mean of the full sample, and $\hat{\Xi} := \sum_{j=1}^k \hat{\Xi}_j/n_j$ is a pooled estimate of covariance, with the $\hat{\Xi}_j$'s denoting the individual covariance matrices estimates of each subsample.

As previously noted, this central limit theorem and such corollaries hold only if the population Fréchet mean(s) is unique. This depends crucially on the nontrivial geometry of the space of unlabeled networks. The following section deals exclusively with this issue.

4. Geometric requirements for uniqueness of the Fréchet mean.

Underlying the central limit theorem in Theorem 3.2, the basic question is: which compact subsets $K'$ of $U_d$ have a unique Fréchet mean?

We have seen in Section 2 that $U_d$ may be difficult to work with, while a fundamental domain $F \subset \mathcal{O}_D$ for the action of $\Sigma_d$ on the space of labeled networks $\mathcal{O}_D$ seems more tractable. Indeed, finding the Fréchet mean for a distribution supported in $F$ is a standard center of mass calculation in Euclidean space. However, it is not clear that this Fréchet mean “upstairs” in $F$ projects to the Fréchet mean “downstairs” in the quotient space $U_d = \mathcal{O}_D/\Sigma_d$, because the metric used to compute Fréchet means downstairs is the Procrustean distance, which may or may not equal the Euclidean distance.

In this section, we find a fundamental domain $F$ by a standard procedure (Lemma 4.1), and find compact subsets $K \subset F$ for which the Fréchet mean upstairs is guaranteed to project to the Fréchet mean of $K' \subset U_d$, where $K' = q(K)$ is the projection of $K$ under the quotient/projection map $q : \mathcal{O}_D \to U_d = \mathcal{O}_D/\Sigma_d$. This is the content of the main result in this section (Theorem 4.1). We also show that this result in our special setup is an improvement of the best result for general Riemannian manifolds due to Afsari [1] (see Figure 6).

We now discuss the construction of a fundamental domain $F$. A fundamental domain is characterized by: (i) every weight vector $x$ can be permuted by some $\sigma \in \Sigma_d$ to a network $\sigma \cdot x$ in $F$; (ii) if $\bar{w} \in \mathcal{O}_D$ has $\bar{w} \in F \cap \sigma F$ for $\sigma \in \Sigma_d, \sigma \neq \text{Id}$, then $\bar{w} \in \partial F$. (As a technical note, we always consider $\partial F$
with respect to the induced topology on $\mathcal{O}_D$ from the standard topology on $\mathbb{R}^D$. ) Once $F$ has been constructed, we are guaranteed that the projection map $q : \mathcal{O}_D \to \mathcal{U}_d, q(\vec{w}) = [\vec{w}]$ restricts to a surjective map $q : F \to \mathcal{U}_d$ which is a homeomorphism from the interior $F^o$ of $F$ to $q(F^o)$. (In fact, $q$ is a diffeomorphism on this region by definition of the smooth structure on $q(F^o)$.)

It is convenient to center a choice of fundamental domain on a weight vector with trivial stabilizer.

**Definition 4.1.** A vector $\vec{w} = (w_1, \ldots, w_D) \in \mathcal{O}_D$ is distinct if it has trivial stabilizer for the action of $\Sigma_d$: i.e., if $\sigma \cdot \vec{w} \neq \vec{w}$ for all $\sigma \in \Sigma_d, \sigma \neq \text{id}$.

A vector with trivial stabilizer is also called a vector with trivial automorphism group. Weight vectors with all different entries are distinct, which implies that the distinct vectors are dense in $\mathcal{O}_D$.

For example, consider the two graphs $G_1$ and $G_2$ in Figure 5. Both share the same connectivity pattern (i.e., are isomorphic), but have different weight vectors. The weight vector $\vec{w}^1 = (20, 20, 7, \ldots)$ of $G_1$ satisfies $\sigma \cdot \vec{w}^1 = \vec{w}^1$ for $\sigma = (23) \in \Sigma_7$. In contrast, for all $\sigma \in \Sigma_7 \setminus \{\text{id}\}$, $\sigma \cdot \vec{w}^2 \neq \vec{w}^2$, where $\vec{w}^2$ is the weight vector of $G_2$, because the two 20’s belong to nodes with different valences. Thus even though $\vec{w}^1, \vec{w}^2$ have the same set of weights, $\vec{w}^2$ is distinct, while $\vec{w}^1$ is not.

We now explain a standard procedure to construct a fundamental domain as one region in the Voronoi diagram of the orbit of a distinct vector. (Ge-
ometers call this a Dirichlet domain.) Let $d_P$ be the Procrustean distance on $O_D/\Sigma_d$. From now on, we just write $\bar{w}$ instead of $[\bar{w}]$ for elements of $U_d$.

