Supplement to "Averages of Unlabeled Networks: Geometric Characterization and Asymptotic Behavior", by Kolaczyk, Lin, Rosenberg, Walters, and Xu

Supplement C

Improvements to Theorem 4.5

In this Supplement, we give two types of improvements to Thm. 4.5, which guarantees the uniqueness of the Fréchet mean for smooth distributions compactly supported inside the image in $\mathcal{U}_d$ of the $F_{a/4}$ cone in the fundamental domain F. In §2, we prove that distributions whose support is mostly inside the $F_{a/4}$ cone in a Sobolev sense also have unique Fréchet means. In §3, we show how to embed any compact subset K of $\mathcal{U}_d$ into the set $\mathcal{B}(K)$ of bounded functions on K such that any smooth distribution supported in K has a unique Fréchet mean in $\mathcal{B}(K)$. We relate this theory to the running Example 2.1.

1. Distributions with support close to the $\boldsymbol{F_{a/4}}$ cone. The reader may just want to read the statement of results in §2.1, since the proofs in §2.2 are technical.

1.1. *Statement of results.* In Thm. 4.5, we proved that probability distributions Q with compact support inside the $F_{a/4}$ cone have a unique Fréchet mean. In this Supplement, we extend this result to probability measures Q' which are close to such a Q in an appropriate Sobolev norm. In practical terms, this means that distributions Q' with small tails outside the $F_{a/4}$ cone also have a unique Fréchet mean (Thm. 1.1).

To set the notation, let $H^{0,\infty}$ denote the completion of the smooth, compactly supported functions on the space of unlabeled networks $\mathcal{U}_d$ is the sup norm, and let $B_g^{2,\infty}(\eta)$ denote the η-ball around g in the $H^{2,\infty}$ norm. Recall that

$$\|f\|_{2,\infty} = \sup_{x\in \operatorname{supp}(f)} \sup_{|\alpha|\leq 2} \|\partial^\alpha f(x)|,$$

where $\alpha = (\alpha^1, \ldots, \alpha^D)$ is a multi-index. Here we are identifying functions on $\mathcal{U}_d$ with functions on a fundamental domain $F \subset \mathbb{R}^D$ which are invariant under the permutation group Σ_d. We also denote the usual L^2-Sobolev spaces by $H^s(\mathcal{U}_d)$. The ball $B_g^3(\zeta)$ around $g \in H^3(\mathcal{U}_d)$ is

$$B_g^3(\zeta) = \{f \in H^3(\mathcal{U}_d) : \|f - g\|_{H^3} < \zeta\}.$$

We first prove that a function Sobolev close to a function with a unique minimum has a unique minimum, provided some technical conditions hold.

PROPOSITION 1.1. *Let g be a smooth, compactly supported function on a compact, connected set $E \subset F$, such that g has a unique minimum at x_0 in the interior $\mathring{E}$ of E. Assume that x_0 is isolated among the critical points of g, and that $D^2 g = \mu \cdot Id$ for some $\mu > 0$ at x_0. Then there exists $\eta > 0$ and a neighborhood $B^3_g(\zeta)$ of g such that every compactly supported continuous function $h \in B^3_g(\zeta) \cap \mathcal{C}_c(E)$ has a unique minimum, provided*

(i) there exists $x^* \in \mathring{E}$ and $\epsilon > 0$ such that h has at least fourth order continuous partial derivatives on the ball $B_\epsilon(x^*)$;

(ii)

$$\sup_{|\alpha| \leqslant 2} |\partial^\alpha (h - g)(x^*)| < \frac{\eta}{4}. \tag{1.1}$$

This is proved in Proposition 1.5. We then apply this to Fréchet functions (see Corollary 1.7).

COROLLARY 1.2. *Let Q be a smooth probability distribution with support inside a compact set $E \subset F_{a/4}$ with Fréchet function $f_Q(x) = \int_E d_P^2(x, y)\nu_0(y)dy$ with respect to the Procrustean distance. Then there exists $\zeta > 0$ such that every $f \in B^3_{f_Q}(\zeta) \cap C_c(F)$ has a unique minimum.*

We will prove that the Fréchet function is in H^3 and that the Fréchet function depends H^3-continuously on the choice of $Q \in H^3 \cap C_c(F)$. This implies the main result (see Theorem 1.2):

THEOREM 1.1. *Let Q be a smooth probability distribution with support inside a compact set $E \subset F_{a/4}$. There exists $\zeta > 0$ such that for every $Q' \in B^3_Q(\zeta) \cap C_c(F)$, the Fréchet function $f_{Q'}$ has a unique minimum.*

For completeness, we include a final result that the Fréchet function with respect to the Procrustean distance lies in the Sobolev space H^3 for Q compactly supported (Lemma 1.5).

1.2. *Proofs of the main results.* Let $H_{0,\infty}$ denote the completion of the smooth, compactly supported functions on $\mathcal{U}_d$ is the sup norm, and let $B^{2,\infty}_g(\eta)$ denote the η-ball around g in the $H^{2,\infty}$ norm. Recall that

$$\|f\|_{2,\infty} = \sup_{x \in \operatorname{supp}(f)} \sup_{|\alpha| \leq 2} \|\partial^\alpha f(x)|,$$

where α is a multi-index.

PROPOSITION 1.3. *Let g be a smooth, compactly supported function on $\mathcal{U}_d$ with a unique minimum at x_0. Assume that x_0 is isolated among the critical points of g, and that the Hessian satisfies $D^2g = \mu \cdot \mathrm{Id}$ for some $\mu > 0$ at x_0. Then there exists a neighborhood $B_g^{2,\infty}(\eta)$ of g such that every compactly supported smooth function $h \in B_g^{2,\infty}(\eta) \cap C_c^\infty(\mathcal{U}_d)$ has a unique minimum.*

By definition, a smooth function on $\mathcal{U}_d$ is a σ_d-invariant smooth function on $\mathcal{O}_D$.

REMARK 1.4. It is easy to check that for the Fréchet function $f_Q(x) = \int_E d_E^2(x,y)Q(y)dy$, with Q a smooth distribution supported in a compact set $E \subset F$, a fundamental domain for $\mathcal{U}_d$, we have f_Q is smooth and $D^2 f_Q = 2 \cdot \mathrm{Id}$.

