SUPPLEMENTARY MATERIAL TO "FUNCTIONAL DATA ANALYSIS FOR DENSITY FUNCTIONS BY TRANSFORMATION TO A HILBERT SPACE"

The Wasserstein metric, Wasserstein-Fréchet mean, simulation results and additional proofs

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S.1. The Wasserstein Metric. The equivalence of the metrics

$$d_Q(f,g)^2 = \int_0^1 (F^{-1}(t) - G^{-1}(t))^2 \, dt \quad \text{and} \quad d_W(f,g)^2 = \inf_{X \sim f, Y \sim g} E(X-Y)^2$$

is well known. It can be easily seen by applying a covariance identity due to [28]. If $X \sim F$, $Y \sim G$ and $(X,Y) \sim H$, then this identity states that

$$\mathrm{Cov}(X,Y) = \int\int \{H(u,v) - F(u)G(v)\} \, du \, dv.$$

Expanding the expectation $E(X-Y)^2$, one finds that the distance is obtained by maximizing $E(XY)$, or, equivalently, by maximizing $\mathrm{Cov}(X,Y)$. For a random variable U that is uniformly distributed on $[0,1]$, take $X^* = F^{-1}(U)$ and $Y^* = G^{-1}(U)$. Then $X^* \sim F$, $Y^* \sim G$ and the distribution function of (X^*, Y^*) is given by $H^*(u,v) = \min(F(u), G(v))$. Clearly, for any joint distribution of $X \sim F$ and $Y \sim G$, we have $H \le H^*$. By Hoeffding's inequality, this means $\mathrm{Cov}(X,Y) \le \mathrm{Cov}(X^*, Y^*)$. Thus,

$$\begin{aligned} d_W(f,g)^2 = E[(X^* - Y^*)^2] &= E[(F^{-1}(U) - G^{-1}(U))^2] \\ &= \int_0^1 (F^{-1}(t) - G^{-1}(t))^2 \, dt. \end{aligned}$$

Let Q be the quantile process corresponding to the density process $f \sim \mathfrak{F}$ and set $Q_\oplus(t) = E(Q(t))$. For $q_\oplus = Q'_\oplus$ and $F_\oplus = Q_\oplus^{-1}$, the *Wasserstein-Fréchet* mean is

$$f_\oplus(x) = \frac{1}{q_\oplus(F_\oplus(x))}.$$

Its estimation can thus be reduced to estimating the function $q_\oplus$. Due to the restrictions on the space $\mathcal{F}$ (see assumption (A1)), we can pass differentiation inside the expectation so that $E(Q'(t)) = q_\oplus(t)$. This suggests averaging the quantile densities of the sample to obtain an estimator for $q_\oplus$.

Starting with either the densities, f_i, or their estimates, $\check{f}_i$, $i = 1, \ldots, n$, we therefore use the corresponding quantile densities (q_i or $\check{q}_i$) to estimate $q_\oplus$ by

$$\tilde{q}_\oplus(t) = \frac{1}{n}\sum_{i=1}^n q_i(t), \quad \text{respectively,} \quad \hat{q}_\oplus(t) = \frac{1}{n}\sum_{i=1}^n \check{q}_i(t).$$

Computing the corresponding distribution functions, we thus estimate the Wasserstein-Fréchet mean by

$$\tilde{f}_\oplus(x) = \frac{1}{\tilde{q}_\oplus(\tilde{F}_\oplus(x))}, \quad \text{respectively,} \quad \hat{f}_\oplus(x) = \frac{1}{\hat{q}_\oplus(\hat{F}_\oplus(x))}.$$

As Theorem 2 requires a rate of convergence γ_n for the Wasserstein-Fréchet mean estimator based on fully observed densities, the following result shows that we make take $\gamma_n = n^{-1/2}$ in the case of fully observed densities.

PROPOSITION 3. *Under assumption (A1), the estimator $\tilde{f}_\oplus$ of $f_\oplus$ for the Wasserstein-Fréchet mean satisfies*

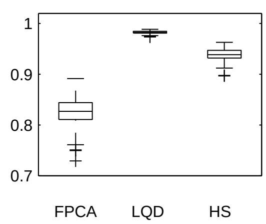
$$d_W(f_\oplus, \tilde{f}_\oplus) = O_p(n^{-1/2}).$$

PROOF. By Thm 3.9 in [9], $d_2(q_\oplus, \tilde{q}_\oplus) = O_p(n^{-1/2})$. As $|Q_\oplus(t) - \tilde{Q}_\oplus(t)| \leq d_2(q_\oplus, \tilde{q}_\oplus)$, we also have

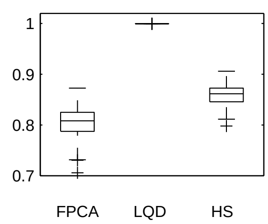
$$d_W(f_\oplus, \tilde{f}_\oplus) = d_2(Q_\oplus, \tilde{Q}_\oplus) = O_p(n^{-1/2}).$$

□

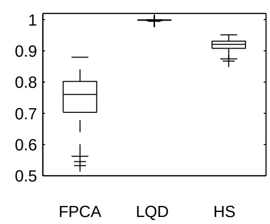
S.2. Simulation Results for the Wasserstein Metric. Figure 7 shows the distribution of fraction of variance explained values in terms of the distance d_W for all simulation settings, similar to Figure 2 in the main text which shows the results for the ordinary L^2 distance. The use of the Wasserstein distance more clearly demonstrates the weakness of ordinary FPCA. The Hilbert sphere method performs relatively better in the context of metric d_W than the L^2 metric, but is still outperformed by the transformation method using the log quantile density transformation, ψ_Q.