**Lemma 4.1.** Fix a distinct vector $\bar{w} \in O_D$. Set

\[ F = F_{\bar{w}} = \{ \bar{w}' \in O_D : d_E(\bar{w}, \bar{w}') \leq d_E(\bar{w}, \sigma \cdot \bar{w}'), \; \forall \sigma \in \Sigma_d \} = \{ \bar{w}' \in O_D : d_E(\bar{w}, \bar{w}') = d_P(\bar{w}, \bar{w}') \} \]

Then

(i) $F$ is a fundamental domain for the action of $\Sigma_d$ on $O_D$.

(ii) $F$ is a solid cone with polyhedral cross section.

In the proof, we use the fact that $\bar{w}$ is distinct just below (4.1).

**Proof.** (i) First, for fixed $\bar{w}_1$, a minimum of $d_E(\bar{w}, \sigma \cdot \bar{w}_1)$ is attained, since $\Sigma_d$ is finite. Thus every network (characterized by its weight vector $\bar{w}_1$) has a permutation in $F$.

Second, we can rewrite $F$ as

\[ F = \{ \bar{w}_1 \in O_D : d_E(\bar{w}, \bar{w}_1) \leq d_E(\sigma \cdot \bar{w}, \bar{w}_1), \; \forall \sigma \in \Sigma_d \}. \]

Let $\bar{w}_1 \in F \cap \sigma F$. Then $\sigma^{-1} \bar{w}_1 \in F$, and

\[
\begin{align*}
    d_E(\bar{w}, \bar{w}_1) &= \min_\tau d_E(\bar{w}, \tau \cdot \bar{w}_1), \\
    d_E(\bar{w}, \sigma^{-1} \bar{w}_1) &= \min_\tau d(\bar{w}, \tau \cdot \sigma^{-1} \bar{w}_1) \\
    &= \min_\tau d(\bar{w}, \tau \cdot \bar{w}_1).
\end{align*}
\]

Thus

\[ d_E(\bar{w}, \bar{w}_1) = d_E(\bar{w}, \sigma^{-1} \bar{w}_1) = d_E(\sigma \cdot \bar{w}, \bar{w}_1), \] (4.1)

so $\bar{w}_1$ is equidistant to $\bar{w}$ and $\sigma \bar{w}$. Since $\bar{w}$ is distinct, $\sigma \bar{w} \neq \bar{w}$ for $\sigma \neq \text{id}$. Thus $\bar{w}_1$ lies on a hyperplane in $O_D$ defined by (4.1), and any ball around $\bar{w}'$ contains points that are closer to $\bar{w}$ than to $\sigma \bar{w}$, and points that are farther from $\bar{w}$ than from $\sigma \bar{w}$. Therefore $\bar{w}_1 \in \partial F$.

(ii) We can construct $F'$ for the action of $\Sigma_d$ on all of $\mathbb{R}^D$ by taking the set of hyperplanes $H_\sigma$ of points equidistant from $\bar{w}$ and $\sigma \bar{w}$ for $\sigma \in \Sigma_d$, and taking the connected component of $O_D \setminus \bigcup_\sigma H_\sigma$ containing $\bar{w}$. Since these hyperplanes all pass through the origin, this component is a solid cone on the origin. The boundary is given by a union of hyperplanes, so the cross section is a polyhedron. (Not all hyperplanes contribute edges to the cross sectional polygon; see the next example.) Moreover, $\Sigma_d$ preserves $O_D$, so a fundamental domain in $O_D$ is given by $F = F' \cap O_D$. The boundary planes of $F$ are either boundary planes of $F'$ or (subspaces of) the boundary of $O_D$.  

\[ \square \]
This Dirichlet/Voronoi fundamental domain depends on a choice of \( \vec{w} \). In particular, for a fixed distinct \( \vec{w}_0 \), we can guarantee that \( \vec{w}_0 \) is in the interior of \( F \) by setting \( \vec{w} = \vec{w}_0 \) in the lemma.

\( F \) is a solid cone cut out by at most \( d! - 1 + D \) hyperplanes, where \( d! - 1 \) is the order of \( \Sigma_d \setminus \{ \text{Id} \} \) and \( D \) is the number of coordinate hyperplanes. Thus this construction of \( F \) is not very practical except in low dimensions. Looking back at Figure 2, the infinite solid cone is the fundamental domain for the distinct vector \((3, 2, 1)\). See Appendix A for an algorithm that computes the fundamental domain and examples for \( d = 3, 4 \).

We now give more information about \( F \). The following result, although interesting, is not used below.

**Proposition 4.2.** Let \( F \) be the fundamental domain associated to a distinct vector \( \vec{w} \in O_D \). All distinct vectors in \( F \) have a representative in the interior \( F^0 \) of \( F \).