PROOF. By the assumption on the Hessian, x_0 is isolated among all local minima of g. It follows easily that (i) there exists $\epsilon > 0$ such that $f_{\nu_0}(x_i) - f_{\nu_0}(x_0) > \epsilon$ for all local minima x_i; (ii) small values of f_{ν_0} come from points close to x_0: there exists δ such that

$$A_\epsilon := f_{\nu_0}^{-1}(F_{\nu_0}(x_0), F_{\nu_0}(x_0) + \epsilon) \subset B_{x_0}(\delta),$$

where this δ-ball is measured in the Procrustean distance.

Assume that such an h has two global minima x', x''. We claim that $x', x'' \in A_\epsilon$, if we set $\eta = \epsilon/2$ as a preliminary estimate. For

$$\|h - g\|_{0,\infty} \le \|h - g\|_{2,\infty} < \epsilon/2$$

implies that $h(x_0) < g(x_0) + \epsilon/2$, while for $z \notin A_\epsilon$,

$$h(z) \ge g(z) - (\epsilon/2) > g(x_0) + \epsilon - (\epsilon/2) = g(x_0) + \epsilon/2.$$

This proves the claim.

Take a smooth curve $\gamma : [0,1] \to A_\epsilon$ with $\gamma(0) = x', \gamma(1) = x''$, $\gamma(t_0) = x_0$ for some t_0. We may assume that $\dot\gamma(t_0) = V$. By reparametrizing, we may assume that $|\dot\gamma(t)| = 1$, and then $\gamma : [0, \mathrm{length}(\gamma)] \to A_\epsilon$ has length at most 3δ, a crude upper bound for the length of paths in A_ϵ going through x_0. Let $G_h(t) = h(\gamma(t))$.

Let a local maximum of G_h occur at t_1, so $\dot{G}_h(t_1) = 0, \ddot{G}_h(t_1) \leq 0$. Thus

$$\begin{aligned} |\ddot{G}_h(t_1) - \ddot{G}_h(t_0)| &\leq |\ddot{G}_h(t_1) - \ddot{G}_g(t_1)| + |\ddot{G}_g(t_1) - \ddot{G}_g(t_0)| \\ &\quad + |\ddot{G}_g(t_0) - \ddot{G}_h(t_0)| \\ &\leq \eta + |\ddot{G}_g(t_1) - \ddot{G}_g(t_0)| + \eta. \end{aligned} \tag{1.2}$$

Reset

$$\eta = \min\{\epsilon/2, 1/4\}.$$

We can choose $\delta = \delta_g$ small enough so that

$$y \in B_{x_0}(\delta), V \in T_y(\mathcal{U}_d), |V| = 1 \Rightarrow D^2 g_y(V, V) \in (3/2, 5/2).$$

Then

$$|\ddot{G}_g(t_1) - \ddot{G}_g(t_0)| = |\ddot{G}_g(t_1) - 2| < \frac{1}{2},$$

so (1.2) becomes

$$|\ddot{G}_h(t_1) - \ddot{G}_h(t_0)| < 2(1/4) + (1/2) = 1.$$

On the other hand, for $h \in B_g^{2,\infty}(1/4)$, we get

$$|\ddot{G}_h(t_0) - 2| = |\ddot{G}_h(t_0) - D^2 g_{x_0}(V, V)| = |D^2 h_{x_0}(V, V) - D^2 g_{x_0}(V, V)| \leq 1/4,$$

so

$$\ddot{G}_h(t_0) \geq \frac{7}{4}.$$

This implies

$$\ddot{G}_h(t_1) \geq \ddot{G}_h(t_0) - 1 \geq \frac{7}{4} - 1 > 0.$$

This contradicts $\ddot{G}_h(t_1) \leq 0$. □

Unlike the Euclidean distance $d_E^2(x, \cdot)$ from a point x, the Procrustean distance $d_P^2(x, \cdot)$ is not smooth outside the $F_{a/4}$ cone. Thus the Fréchet functions we wish to consider do not satisfy the hypothesis for h in the Proposition. The next Proposition addresses this issue.

For notation, we denote the usual L^2-Sobolev spaces by $H^s(\mathcal{U}_d)$. The ball $B_g^3(\zeta)$ around $g \in H^3(\mathcal{U}_d)$ is

$$B_g^3(\zeta) = \{f \in H^3(\mathcal{U}_d) : \|f - g\|_{H^3} < \zeta\}.$$

We also use standard multi-index notation $\alpha = (\alpha^1, \ldots, \alpha^D)$.

Fix a closed, path connected set $E \subset F$, where F is a fundamental domain for $\mathcal{U}_d$. We assume that $E \cap \partial F = \emptyset$. Thus the projection E' of E into $\mathcal{U}_d$ is closed and path connected. A function g on E' corresponds to a function on E, so derivatives of g really mean derivatives of this function on E.

For convenience, we restate Proposition 1.1.

PROPOSITION 1.5. *Let g be a smooth, compactly supported function on $E' \subset \mathcal{U}_d$ with a unique minimum at x_0. Assume that x_0 is isolated among the critical points of g, and that $D^2 g = \mu \cdot Id$ for some $\mu > 0$ at x_0. Fix η as Proposition 1.3. Then there exists a neighborhood $B^3_g(\zeta)$ of g such that every continuous function $h \in B^3_g(\zeta) \cap C_c(E')$ has a unique minimum, provided*
(i)

$$\exists x^* \in \mathring{E}', \sup_{|\alpha| \leqslant 2} |\partial^\alpha (h-g)(x^*)| < \frac{\eta}{4}, \tag{1.3}$$

(ii) h is at least fourth order continuously differentiable on some ball $B_\epsilon(x^*)$.

The proof of the Proposition is broken down into Lemmas 1.1 - 1.4.