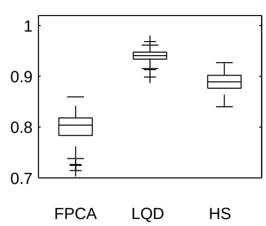
(a) Setting 1 - $K = 1$



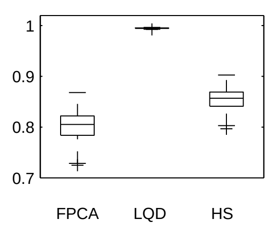
(b) Setting 2 - $K = 1$



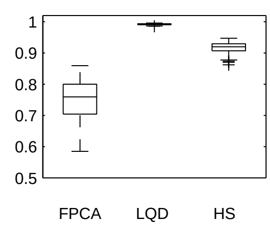
(c) Setting 3 - $K = 2$



(d) Setting 1 - $K = 1$



(e) Setting 2 - $K = 1$



(f) Setting 3 - $K = 2$

Fig 7: Boxplots of fraction of variance explained for 200 simulations, using the Wasserstein metric, d_W. The first row corresponds to fully observed densities and the second corresponds to estimated densities. The columns correspond to settings 1, 2 and 3 from left to right (see Table 1). The methods are denoted by 'FPCA' for ordinary FPCA on the densities, 'LQD' for the transformation approach with ψ_Q and 'HS' for the Hilbert sphere method.

S.3. Listing of All Assumptions. The following is a systematic compilation of all assumptions, subsets of which are used for various results and some of which have been stated in the main text. Recall that d_2 and d_∞ denote the L^2 and uniform metrics, respectively, and $\|\cdot\|_2$ and $\|\cdot\|_\infty$ denote the corresponding norms.

(A1) For all $f \in \mathcal{F}$, f is continuously differentiable. Moreover, there is a constant $M > 1$ such that, for all $f \in \mathcal{F}$, $\|f\|_\infty$, $\|1/f\|_\infty$ and $\|f'\|_\infty$ are all bounded above by M.

(D1) For a sequence $b_N = o(1)$, the density estimator $\check{f}$, based on an i.i.d. sample of size N, satisfies $\check{f} \geq 0$, $\int_0^1 \check{f}(x)\, dx = 1$ and

$$\sup_{f\in\mathcal{F}} E(d_2(f, \check{f})^2) = O(b_N^2).$$

(D2) For a sequence $a_N = o(1)$ and some $R > 0$, the density estimator $\check{f}$, based on an i.i.d. sample of size N, satisfies

$$\sup_{f\in\mathcal{F}} P(d_\infty(f, \check{f}) > Ra_N) \to 0.$$

(S1) Let $\check{f}$ be a density estimator that satisfies (D2), and suppose densities $f_i \in \mathcal{F}$ are estimated by $\check{f}_i$ from i.i.d. samples of size $N_i = N_i(n)$, $i = 1, \ldots, n$, respectively. There exists a sequence of lower bounds $m(n) \leq \min_{1\leq i\leq n} N_i$ such that $m(n) \to \infty$ as $n \to \infty$ and

$$n \sup_{f\in\mathcal{F}} P(d_\infty(f, \check{f}) > Ra_m) \to 0$$

where, for generic $f \in \mathcal{F}$, $\check{f}$ is the estimated density from a sample of size $N(n) \geq m(n)$.

(K1) The kernel κ is of bounded variation and is symmetric about 0.

(K2) The kernel κ satisfies $\int_0^1 \kappa(u)\, du > 0$, and $\int_{\mathbb{R}} |u|\kappa(u)\, du$, $\int_{\mathbb{R}} \kappa^2(u)\, du$ and $\int_{\mathbb{R}} |u|\kappa^2(u)\, du$ are finite.

(T0) Let f, $g \in \mathcal{G}$ with f differentiable and $\|f'\|_\infty < \infty$. Set

$$D_0 \geq \max\left(\|f\|_\infty, \|1/f\|_\infty, \|g\|_\infty, \|1/g\|_\infty, \|f'\|_\infty\right).$$

There exists C_0 depending only on D_0 such that

$$d_2(\psi(f), \psi(g)) \leq C_0\, d_2(f, g), \quad d_\infty(\psi(f), \psi(g)) \leq C_0\, d_\infty(f, g).$$

(T1) Let $f \in \mathcal{G}$ be differentiable with $\|f'\|_\infty < \infty$ and let D_1 be a constant bounded below by $\max(\|f\|_\infty, \|1/f\|_\infty, \|f'\|_\infty)$. Then $\psi(f)$ is differentiable and there exists $C_1 > 0$ depending only on D_1 such that $\|\psi(f)\|_\infty \leq C_1$ and $\|\psi(f)'\|_\infty \leq C_1$.