**Proof.** See Supplement A. \( \square \)

**Remark 4.3.** Any nondistinct vector \( \vec{w}' \) has an arbitrarily close distinct vector \( \vec{w} \). Then \( d_P(\vec{w}, \vec{w}') = d_E(\vec{w}, \vec{w}') \), and this remains true for vectors close to \( \vec{w} \). Therefore, \( \vec{w}' \) is in the interior \( F^0 \) of \( F = F_{\vec{w}} \). Thus for any nondistinct vector \( \vec{w}' \), we can find a fundamental domain that contains \( \vec{w}' \) in its interior.

The next lemma gives a sense of the minimal size of \( F \). Let \( F_c \) denote the solid cone with vertex at the origin, axis \( \vec{w} \), and cone angle \( c \). Let \( a = a_{\vec{w}} \) be the smallest angle between \( \vec{w} \) and \( \sigma \cdot \vec{w} \) for \( \sigma \in \Sigma_d \), for \( \sigma \neq \text{id} \). Of course, \( a/2 \) is the smallest angle between \( \vec{w} \) and a hyperplane boundary of \( F \).

**Lemma 4.2.** \( F \) contains the solid cone \( F_{a/2} \).

**Proof.** We claim that for vectors \( \vec{u}, \vec{\ell}, \vec{v} \), the angles formed by them satisfy

\[
\angle(\vec{u}, \vec{\ell}) + \angle(\vec{\ell}, \vec{v}) \geq \angle(\vec{u}, \vec{v}).
\]

To prove this, we may assume the \( \vec{u}, \vec{v}, \vec{\ell} \) are unit vectors. Let \( \vec{\ell}' \) be the projection of \( \vec{\ell} \) into the plane of \( \vec{u} \) and \( \vec{v} \). Assume that \( \angle(\vec{u}, \vec{\ell}') + \angle(\vec{\ell}', \vec{v}) = \angle(\vec{u}, \vec{v}) \). Then \( \cos(\angle(\vec{u}, \vec{\ell}')) = \vec{u} \cdot \vec{\ell}' / |\vec{\ell}'| \geq \vec{u} \cdot \vec{\ell}' \), and \( \cos(\angle(\vec{u}, \vec{\ell})) = \vec{u} \cdot \vec{\ell} = \vec{u} \cdot \vec{\ell}' + \vec{u} \cdot (\vec{\ell} - \vec{\ell}') = \vec{u} \cdot \vec{\ell}' \), since \( \vec{\ell} - \vec{\ell}' \) is normal to the \( (\vec{u}, \vec{v}) \)-plane. Thus \( \angle(\vec{u}, \vec{\ell}') \leq \angle(\vec{u}, \vec{\ell}) \). Similarly, \( \angle(\vec{\ell}', \vec{v}) \leq \angle(\vec{\ell}, \vec{v}) \). Thus \( \angle(\vec{u}, \vec{\ell}) + \angle(\vec{\ell}', \vec{v}) \geq \angle(\vec{u}, \vec{\ell}') + \angle(\vec{\ell}', \vec{v}) = \angle(\vec{u}, \vec{v}) \). The other possibility is that \( \angle(\vec{u}, \vec{\ell}) - \angle(\vec{\ell}', \vec{v}) = \angle(\vec{u}, \vec{v}) \) or the same with \( \vec{u} \) and \( \vec{v} \) switched. In this case, \( \cos(\angle(\vec{u}, \vec{\ell}')) = \vec{u} \cdot \vec{\ell}' \leq \cos(\angle(\vec{u}, \vec{\ell}')) \) implies \( \angle(\vec{u}, \vec{\ell'}) \geq \angle(\vec{u}, \vec{\ell}). \)
Thus for a fixed permutation \( \sigma \), we have 
\[
\angle(\vec{\ell}, \vec{u}) + \angle(\vec{u}, \sigma \cdot \vec{\ell}) \geq \angle(\vec{\ell}, \sigma \cdot \vec{\ell}) \geq a. 
\]
Therefore
\[
\vec{u} \in F_{a/2} \implies \angle(\vec{u}, \sigma \cdot \vec{\ell}) \geq a/2. 
\]

We may assume that \( |\vec{\ell}| = |\vec{u}| \). Because \( \vec{u} \) and the \( \sigma \cdot \vec{\ell} \) all lie on the sphere of radius \( |\vec{\ell}| \), the distances between \( \vec{u}, \vec{\ell}, \sigma \cdot \vec{\ell} \) are proportional to the angles they form with the origin. Thus (4.2) implies that 
\[
d_E(\vec{u}, \sigma \cdot \vec{\ell}) \geq d_E(\vec{u}, \vec{\ell}), 
\]
so \( \vec{u} \in F \).

Although the topology of the interior \( F^o \) “upstairs” and its image \( q(F^o) \) “downstairs” are the same, their geometries are very different; this underlies the difference in general between the Fréchet means upstairs and downstairs.