LEMMA 1.1. *For fixed $h \in B^3_g(\zeta) \cap C_c(E')$ and for η as in Proposition 1.3 and $x^* \in \mathring{E}'$, there exists $p \in C_c^\infty(E')$ such that for fixed $\tilde{\zeta} > 0$:*

$$\|p - h\|_{H^3} < \tilde{\zeta}, \tag{1.4}$$

$$\sup_{|\alpha| \leqslant 2} |\partial^\alpha (p-h)(x^*)| < \frac{\eta}{4}. \tag{1.5}$$

PROOF. We will do the proof on $E \subset F$, and then the final result is valid on E'. Thus in the proof Sobolev spaces on $\mathcal{U}_d$ are replaced by Sobolev spaces on F for functions which descend to $\mathcal{U}_d$, $B^3_g(\zeta)$ is a subset of these Sobolev spaces on F, $x^* \in \mathring{E}$, etc.

Since Sobolev spaces are completions of spaces of compactly supported smooth functions, we can find $p_0 \in C_c^\infty(E)$ such that $\|p_0 - h\|_{H^3} < \tilde{\zeta}$, for some fixed $\tilde{\zeta}$ which will vary from line to line in the proof.

Define $p_1(x)$ on E by the truncated Taylor expansion

$$p_1(x) = h(x^*) + \sum_{1 \leqslant |\alpha| \leqslant 4} \frac{\partial^\alpha h(x^*)}{\alpha!} (x - x^*)^\alpha.$$

For $|\alpha| \leqslant 4$,

$$\partial^\alpha (p_1 - h)(x^*) = 0. \tag{1.6}$$

Since p_1 is a smooth function and since x^* is an interior point, for fixed $\tilde{\zeta} > 0$, there exists $\delta > 0$ such that $B_\delta(x^*) \subset E$ and

$$\sup_{x \in B_\delta(x^*)} \sup_{|\alpha| \leqslant 2} |\partial^\alpha p_1(x) - \partial^\alpha h(x^*)| < \tilde{\zeta}. \tag{1.7}$$

Define $\bar{p}_0 \in L^1(\mathbb{R}^D)$ by

$$\bar{p}_0(x) = \begin{cases} p_1(x), & x \in B_\delta(x^*), \\ p_0(x), & x \in E \backslash B_\delta(x^*), \\ 0, & x \notin E. \end{cases}$$

Pick a positive smooth function $\phi \in C_c^\infty(B_\delta(0))$ with $\int_{\mathbb{R}^D} \phi(x)dx = 1$. For the smooth function

$$p = \phi * \bar{p}_0,$$

we have

$$\partial^\alpha p = \phi * \partial^\alpha \bar{p}_0.$$

We show that this p satisfies (1.4) and (1.5). For (1.5), we have

$$\begin{aligned} |p(x^*) - h(x^*)| = |\phi * \bar{p}_0(x^*) - h(x^*)| &\leqslant \int_{\mathbb{R}^D} |\phi(y)||\bar{p}_0(x^* - y) - h(x^*)|dy \\ &= \int_{\mathbb{R}^D} |\phi(y)||p_1(x^* - y) - h(x^*)|dy \\ &< \tilde{\zeta} \int_{\mathbb{R}^D} \phi(y)dy = \tilde{\zeta}, \end{aligned} \tag{1.8}$$

for δ small enough. In the second line the support of ϕ implies $x^* - y \in B_\delta(x^*)$, so $\bar{p}_0$ becomes p_1. By the same argument, we have

$$\sup_{|\alpha| \leqslant 2} |\partial^\alpha (p - h)(x^*)| < \tilde{\zeta}. \tag{1.9}$$

Since $\tilde{\zeta}$ is arbitrary, (1.5) follows.

We now verify that p satisfies (1.4). In the estimates below, we always shrink the various choices of δ so that (1.9) still holds. Note that as δ shrinks, the sup norm of ϕ increases, but we only use $\int \phi = 1$ in (1.8), which is valid for all δ.

For $x \notin B_{2\delta}(x^*)$, we have

$$p(x) = \int_{B_\delta(0)} \phi(y)\bar{p}_0(x-y)dy = \int_A \phi(y)p_0(x-y)dy \text{ with } A + \{x\} = B_\delta(x) \cap E.$$

Also, if we choose δ such that $B_{3\delta}(x^*) \subset E$, then for $x \in B_{2\delta}(x^*)$ and $y \in B_\delta(0)$, we have

$$\phi(y)\bar{p}_0(x-y) = \begin{cases} \phi(y)p_1(x-y), & x-y \in B_\delta(x^*), \\ \phi(y)p_0(x-y), & x-y \notin B_\delta(x^*). \end{cases}$$

Therefore

$$\begin{aligned}
&\int_E |p(x)-h(x)|^2 dx \\
&= \int_{B_{2\delta}(x^*)} |\phi * \bar{p}_0(x) - h(x)|^2 dx + \int_{E\setminus B_{2\delta}(x^*)} |\phi * \bar{p}_0(x) - h(x)|^2 dx \\
&\leq \int_{B_{2\delta}(x^*)} |\phi * p_1(x) - h(x)|^2 dx + \int_{B_{2\delta}(x^*)} |\phi * p_0(x) - h(x)|^2 dx \\
&\quad + \int_{E\setminus B_{2\delta}(x^*)} |\phi * p_0(x) - h(x)|^2 dx \\
&= \int_{B_{2\delta}(x^*)} |\phi * p_1(x) - h(x^*) + h(x^*) - h(x)|^2 dx \\
&\qquad\quad + \int_E |\phi * p_0(x) - p_0(x) + p_0(x) - h(x)|^2 dx \\
&\leq 2\int_{B_{2\delta}(x^*)} |\phi * p_1(x) - h(x^*)|^2 dx + 2\int_{B_{2\delta}(x^*)} |h(x^*) - h(x)|^2 dx \\
&\quad + 2\int_E |\phi * p_0(x) - p_0(x)|^2 dx + 2\int_E |p_0(x) - h(x)|^2 dx \\
&:= \text{(I)} + \text{(II)} + \text{(III)} + \text{(IV)}.
\end{aligned}$$

(I) can be made less that $\tilde{\zeta}/4$ by the estimates in (7). (II) can be made less that $\tilde{\zeta}/4$ by the continuity of h, again shrinking δ as necessary.

For (III), p_0 is a smooth function on compact set E and hence its derivatives of any order are uniformly continuous. Therefore

$$\sup_{|\alpha|\leqslant 3} |\partial^\alpha p_0(x) - \partial^\alpha p_0(y)| < \sqrt{\frac{\tilde{\zeta}}{4\mathrm{Vol}(E)}}, \forall y \in B_\delta(x). \tag{1.10}$$

shrinking δ finitely many times as necessary. Hence we can estimate

$$\int_E \left[\int_{B_\delta(0)} |p_0(x-y) - p_0(x)|\phi(y)dy\right]^2 dx < \int_E \int_{B_\delta(0)} \frac{\tilde{\zeta}}{4\mathrm{Vol}(E)} \cdot \phi(y)dy < \frac{\tilde{\zeta}}{4}.$$

(IV) is controlled by the choice of p_0 with respect to the H^3-norm. Since $\tilde{\zeta}$ is chosen arbitrarily, we can make $\int_E |p_0(x) - h(x)|^2 dx$ as small as possible.

By the same procedure, we can also control $\int_E |\partial^\alpha(\bar{p}-h)(x)|^2 dx, |\alpha| \leqslant 3$. $\square$

The next Lemma and Corollary show that every p satisfying (1.4) and (1.5) has a unique minimum.

LEMMA 1.2. *Let g be as in Proposition 1.3 and h as in Proposition 1.5, so $g \in C_c^\infty(F)$ and $h \in B_g^3(\zeta) \cap C_c^\infty(E)$. For η as in Proposition 1.3 and for $p \in C_c^\infty(E)$ satisfying (1.4) and (1.5), we have*

$$\|p-g\|_{2,\infty} < \eta \tag{1.11}$$

on E.

PROOF. By the assumptions on h, we have

$$\|p-g\|_{H^3} \leq \|p-h\|_{H^3} + \|h-g\|_{H^3} < \tilde{\zeta} + \zeta, \tag{1.12}$$

for arbitrarily small $\zeta, \tilde{\zeta}$, and

$$\sup_{|\alpha|\leqslant 2} |\partial^\alpha(p-g)(x^*)| \leq \sup_{|\alpha|\leqslant 2} |\partial^\alpha(p-h)(x^*)| + \sup_{|\alpha|\leqslant 2} |\partial^\alpha(h-g)(x^*)| < \frac{\eta}{2}. \tag{1.13}$$

By (1.13), the estimate (1.11) holds at $x^* \in \mathring{E}$.

Claim: For fixed $x \in E$, there exists a "cross section" $S = S_x$ diffeomorphic to an open ball in $\mathbb{R}^{D-1}$ with (i) the $(D-1)$-dimensional volume $\mathrm{Vol}_{D-1}(S_x)$ bounded below by a positive constant M independent of x; (ii) for all $s \in S_x$, there exists a unique path from x to x^* passing through s and lying in E.

For the claim, take a smooth, simple path $\gamma_x : [0,1] \to E$ with $\gamma_x(t) \notin \partial E, \forall t \neq 0$, $\gamma_x(0) = x$, $\gamma_x(1) = x^*$. We then take a maximal tubular neighborhood $T_x \subset F$ of γ_x with a diffeomorphism $\alpha = \alpha_x$ such that

$$\alpha : T_x \xrightarrow{\cong} [0,1] \times B_1(0),\ B_1(0) \subset \mathbb{R}^{D-1}.$$

Define the fiber $T_{t,x} := \alpha^{-1}(t)$. Consider a smooth function $f : [0,1] \to \mathbb{R}^+$ such that

$$f(0) = f(1) = 0;\ f(t) > 0\ \forall t \neq 0,1;\ f(t)T_{t,x} \subset E.$$

Define β such that $B_\beta(x^*) \subset E$. After a possible reparametrization, we can assume $\gamma_x(0.9) \subset B_\beta(x^*)$.

For fixed $t \in [0,1]$, set

$$S_x = \{y \in E : y \in f(t)T_{t,x}\}.$$

A choice of $V \in B_1(0)$ gives a section $s_{V,x}(t) = \alpha^{-1}(t,V)$ of T_x. For a fixed $t_0 \in [0,1]$, set

$$S_x(t_0) = \{f(t_0)s_{V,x}(t_0) : V \in B_1(0)\}.$$

For fixed V, the path $\gamma_{x,V} = f(t)s_{V,x}(t)$ is the path from x to x^* passing once through $S_x(t_0)$. This proves (ii).

For (i), for fixed ϵ we take a finite cover of the compact set E by closed ϵ - balls $B_1, \dots, B_m$. For x in $\overline{B_i} \setminus \cup_{j=1}^{i-1}\overline{B_j}$, we can choose γ_x from x to x^* depending continuously on x in the compact-open topology on paths ending at x^*. We now set $t_0 = 0.9$. On each $\overline{B_i}$, the radius of $T_{0.9,x}$ depends continuously on x by the Weyl Tubular Neighborhood Theorem, so $\mathrm{Vol}_{D-1}(T_{0.9,x})$ is bounded below by a positive constant. Since there are a finite number of B_i, this proves (i) and the Claim.

It follows that there exists $M > 0$ such that

$$\mathrm{Vol}_{D-1}(S_x(t_0)) \geqslant M, \forall x \in E, \tag{1.14}$$

for $t_0 \neq 0, 1$.