Example 4.4 (Example C = \( \mathbb{R}^2/\mathbb{Z}_4 \) continued). \( F^o \) is the open first quadrant. Let \( \vec{v}, \vec{\ell} \in F^o \) cut out angles \( \alpha, \beta \) with the positive \( x \)-axis, respectively. By the law of cosines, the Euclidean distance between \( \vec{v}, \vec{\ell} \) is less than the distance between \( \vec{v} \) and \( R_{\pi/2} \vec{\ell} \), the rotation of \( \vec{\ell} \) by \( \pi/2 \) radians counterclockwise, iff \( |\alpha - \beta| < \pi/4 \). Thus for \( |\alpha - \beta| > \pi/4 \), 
\[
d_E(\vec{v}, \vec{\ell}) \neq d_P([\vec{v}], [\vec{\ell}]). 
\]
Thus distances upstairs and downstairs are different.

This affects the Fréchet means. Let \( \nu = (4/3\pi) r \, dr \, d\theta \) be the uniform probability measure on \( F \) supported on \( \{(r, \theta) \in [1, 2] \times [0, \pi/2]\} \). The Fréchet mean upstairs on \( F \) is the center of mass \( (3/2, 3/2) \). The cone \( C \) has a circle action which rotates points equidistant from the vertex, and the Procrustean distance is clearly invariant under this action. This implies that if \( [(r_0, \theta_0)] \) is a Fréchet mean on \( C \), so is \( [(r_0, \theta)] \) for all \( \theta \). Therefore, we can compute the Fréchet mean at \( \theta = \pi/4 \). Since \( |(\pi/4) - \beta| \leq \pi/4 \) in \( F \), 
\[
d_E((r_0, \pi/4), (r, \theta)) = d_P((r_0, \pi/4), (r, \theta)) \text{ for all } (r, \theta) \in F. 
\]
The previous computation gives \( r_0 = 3/2 \). We conclude that the Fréchet mean downstairs on \( C \) is the entire circle \( r = 3/2 \).

We now find a sub-cone of \( F \) such that the Fréchet mean of a compact convex set \( K \) inside this sub-cone projects to the unique Fréchet mean of the associated quotient space \( K' = q(K) \) inside \( U_d \). As explained at the beginning of this section, this allows us to derive a central limit theorem on \( K' \).

Theorem 4.1. \( K \) be a compact convex subset of the closed cone \( F_{a/4} \), and let \( Q \) be a distribution supported on \( K \). Let \( Q' = q_*Q \) be the pushdown measure on \( K' = q(K) \). Then the Fréchet mean of \( K \) projects to the unique Fréchet mean \( \mu_K' \) of \( K' \). In other words, let \( K' \subset U_d \) be such that there
exists a compact convex set $K \subset F_{a/4}$ with $q : K \to K'$ a homeomorphism. Then the Fréchet mean $\mu_{K'}$ of $K'$ is unique and satisfies $q(\mu_K) = \mu_{K'}$.

See Figure 5 for a schematic picture.

**Proof.** Take $\vec{u}, \vec{v} \in F_{a/4}$ with $|\vec{u}| = |\vec{v}| = 1$. As in the previous lemma, $\angle(\vec{u}, \vec{e}) + \angle(\vec{e}, \vec{v}) \geq \angle(\vec{u}, \vec{v})$, with equality iff $\vec{u}, \vec{v}, \vec{e}$ are coplanar. Thus

$$\angle(\vec{u}, \vec{v}) \leq 2(a/4).$$

On the other hand, for $\sigma \neq \text{id}$, we have as above

$$\angle(\vec{u}, \sigma \cdot \vec{v}) + \angle(\sigma \cdot \vec{v}, \sigma \cdot \vec{e}) \geq \angle(\vec{u}, \sigma \cdot \vec{e}) \Rightarrow \angle(\vec{u}, \sigma \cdot \vec{v}) \geq \angle(\vec{u}, \sigma \cdot \vec{e}) - \angle(\vec{v}, \vec{e}).$$

Let the plane containing $\vec{0}, \vec{u}, \sigma \cdot \vec{e}$ intersect $\partial F$ at a line containing the unit vector $\vec{z}$. Then

$$\angle(\vec{u}, \sigma \cdot \vec{e}) = \angle(\vec{u}, \vec{z}) + \angle(\vec{z}, \sigma \cdot \vec{e}) \geq (a/2 - a/4) + a/2 = 3a/4.$$

Therefore

$$\angle(\vec{u}, \sigma \cdot \vec{v}) \geq 3a/4 - a/4 = a/2 \geq \angle(\vec{u}, \vec{v}).$$

Since $|\vec{u}| = |\vec{v}| = |\sigma \cdot \vec{v}| = 1$, the distance between these vectors is proportional to their angles. This implies that

$$d^2_P(\vec{u}, \vec{v}) = d^2_P([\vec{u}],[\vec{v}])$$

on $F_{a/4}$.