Let D_a denote the directional derivative in the direction a. For fixed $x \neq x^*$ and for each $V \in B_1(0)$, we have

$$\begin{aligned} |p(x) - g(x)| &\leq |p(x) - g(x) - p(x^*) + g(x^*)| + |p(x^*) - g(x^*)| \\ &\leq \int_{\gamma_{x,V}} |D_{\dot\gamma_{x,V}}(p-g)(s)|ds + \frac{\eta}{2}. \end{aligned}$$

Thus

$$\begin{aligned} |p(x) - g(x)| &\leq \int_{\gamma_{x,V}} |D_{\dot\gamma_{x,V}}(p-g)(s)|ds + \frac{\eta}{2} \\ &= \frac{1}{\mathrm{Vol}_{D-1}(S_x(t_0))} \int_{S_x(t_0)} dV \int_{\gamma_{x,V}} |D_{\dot\gamma_{x,V}}(p-g)(s)|ds + \frac{\eta}{2} \\ &= \frac{1}{\mathrm{Vol}_{D-1}(S_x(t_0))} \int_{S_x} |D_{\dot\gamma_{x,V}}(p-g)(s)|dV ds + \frac{\eta}{2} \\ &\leq \frac{1}{M} \left(\int_E dx\right)^{\frac{1}{2}} \left(\int_E |D_{\dot\gamma_{x,V}}(p-g)(x)|^2 dx\right)^{\frac{1}{2}} + \frac{\eta}{2} \\ &\leq \frac{\mathrm{Vol}(E)^{\frac{1}{2}}}{M} \left(\mathrm{Vol}(E)^{\frac{1}{2}} \|\partial^\alpha(p-g)\|_\infty\right) + \frac{\eta}{2} \\ &\leq \frac{\mathrm{Vol}(E)}{M} \|p-g\|_{H^3} + \frac{\eta}{2}. \end{aligned}$$

By (1.12), for $\zeta, \tilde{\zeta}$ small enough, we have

$$|p(x) - g(x)| < \eta, \forall x \in E, x \neq x^*.$$

The same estimate works for $|\alpha| \leqslant 2$, just by replacing $D_{\dot{\gamma}_{x,V}}(p-g)(x)$ with $D_{\dot{\gamma}_{x,V}}(\partial^\alpha p - \partial^\alpha g)(x)$. The (1.11) holds for all $x^* \neq x \in E$, and (1.13) says that (1.11) holds at x^*. □

LEMMA 1.3. *In the notation of Lemma 1.1, let $\{p_n\} \subset C_c^\infty(E)$ be a sequence with each p_n satisfying (1.4) and (1.5) with $\tilde{\zeta} = \tilde{\zeta}_k \to 0$ as $k \to \infty$. Then a subsequence of $\{p_n\}$ converges to h uniformly.*

PROOF. The proof follows a standard Arzela-Ascoli argument. In the proof, we use the notation of the previous Lemma.

By (1.5), the sequence $\{p_n(x^*)\}$ is bounded, so there exists a subsequence $\{p_{n_k}(x^*)\}$ with $\lim_{k\to\infty} p_{n_k}(x^*) = p_0 \in \mathbb{R}$.

To apply Arzela-Ascoli, we need to show that this subsequence $\{p_{n_k}\}$ is equicontinuous and uniformly bounded. For uniform boundedness, take $x \in E, x \neq x^*$. As in Lemma 1.2,

$$\begin{aligned}
|p_{n_k}(x) - p_{n_l}(x)| &\leqslant |p_{n_k}(x) - p_{n_l}(x) - p_{n_k}(x^*) + p_{n_l}(x^*)| \\
&\qquad + |p_{n_k}(x^*) - p_{n_l}(x^*)| \\
&\leq \int_{\gamma_{x,V}} |D_{\dot{\gamma}_{s,V}}(p_{n_k} - p_{n_l})(y)| dy + |p_{n_k}(x^*) - p_{n_l}(x^*)| \\
&\leq \frac{\mathrm{Vol}(E)}{M} \|p_{n_k} - p_{n_l}\|_{H^3} + |p_{n_k}(x^*) - p_{n_l}(x^*)|.
\end{aligned} \tag{1.15}$$

Since $\{p_{n_k}\}$ forms a Cauchy sequence in H^3 - norm and $\{p_{n_k}(x^*)\}$ is a Cauchy sequence in $\mathbb{R}$, we conclude that

$$|p_{n_k}(x) - p_{n_l}(x)| \xrightarrow{k,l\to\infty} 0, \forall x \in E. \tag{1.16}$$

Note that this convergence is uniform since the last line of (1.15) is independent of the choice of x. Since each p_{n_k} is bound on the compact set E, it follows easily from (1.16) that $\{p_{n_k}\}$ is uniformly bounded.

For equicontinuity, fix $\epsilon > 0$ and take $N = N(\epsilon) \gg 0$. The functions $p_{n_1}, \ldots, p_{n_N}$ are uniformly continuous on E, and hence equicontinuous. For $k \geq N$, by (1.16) there exists $\delta > 0$ such that for $|x - y| < \delta$,

$$|p_{n_k}(x) - p_{n_k}(y)| \leqslant |p_{n_k}(x) - p_{n_N}(x)| + |p_{n_N}(x) - p_{n_N}(y)| + |p_{n_N}(y) - p_{n_k}(y)| < \epsilon.$$

By Arzela-Ascoli, we conclude that the sequence $\{p_{n_k}\}$ converges uniformly to some function $\tilde{h}$. We prove that $\tilde{h} = h$. By this uniform convergence, for $\epsilon > 0$, we have $|p_{n_k}(x) - \tilde{h}(x)| < \epsilon$ for $k \gg 0$, which implies

$$\|p_{n_k} - \tilde{h}\|_{L^2} \xrightarrow{k\to\infty} 0.$$

On the other hand, $\|p_{n_k} - h\|_{H^3} \to 0$ implies $\|p_{n_k} - h\|_{L^2} \xrightarrow{k\to\infty} 0$. Since h and $\tilde{h}$ are continuous, we must have $\tilde{h} = h$. $\square$

The next Lemma completes the proof of Proposition 1.5, *i.e.*, Proposition 1.1.

LEMMA 1.4. *If h satisfies the hypotheses in Proposition 1.5, then h has a unique minimum in E.*

PROOF. Suppose that h attains its global minimum at two isolated points x_1 and x_2. Choose $\epsilon > 0$ such that $B_\epsilon(x_1) \cap B_\epsilon(x_2) = \emptyset$. By Lemma 1.3, we can find a sequence $\{p_i\}_{i\in\mathbb{N}}$ such that $p_n \to h$ uniformly and each p_i satisfies (1.4) and (1.5). By Remark 1.4, each p_i has a unique minimum, say at y_i. Due to the uniform convergence of $\{p_i\}$, $\{y_i\}$ converges to either x_1 or x_2.

Assume that $y_i \to x_1$. By the uniqueness of the minimum for p_i, for all i, there exists ϵ_i such that for $\epsilon' < \epsilon_i$, there exists δ such that

$$p_i(x) \in (p_i(y_i) - \delta, p_i(y_i) + \delta) \Rightarrow x \in B_{\epsilon'}(y_i). \tag{1.17}$$

By the equicontinuity of the $\{p_i\}$, we can take $\epsilon_i = \epsilon_1$ independent of i.

On the other hand,

$$|p_i(y_i) - p_i(x_2)| \le |p_i(y_i) - p_i(x_1)| + |p_i(x_1) - h(x_1)| + |h(x_2) - p_i(x_2)| \to 0,$$

as $i \to \infty$. Thus $x_2 \in B_{\epsilon'}(y_i)$ for $i \gg 0$ by (1.17). For $\epsilon' < \epsilon/2$ and $i \gg 0$, we conclude that $x_2 \in B_\epsilon(x_1)$, a contradiction. $\square$

We can now prove the Euclidean version of Corollary 1.2

COROLLARY 1.6. *Let Q be a smooth probability distribution on F with compact support in E such that the Fréchet function $f_Q(x) = \int_E d_E^2(x,y)Q(y)dy$ has a unique minimum at x_0. Then there exists ζ such that every continuous function $f \in B^3_{f_Q}(\zeta) \cap C_c(E)$ has a unique minimum.*

Proof. We cannot directly apply Proposition 1.1, since f_Q does not have compact support. However, for fixed E, the minimum of f_Q occurs inside the diam(E)-neighborhood N of E, since $x_0 \notin N$ implies $d_E(x_0, y) > d_E(x, y)$ for all $x, y \in E$. Thus we may consider f_Q restricted to N and replace E with N in the Proposition. Recall from Remark 2.3 that f_Q satisfies the hypothesis of Proposition 1.1. $\square$

This gives a proof of Corollary 1.2.

Corollary 1.7. *Let Q be a smooth probability distribution with support inside a compact set $E \subset F_{a/4}$ with Fréchet function $f_Q(x) = \int_E d_P^2(x, y)\nu_0(y)dy$ with respect to the Procrustean distance. Then there exists $\zeta > 0$ such that every $f \in B^3_{f_Q}(\zeta) \cap C_c(F)$ has a unique minimum.*

Proof. For $x, y \in F_{a/4}$, we know $d_P(x, y) = d_E(x, y)$. Therefore f_Q is the same for the Euclidean and Procrustean distances. By Remark 1.4 and Lemma 1.5, we can apply Proposition 1.5 to f_Q. Thus continuous compactly supported functions that are H_3 close to f_Q have unique minima. $\square$

We can now prove Theorem 1.1.

Theorem 1.2. *Let Q be a smooth probability distribution with support inside a compact set $E \subset F_{a/4}$. There exists $\zeta > 0$ such that for every $Q' \in B^3_Q(\zeta) \cap C_c(F)$, the Fréchet function $f_{Q'} = \int_E d_P^2(x, y)Q'(y)dy$ has a unique minimum.*

Proof. By Corollary 1.7, the theorem follows by proving that the function $F : Q \to f_Q$ is continuous on H_3, as then Q' close to Q implies $f_{Q'}$ is close to f_Q. (As in the proof of Corollary 1.6, the fact that f_Q does not have compact support is not a problem.)

The continuity of F proceeds as before. For $|\alpha| \le 3$, estimates on $|\partial^\alpha f_{Q_1} - \partial^\alpha f_{Q_2}|$ reduce to estimates on $|Q_1 - Q_2|$ inside the integrand. $\square$

We end by estimating the smoothness of the Fréchet integral f_Q with respect to the Procrustean distance. Namely, we show that f_Q has third order weak derivatives, which matches up with one of the hypotheses in Proposition 1.1. This indicates that improvements to Theorem 1.1 is possible: if f_Q is H^3-close to a smooth function on F with a unique minimum, then f_Q has a unique minimum.

Lemma 1.5. *The Fréchet function $f_Q(x) = \int_E d_P^2(x, y)Q(y)dy$ with respect to the Procrustean distance lies in H^3.*

PROOF. We show that f_Q has weak third derivatives; the argument for lower order derivatives is similar.

The Fréchet function is

$$f_Q(x) = \int_E \min_{\sigma\in\Sigma_d}\{|\sigma\cdot x - y|^2\}Q(y)dy.$$

Since Σ_d is a finite set, for ease of notation we just consider the two element set $\Sigma_2 = \{\sigma_1, \sigma_2\}$. Take $|\alpha| = 3$, set $\alpha = \beta+\gamma, |\beta| = 2, |\gamma| = 1$. Then

$$\begin{aligned}
\partial_x^\alpha f_Q(x) &= \partial_x^\alpha \int_{\mathbb{R}^D} \min(|\sigma_1\cdot x - y|^2, |\sigma_2\cdot x - y|^2)Q(y)dy\\
&= \partial_x^\gamma \int_{\mathbb{R}^D} \partial_x^\beta \min(|\sigma_1\cdot x - y|^2, |\sigma_2\cdot x - y|^2)Q(y)dy\\
&= \partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta \min(|\sigma_1\cdot x - y|^2, |\sigma_2\cdot x - y|^2)Q(y)dy\\
&= \frac{1}{2}\partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta \big(|\sigma_1\cdot x - y|^2 + |\sigma_2\cdot x - y|^2\\
&\qquad - ||\sigma_1\cdot x - y|^2 - |\sigma_2\cdot x - y|^2|\big)\, Q(y)dy\\
&= \frac{1}{2}\partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta (|\sigma_1\cdot x - y|^2 + |\sigma_2\cdot x - y|^2)Q(y)dy\\
&\qquad + \frac{1}{2}\partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta ||\sigma_1\cdot x - y|^2 - |\sigma_2\cdot x - y|^2|Q(y)dy\\
&:= A + B.
\end{aligned}$$

The second line uses dominated convergence; the third line uses the symmetry of the integrand in x, y; the fourth line uses $\min\{f, g\} = |f+g| - |f-g|$.