As a compact convex subset of Euclidean space, $K$ has a unique Fréchet mean. It follows that $K'$ is compact convex. $q : K \to K'$ is a homeomorphism, so for $[\vec{x}] \in K'$, the Fréchet functions on $K'$ and $K$ satisfy

$$f([\vec{x}]) = \int_{K'} d^2_P([\vec{x}],[\vec{y}]) q_* Q(d[\vec{y}]) = \int_{K} d^2_E(\vec{x}, \vec{y}) Q(d\vec{y}) = f(\vec{x}).$$

Thus the Fréchet mean $\mu_K$ of $f$ on $K$ projects to $\mu_{K'}$, the unique Fréchet mean of $f$ on $K'$.

It follows from the proof that the distance function $d^2_P$ is convex on the projection of the $F_{a/4}$ cone.

From Thm. 4.1, we derive the main result Thm. 3.2.

We now prove that Thm. 4.1 is a quantitative improvement over the optimal estimate for general Riemannian manifolds due to Afsari:
Fig 6. $K \subset F_a/4$, the blue cone. $K$ and $K'$ are homeomorphic via $q$. The Euclidean distance between points $\vec{x}, \vec{y} \in F_a/4$ is the same as the Procrustean distance between their orbits $[\vec{x}], [\vec{y}]$, so $K$ and $K'$ are actually isometric. The Fréchet means of $K$ and $K'$ are related by $\mu_{K'} = q(\mu_K)$. In particular, the Fréchet mean of $K'$ is unique.
Theorem 4.2. [1, Thm. 2.1] Let $M$ be a complete Riemannian manifold with sectional curvatures at most $\Delta$ and injectivity radius $\iota_M$. Set

$$\rho_0 = \frac{1}{2} \min \{\iota_M, \frac{\pi}{\Delta}\},$$

with the convention that $\frac{\pi}{\Delta} = \infty$ if $\Delta \leq 0$. For any $\rho < \rho_0$, a geodesic ball of radius $\rho$ in $M$ has a unique Fréchet mean.

The injectivity radius is the supremum of $r > 0$ such that every geodesic ball of radius $r$ is a topological ball. Afsari’s theorem does not apply to $U_d$, which is not a manifold. We also cannot apply this theorem to the more tractable interior $F^o_w$ of $F_w$, which is diffeomorphic to $U_d$ minus a set of measure zero, because $F^o_w$ is not complete in the Euclidean metric, and has zero injectivity radius.

However, we can compare Afsari’s result to Thm. 4.1 on (the locally complete) geodesic balls inside $F^o_a$, as these are ordinary Euclidean balls. The Euclidean metric has zero curvature, so $\pi/\Delta = \infty$ in our convention. Therefore, we need the injectivity radius of the smooth points of cone $F^o_a$. Take $\vec{v}$ lying on the cone axis. A ball $B_{\vec{v}}$ centered at $\vec{v}$ and tangent to the cone at a point $P$ determines a right triangle $\Delta O\vec{v}P$. This ball has radius $|\vec{v}| \sin(a/2)$, so this is the injectivity radius $\iota_{B_{\vec{v}}}$ in Thm. 4.2. Thus Afsari’s theorem applies to a ball of half this radius, denoted $B_{\vec{v}}(|\vec{v}| \sin(a/2)/2)$.

For Thm. 4.1, we can take any compact set $K$ inside $F^o_{a/4}$. To show that this Theorem improves the general Afsari result, we find such a $K$ containing $B_{\vec{v}}(|\vec{v}| \sin(a/2)/2)$. This follows if the $F^o_{a/4}$ cone contains the cone containing $B_{\vec{v}}(|\vec{v}| \sin(a/2)/2)$, which has cone angle $\sin^{-1}(\sin(a/2)/2)$. Since $\sin$ is increasing for $a \in (0, \pi/2)$, it suffices to show that

$$\sin(a/4) \geq \sin(a/2)/2.$$  \hspace{1cm} (4.3)

This follows from $2 \sin(a/4) \geq 2 \sin(a/4) \cos(a/4) = \sin(a/2)$.

As a result, $K' = q(K) \subset U_d$ has a unique Fréchet mean, even though its radius is larger than the bound in Thm. 4.2. This just says that the Afsari bound, which is universal for all Riemannian manifolds, may have an improvement on specific manifolds.

Figure 6 illustrates this improvement.

We end this section with an example of the difficulties of handling a graph with a non-distinct weight vector.

Example 4.5. As in Figure 2, take the distinct weight vector $\vec{w} = (3, 2, 1)$. The fundamental domain is $F = F_{\vec{w}} = \{x \geq y \geq z\}$. The proof
Fig 7. A cross-section of the fundamental domain $F$ showing the improvement of Thm. 4.1 over the Afsari result. The Afsari work gives a unique Fréchet mean of the image in $U_d$ to the ball of radius $r_*/2$, where $r_*$ is the injectivity radius at $\vec{v}$. Thm. 4.1 gives a unique Fréchet mean to the image in $U_d$ of the larger compact set $K'$ inside the $a/4$ cone. The boundary of $K'$ can extend down to $\vec{0}$, outwards as far as the walls of the $a/4$ cone, and to any finite height.
of Corollary 4.2 shows that every $\vec{w}_1 \in F_{a/2}$ has a neighborhood $U$ on which
\[ d_P([\vec{w}_2], [\vec{w}_3]) = d_E(\vec{w}_2, \vec{w}_3), \]
for all $\vec{w}_2, \vec{w}_3 \in U$.