A is smooth, so we have to check B. For $\langle\cdot,\cdot\rangle$ the usual inner product on $\mathbb{R}^D$,

$$B = \partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta |\langle \sigma_1\cdot x - \sigma_2\cdot x, y\rangle| Q(y)dy.$$

Now $g(y) = \langle \sigma_1\cdot x - \sigma_2\cdot x, y\rangle$ is linear in y. For $\beta = (\xi, \zeta)$ as a multi-index, we have

$$\begin{aligned}
B &= \partial_x^\gamma \int_{\mathbb{R}^D} \partial_y^\beta |\langle \sigma_1\cdot x - \sigma_2\cdot x, y\rangle| Q(y)dy\\
&= \partial_x^\gamma \int_{\mathbb{R}^D} \left.\frac{d^2|z|}{dz^2}\right|_{z=g(y)} \partial_y^\xi g(y)\partial_y^\zeta g(y) Q(y)dy\\
&= 2\partial_x^\gamma \int_{\mathbb{R}^D} \delta_{\sigma_1\cdot x - \sigma_2\cdot x}(y)\partial_y^\xi g(y)\partial_y^\zeta g(y)Q(y)dy,
\end{aligned}$$

where $\delta_{\sigma_1\cdot x-\sigma_2\cdot x}(y)$ is the Dirac delta function. The integration in the last line is well-defined in the distributional/weak sense since Q has compact support. Thus B exists in the weak sense. $\square$

2. Isometric embeddings and uniqueness of Fréchet means. In this section we prove that for any compactly supported distribution on $\mathcal{U}_d$, there is a unique Fréchet mean after isometrically embedding the support of the distribution in a vector space of bounded functions. The main point is that we can use convexity techniques in the vector space. As a corollary, the consistency result (Theorem 3.2) in the main text extends to this embedding.

Let $K \subset \mathcal{U}_d$ be a compact set. For a distribution Q supported on K, consider the integrand in the Fréchet function $F(x) = \int_K d^2(x,y)Q(dy)$ as (the square of) bounded function of x:

$$f_x \in \mathcal{B}(K), \quad f_x(y) = d(x,y).$$

In general, we consider an arbitrary compact metric measure space (K, d, Q). We can rewrite the Fréchet function as

$$F(x) = \|f_x\|^2_{2,Q},$$

the square of the L^2 norm of f_x with respect to Q.

Let $\imath : K \to \mathcal{B}(K)$ be $\imath(x) = f_x$. This is clearly a continuous injection $(K,d) \to (\mathcal{B}(K), d_\infty)$, where d_∞ is the metic associated to the L^∞ norm $\|\cdot\|_\infty$. In fact, $\imath$ is an isometric injection.

Lemma 2.1. *$\imath : (K,d) \to (\mathcal{B}(K), d_\infty)$ is an isometry.*

This is well-known, but we include the quick proof.

Proof. For $x, z \in K$,

$$\begin{aligned} d_\infty(\imath(x), \imath(z)) &= \|\imath(x) - \imath(z)\|_\infty = \max_{y\in K} |d(x,y) - d(z,y)| \\ &\geq |d(x,z) - d(z,z)| = d(x,z). \end{aligned}$$

Also, we either have, for some $y_0 \in K$,

$$d_\infty(\imath(x), \imath(z)) = \max_{y\in K} |d(x,y) - d(z,y)| = d(x,y_0) - d(z,y_0)| \leq d(x,z),$$

or

$$d_\infty(\imath(x), \imath(z)) = \max_{y\in K} |d(x,y) - d(z,y)| = -d(x,y_0) + d(z,y_0)| \leq d(x,z).$$

Thus $d_\infty(\imath(x), \imath(z)) = d(x,z)$. $\square$

Consider $(\mathcal{B}(K), d_\infty, \imath_*Q)$, where $\imath_*Q(A) = Q(\imath^{-1}(A))$ is the pushforward measure. $\imath : K \to \mathcal{B}(K)$ is (Q, i_*Q) measurable, so for any continuous function g on $\mathcal{B}(K)$, we have

$$\int_{\mathcal{B}(K)} g \; d\imath_*Q = \int_K g \circ \imath \; dQ.$$

In our case where $K \subset \mathcal{U}_d$, we can write

$$\int_{\mathcal{B}(K)} g \; d\imath_*Q = \int_{\mathcal{U}_d} g \circ \imath \; dQ,$$

since Q has support on K. In particular,

$$F(x) = \int_{\mathcal{U}_d} d^2(x, y) \; Q(dy) = \int_{\mathcal{B}(K)} \|f_x - f_y\|^2 \; i_*Q(df_y).$$

Thus F on K (or really $F \circ \imath^{-1}$ on $\imath(K)$) extends to a continuous function $\overline{F} : \mathcal{B}(K) \to \mathbb{R}$:

$$\overline{F}(f) = \int_{\mathcal{B}(K)} \|f - g\|^2 i_*Q(dg) = \int_{\mathcal{B}(K)} \|f - f_y\|^2 \; i_*Q(df_y).$$

Let $\mathcal{C} = \mathcal{C}(K)$ be the closed convex hull of $\imath(K)$ in $\mathcal{B}(K)$. Recall that a real valued function f on a vector space V is convex if $f(tx + (1-t)x') \leq tf(x) + (1-t)f(x')$ for $x, x' \in V$, $t \in [0, 1]$, and is strongly convex if $f(tx + (1-t)x') < tf(x) + (1-t)f(x')$ for $x, x' \in V$, $t \in (0, 1)$.

LEMMA 2.2. *Let K be a compact set, and let f be a strongly convex function on $(\mathcal{B}(K), d_\infty)$. Then f has a unique minimum in $\mathcal{C}(K)$.*

PROOF. The closed convex hull $\mathcal{C}(K)$ of the compact set $\imath(K)$ in the Banach space $\mathcal{B}(K)$ is compact [**?** , Thm. 5.35] and of course convex. A strongly convex function on a compact convex set has a unique minimum. $\square$

Now we prove that there is a unique Fréchet mean for $\overline{F}$ in $\mathcal{C}(K)$.

THEOREM 2.1. *Let $(\mathcal{C}, d', \mu)$ be a compact convex metric measure space, with μ a finite Borel measure (for the metric topology). Let $\overline{F} : \mathcal{C} \to \mathbb{R}$ be the Fréchet function $\overline{F}(x) = \int_{\mathcal{C}} d'(x, y)^2 \; \mu(dy)$. Then $\overline{F}$ has a unique minimum. In particular, for $\mathcal{C} = \mathcal{C}(K) \subset \mathcal{B}(K)$, $d' = d_\infty$, and $\mu = i_*Q$, where Q is a Borel measure on K, the Fréchet function for (K, d_P) extends to a function on $\imath(K)$ with a unique minimum in $\mathcal{C}(K)$.*

Corollary 2.1. *If K is a compact subset of the space $\mathcal{U}_d$ of unlabeled networks, the consistency result for the Fréchet mean (Theorem 3.2 in the article) holds on the closed convex hull of $\imath(K)$.*

The proof of the corollary follows from the fact that $\mathcal{C}(K)$ is compact and [**?** , Cor. 2.4]

Proof. A distance function $x \mapsto d(x, \cdot)$ on a vector space V is always convex, and its square $x \mapsto d^2(x, \cdot)$ is always strongly convex: (These are easy consequences of the triangle inequality.) For any compactly supported finite measure μ on $\mathcal{C}$, we get

$$\overline{F}_\mu(tf + (1-t)g) := \int_{\mathcal{C}} d^2_\infty(tf + (1-t)g, h)\ \mu(dh) < t\overline{F}_\mu(f) + (1-t)\overline{F}_\mu(g).$$

Thus $\overline{F}_\mu$ is strongly convex. (Note that the integral defining $\overline{F}_\mu(x)$ exists, since the integrand is continuous and hence μ-measurable, and μ is finite and compactly supported.)

We claim that $\overline{F}_\mu$ is continuous on $\mathcal{C}$. Let $f_n \to f$ in $\mathcal{C}$. Then $h_n := d^2_\infty(f_n, \cdot) \to h := d^2_\infty(f, \cdot)$. We have $|d^2_\infty(f_n, g)| \leq \mathrm{diam}(\mathcal{C})$, which is finite since $\mathcal{C}$ is compact. Since the h_n and constant functions are μ-measurable, dominated convergence implies $F_\mu(f_n) = \int_{\mathcal{C}} h_n\ d\mu \to \int_{\mathcal{C}} h\ d\mu = F_\mu(f)$.

Since $\overline{F}_\mu$ is continuous on $\mathcal{C}$, by the last Lemma it has a unique minimum.

For the particular case, note that Q Borel and $\imath$ continuous imply that $i_* Q$ is Borel. □

Corollary 2.2. *For $K \subset \mathcal{U}_d$, the unique Fréchet minimum of $\overline{F}$ on $\mathcal{C}(K)$ lies within the closed ball of radius $2 \cdot \mathrm{diam}(K)$ of $\imath(K)$.*

Proof. The minimum x_0 of $\overline{F}$ lies in $\mathcal{C}(K)$, so there exist $x_n \to x_0$ with each $x_n = \sum_{i=1}^k t_i y_i$ for some $k, t_i \in [0, 1]$, $y_i \in \imath(K)$ with $\sum t_i = 1$ and k, t_i, y_i depending on n. We have

$$\begin{aligned} \|y_1 - x_n\|_\infty &\leq (1 - t_1)\|y_1\|_\infty + t_2\|y_2\|_\infty + \dots t_k\|y_k\|_\infty \\ &\leq (1 + t_1)\|y_1\|_\infty + t_2\|y_2\|_\infty + \dots t_k\|y_k\|_\infty \\ &\leq 2 \max_i \|y_i\|_\infty \end{aligned}$$

Now $\|y_i\|_\infty = \max_{x \in K} d_K(y_i, x) \leq \mathrm{diam}(K)$, so $\|y_i - x_0\|_\infty \leq 2 \cdot \mathrm{diam}(K)$. □

REMARK 2.3. Set $K' = \imath(K) \cup \{x_0\}$, where x_0 is the minimum for the Fréchet function $\overline{F}$ on $\mathcal{C}(K)$. Then $\overline{F}|_{K'}$ has a unique minimum at x_0. Note that K' is $\imath(K)$ plus one more point, and has the natural metric

$$d'_P(x,y) = \begin{cases} d_\infty(\imath(x), \imath(y)) = d_P(x,y), & x, y \in K, \\ d_\infty(x_0, \imath(y)) = \max_{z\in K} |x_0(z) - d_P(y,z)|, & y \in K. \end{cases}$$

So in this sense we can say that "K plus one point" has a unique Fréchet mean.

EXAMPLE 2.4. In Example 3.1 in the paper, we produce a distribution on the cone $C = \mathbb{R}^2/\mathbb{Z}_4$ whose Fréchet mean set is a circle inside C. If we choose a symmetric compact set $K = \{(r,\theta) : r \in [a,b], \theta \in [0, 2\pi]\}$ in C, and choose a distribution with support in K and with no θ dependence, as in (3.5), then the Fréchet set is again a circle $S = \{(r,\theta) : r = r_0\}$ inside K. As a general principle, the S^1 invariance of the distribution and the distance function on K leads to the S^1 invariance of the Fréchet set.

The S^1 rotational action on C extends to an isometric S^1 action on $\mathcal{B}(K)$ in the sup norm. This implies that the unique Fréchet mean f_* of the extended Fréchet function is S^1-invariant. The natural guess for f_* is

$$f_* = \lim_{n\to\infty} \frac{1}{n} \sum_{k=1^n} d_\infty(x_k, \cdot), \tag{2.1}$$

where $x_k = r_0 \exp(2\pi i k/n) \in S$. More generally, we conjecture that if x_k is sampled iid with respect to the uniform measure on S, then (2.1) holds almost surely, and the corresponding central limit theorem holds.

It is natural to try to produce a unique Fréchet mean inside K by taking the closest point in $i(K)$ to f_*. However, if our conjecture holds, then all points on S are equidistant to f_*. This makes sense: no original Fréchet set element should be singled out in this S^1 invariant procedure.