In fact, we can take $U = F_{a/2}$ (See Example B.1 for a stronger statement.)

We now show that the vector $(1, 1, 1) \in \partial F$ has no neighborhood $U$ in $F$ on which (4.4) holds. Note that the stabilizer group of $(1, 1, 1)$ is all of $\Sigma_3$.

Take $\vec{w}_2 = (1 + a_1, 1 + a_2, 1 + a_3)$ with $a_1 > a_2 > a_3 > 0$, and $\vec{w}_3 = (1 + b_1, 1 + b_2, 1 + b_3)$ with $b_1 > b_2 > b_3 > 0$. For small $a$'s and $b$'s, these vectors will be arbitrarily close to $(1, 1, 1)$. Then
\[ d^2_E(\vec{w}_2, \vec{w}_3) = \sum_{i=1}^{3} (a_i - b_i)^2. \]

Take
\[ b_1 \approx a_2, \ b_2 \approx a_3 \approx b_3 \]
and let $\sigma = (132)$. Then
\[ d^2_P([\vec{w}_2], [\vec{w}_3]) < d^2_E(\vec{w}_2, \vec{w}_3) \]
if
\[ \sum_{i=1}^{3} (a_i - b_i)^2 > \sum_{i=1}^{3} (a_i - b_{\sigma(i)})^2. \]

The left hand side of (4.7) is approximately $(a_1 - a_2)^2 + (a_2 - a_3)^2$, and the right hand side is approximately $(a_1 - a_3)^2$. Thus (4.7) holds if
\[ (a_1 - a_2)^2 + (a_2 - a_3)^2 > (a_1 - a_3)^2, \ i.e. \ if \ a_2^2 + 2a_1a_3 > a_2a_1 + a_2a_3. \]

Since $a_2^2 > a_2a_3$, we just need
\[ 2a_3 > a_2. \]

So once we choose the $a$'s and $b$'s to satisfy (4.5),(4.8), we obtain (4.6), which proves the claim.

We conclude that there is no neighborhood $U$ of $(1, 1, 1)$ inside $\mathbb{R}^3$ (not just inside $F$) on which Euclidean distances in $U$ agree with Procrustean distances in $q(U) \subset U_3$. This illustrates the impossibility of applying [1] to the singular point $[(1, 1, 1)]$ of $U_3$. 
5. Discussion. Our work pertains to the geometric and statistical foundations of unlabeled networks. Specifically, we characterize the geometry of the space of such networks, define an appropriate notion of means or averages of unlabeled networks, and derive the asymptotic behavior of the empirical average network. This last result is a necessary precursor for the development of a variety of statistical inference tools in analogy to those encountered in a typical ‘Statistics 101’ course, as we demonstrate in the context of hypothesis testing. A key technical contribution of our work is that of providing broader conditions than available from general results on manifolds for uniqueness of the Fréchet mean network of a distribution on the space of unlabeled networks.

Our work here sets the stage for a program of additional research with multiple components. Firstly, we expect that the asymptotic theory we develop can be extended in interesting ways. For example, it is desirable to extend Thm. 4.1 and the subsequent CLT to distributions with larger support. Intuitively, a distribution with support close enough to a distribution with a unique Fréchet mean should itself have a unique Fréchet mean. For smooth distributions, some Sobolev notion of closeness may work. More broadly, when the uniqueness condition fails, there is a possibility of establishing a limit theorem based on the set distance between the sample Fréchet means and the population Fréchet means, in the spirit of analogous work done for the estimation of level sets [12, 26]. However, the Hausdorff distance between the two does not necessarily go to zero, as in the counterexample in [8], so these limit theorems will be more subtle.

There is also work to be done relating to the task of calculating the Fréchet mean(s) for a sample of unlabeled networks and applying our results in practice (e.g., comparing the means of two subpopulations). An initial challenge to implementation of the theory we have developed is the topological complexity of the space $U_d$ of unlabeled networks, as noted in the Appendices. Further understanding of the topology of $U_d$, in particular its homology groups, could lead to interesting phenomena not present for the contractible space of labeled networks $O_d$. Related to these directions too is the need for a better understanding of the sensitivity of our results to the choice of metric on $O_d$; in particular, the cut distance [25], which is more refined than the Euclidean distance, is an intriguing candidate.

Finally, although our work here assumed weighted undirected networks, it would be important to investigate how the finite set of undirected binary networks fits into our theory. In particular, the definition and uniqueness of Fréchet means needs to be elaborated. It is crucial to understand the placement of the binary graphs inside the fundamental domains we con-
constructed; preliminary work indicates that binary graphs are unfortunately widely scattered throughout a fundamental domain.

APPENDIX A: COMPUTING FUNDAMENTAL DOMAINS

In the two appendices, we discuss the computational difficulties of implementing the theory in Section 4. In this appendix, we show that the fundamental domain $F_{\vec{w}}$ is highly sensitive to the choice of distinct vector $\vec{w}$ as axis.

We use a Dirichlet fundamental domain for the action of $\Sigma_d$ on $\mathbb{R}_{\geq 0}^D$. By Lemma 4.1, $F = F_{\vec{w}} = \bigcap_{\sigma \in \Sigma_d} \{ z \in \mathbb{R}_{\geq 0}^D : d_E(\vec{w}, \vec{z}) \leq d_E(\vec{w}, \sigma \vec{z}) \}$ for a distinct vector $\vec{w} \in \mathbb{R}_{\geq 0}^D$. This is the intersection of $d! + D - 1$ half-spaces, where the $D$ coordinate half-spaces are given by the inequalities $z_j \geq 0$.

The cone $F$ is a convex, non-compact polyhedral region in $\mathbb{R}_{\geq 0}^D$. The $d! - 1$ half-space regions are given by the linear inequalities:

$$\sum_{j=1}^D (w_{\sigma(j)} - w_j) z_j \leq 0,$$

for $\sigma \neq \text{Id}$.

Sage provides efficient tools for converting an input system of linear inequalities into a minimal description of the polyhedral output region; see Supplement B.

We consider the simplest nontrivial example of graphs with four vertices: $d = 4$, $D = \binom{4}{2} = 6$.

**Example A.1.** Choose the distinct vector $\vec{w} = (1, 2, 3, 4, 5, 6)$. Sage gives $F_{\vec{w}}$ as the intersection of 7 half-spaces or the convex hull of 7 rays [see Figure 8].

**Example A.2.** Now choose $\vec{w} = (1, 2, 3, 4, 5, 6, 1)$. $F_{\vec{w}}$ is now described as the convex hull of 79 rays, or the intersection of 18 half-spaces [see Figure 9].

APPENDIX B: COMPUTATION OF THE FRÉCHET INTEGRAL

In this Appendix, we highlight the difficulty of computing the Fréchet integral $f([\vec{x}]) = \int_{U_q} d_p^2([\vec{x}], [\vec{y}]) dQ'([\vec{y}])$ for all $[\vec{x}]$. (Here $Q' = q_s Q$ in the notation of Thm 4.1.) Even when a fundamental domain $F_{\vec{x}}$ has been explicitly determined for a fixed $\vec{x}$, so that $f([\vec{x}]) = \int_{F_{\vec{x}}} d_E^2(\vec{x}, \vec{y}) dQ(\vec{y})$, we have seen in Appendix A that the shape of $F_{\vec{x}}$ depends delicately on $[\vec{x}]$. 
AVERAGES OF UNLABELED NETWORKS

Fig 8. Sage output for computation of a fundamental domain centered at the distinct vector $\vec{w} = (1, 2, 3, 4, 5, 6)$. F.Hrepresentation() lists the half-spaces whose intersection is the fundamental domain. Note that we started with $4! + \binom{4}{2} - 1 = 29$ inequalities, and have narrowed it down to 7. F.Vrepresentation() lists the 7 rays whose convex hull is the fundamental domain.

We can instead divide $\mathbb{R}^D_{\geq 0}$ into $d!$ regions $F_\sigma(\vec{x}) = \{\vec{y} \in \mathbb{R}^D_{\geq 0} : d_P([\vec{x}], [\vec{y}]) = d_E(\vec{x}, \sigma \cdot \vec{y})\}$. Note that $F_\sigma(\vec{x})$ is a fundamental domain for $\sigma \cdot \vec{x}$. Since $F_{\vec{w}} = \bigcup_{\sigma \in \Sigma_d} F_{\vec{w}} \cap F_{\sigma \cdot \vec{x}}$ for a fixed distinct vector $\vec{w}$, the Fréchet integral is given by

$$f(\vec{x}) = \int_{d_4} d_P([\vec{x}], [\vec{y}])dQ'(\vec{y}) = \sum_{\sigma \in \Sigma_d} \int_{F_{\vec{w}} \cap F_{\sigma \cdot \vec{x}}} d_E^2(\vec{x}, \sigma \cdot \vec{y})dQ(\vec{y}).$$

Although on the right hand side we now have a sum of Euclidean integrals for each $\vec{x}$, as in Appendix A it is difficult to explicitly compute $F_{\vec{w}} \cap F_{\sigma \cdot \vec{x}}$.

We illustrate this computation in the simple case $d = 3$. Already for $d = 4$, the computation becomes too lengthy for inclusion here.

Example B.1. $d = 3$. First we show that the fundamental domain $F_{\vec{x}}$ can be chosen to depend only on the ordering $\text{ord}(\vec{x})$ (e.g. from largest to smallest, as in Figure 2) of the components of a distinct vector $\vec{x}$. The Procrustean distance between two points is $d_P([\vec{x}], [\vec{y}]) = \min_{\sigma \in \Sigma_d} d_E(\vec{x}, \sigma \cdot \vec{y})$. To minimize the Euclidean distance, we choose $\sigma$ which reorders $\vec{y}$ to
Fig 9. A partial Sage output for computation of a fundamental domain centered at the distinct vector $\vec{w} = (1, 2, 3, 4, 5, 6, 1)$. \texttt{F.Hrepresentation()} lists the half-spaces whose intersection is the fundamental domain. Note that we started with $4! + (\binom{4}{2} - 1) = 29$ inequalities, and have narrowed it down to 18. \texttt{F.Vrepresentation()} lists the 79 rays whose convex hull is the fundamental domain.

match the ordering of $\vec{x}$, as any other $\sigma$ cannot decrease the distance. (This uses the special fact that $\Sigma_{d=3}$ is the full permutation group of the $D = 3$ set of weight vectors). Therefore, we can choose $F = F_{\vec{x}} = \{ \vec{y} \in \mathbb{R}_3^3 : d_E(\vec{x}, \vec{y}) = d_F(\vec{x}, \vec{y}) \} = \{ \vec{y} \in \mathbb{R}_3^3 : \text{ord}(\vec{y}) = \text{ord}(\vec{x}) \}$ to be independent of the distinct vector $\vec{x}$. The Fréchet integral for a compactly supported probability measure $Q'$ on $U_3$ (or equivalently for $Q$ on $F$) equals

$$f(\vec{x}) = \int_F d_E(\vec{x}, \vec{y})^2 dQ(\vec{y})$$

$$= \|\vec{x}\|^2 \int_F dQ(\vec{y}) - 2\vec{x} \cdot \int_F \vec{y} dQ(\vec{y}) + \int_F \|\vec{y}\|^2 dQ(\vec{y})$$

$$= \|\vec{x}\|^2 - 2\vec{x} \cdot \int_F \vec{y} dQ(\vec{y}) + B$$

$$= \|\vec{x}\|^2 - 2 \sum_i C_i \vec{x}_i + B,$$

where the second integral on the last line is the dot product of a vector and
a vector valued integral, $C_i = \int_{F} y^i dQ(\vec{y})$, and $B = \int_{F} \|\vec{y}\|^2 dQ(\vec{y})$. Thus $f$ is quadratic in $\vec{x}$ on distinct vectors. Since the distinct vectors are dense in Euclidean space, $f$ is quadratic on all vectors. Therefore, $f$ is strictly convex. Since we are minimizing over a convex region, $f$ has a unique global minimum. To explicitly compute it, note that $F$ has eight strata in varying dimensions 0, 1, 2, and 3; these are labeled (1), . . . , (8) in the table below. The restriction to each stratum is smooth away from the lower dimensional boundaries, so we can simply minimize on each open piece to find eight local minima $x^*$.

| # | dim | Region | $x^*$ |
|---|---|---|---|
| (1) | 3 | $x_3 \geq 0$ and $0 < x_1 < x_2 < x_3$ | $(C_1, C_2, C_3)$ |
| (2) | 2 | $x_1 = 0$ and $0 < x_2 < x_3$ | $(0, C_2, C_3)$ |
| (3) | 2 | $0 < x_1 = x_2 < x_3$ | $\left(\frac{1}{7}(C_1 + C_2), \frac{1}{7}(C_1 + C_2), C_3\right)$ |
| (4) | 2 | $0 < x_1 < x_2 = x_3$ | $\left(\frac{1}{2}(C_1 + C_3), \frac{1}{2}(C_1 + C_3), C_2 + C_3\right)$ |
| (5) | 1 | $x_1 = x_2 = 0$ and $x_3 > 0$ | $(0, 0, C_3)$ |
| (6) | 1 | $x_1 = 0$ and $0 < x_2 = x_3$ | $\left(0, \frac{1}{7}(C_2 + C_3), \frac{1}{7}(C_2 + C_3)\right)$ |
| (7) | 1 | $0 < x_1 = x_2 = x_3$ | $(C', C', C')$ |
| (8) | 0 | $x_1 = x_2 = x_3 = 0$ | $(0, 0, 0)$ |

Here $C' = (1/3)(C_1 + C_2 + C_3)$. The true global minimum will depend on the values of $C_1$, $C_2$, and $C_3$.

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SUPPLEMENTARY MATERIAL

Supplement A: Proof of Proposition 4.2. (http://math.bu.edu/people/sr/proof.pdf).

Supplement B: Sage code for computing fundamental domains (https://github.com/KolaczykResearch/fund-domain-networks).

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