(T2) Let d be the selected metric in density space, Y be continuous and X be differentiable on $\mathcal{T}$ with $\|X'\|_\infty < \infty$. There exist constants $C_2 = C_2(\|X\|_\infty, \|X'\|_\infty) > 0$ and $C_3 = C_3(d_\infty(X,Y)) > 0$ such that

$$d(\psi^{-1}(X), \psi^{-1}(Y)) \leq C_2\, C_3\, d_2(X,Y)$$

and, as functions, C_2 and C_3 are increasing in their respective arguments.

(T3) For a given metric d on the space of densities and $f_{1,K} = f_1(\cdot, K, \psi)$ (see (4.5)), $V_\infty - V_K \to 0$ and $E(d(f, f_{1,K})^4) = O(1)$ as $K \to \infty$.

S.4. Additional Proofs.

LEMMA 1. *Let A be a closed and bounded interval of length $|A|$ and assume $X : A \to \mathbb{R}$ is continuous with Lipschitz constant L. Then*

$$\|X\|_\infty \leq 2 \max\left(|A|^{-1/2}\|X\|_2,\ \ L^{1/3}\|X\|_2^{2/3}\right).$$

PROOF OF LEMMA 1. Let t^* satisfy $|X(t^*)| = \|X\|_\infty$ and define $I = [t^* - \|X\|_\infty/(2L), t^* + \|X\|_\infty/(2L)] \cap A$. Then, for $t \in I$, $|X(t)| \geq \|X\|_\infty/2$. If $I = A$,

$$\|X\|_2^2 = \int_A X^2(s)\, ds \geq \frac{|A|\|X\|_\infty^2}{4},$$

so $\|X\|_\infty \leq 2|A|^{-1/2}\|X\|_2$. If $I \neq A$, suppose without loss of generality that $t^* + \|X\|_\infty/(2L) \in A$. Then

$$\|X\|_2^2 \geq \int_{t^*}^{t^*+\|X\|_\infty/(2L)} X^2(s)\, ds \geq \frac{\|X\|_\infty^2}{4} \cdot \frac{\|X\|_\infty}{2L} = \frac{\|X\|_\infty^3}{8L},$$

so $\|X\|_\infty \leq 2L^{1/3}\|X\|_2^{2/3}$. □

LEMMA 2. *Let X be a stochastic process on a closed interval $\mathcal{T} \subset \mathbb{R}$ such that $\|X\|_\infty < C$ and $\|X'\|_\infty < C$ almost surely. Let ν and H be the mean and covariance functions associated with X, and ρ_k and τ_k, $k \geq 1$, be the eigenfunctions and eigenvalues of the integral operator with kernel H. Then $\|\nu\|_\infty < C$, $\|H\|_\infty < 4C^2$ and $\|\rho_k\|_\infty < 4C^2|\mathcal{T}|^{1/2}\tau_k^{-1}$ for all $k \geq 1$. Additionally, $\|\nu'\|_\infty < C$ and $\|\rho_k'\|_\infty < 4C^2|\mathcal{T}|^{1/2}\tau_k^{-1}$ for all $k \geq 1$.*

PROOF. Since the bounds on X and X' are deterministic, $\|\nu\|_\infty$ and $\|H\|_\infty$ are both bounded by the given constants. The bound on $\|\rho_k\|_\infty$ follows since $\rho_k(t) = \tau_k^{-1}\int_{\mathcal{T}} H(s,t)\rho_k(s)\, ds$ and $\|\rho_k\|_2 = 1$. Dominated convergence implies that ν' exists and is bounded by C, and also implies the bound of $4C^2$ for the partial derivatives of H, which then leads to the bounds on ρ_k' for all k. $\square$

LEMMA 3. *Under assumptions (A1) and (T1), with* $\hat{\nu}, \tilde{\nu}, \widehat{H}, \widetilde{H}$ *as in (4.2) and (4.3),*

$$\begin{aligned} &d_2(\nu, \tilde{\nu}) = O_p(n^{-1/2}), && d_2(H, \widetilde{H}) = O_p(n^{-1/2}), \\ &d_\infty(\nu, \tilde{\nu}) = O_p\left(\left(\frac{\log n}{n}\right)^{1/2}\right), && d_\infty(H, \widetilde{H}) = O_p\left(\left(\frac{\log n}{n}\right)^{1/2}\right). \end{aligned} \tag{S.1}$$

Under the additional assumptions (D1), (D2) and (S1), we have

$$\begin{aligned} &d_2(\nu, \hat{\nu}) = O_p(n^{-1/2} + b_m), && d_2(H, \widehat{H}) = O_p(n^{-1/2} + b_m), \\ &d_\infty(\nu, \hat{\nu}) = O_p\left(\left(\frac{\log n}{n}\right)^{1/2} + a_m\right), && d_\infty(H, \widehat{H}) = O_p\left(\left(\frac{\log n}{n}\right)^{1/2} + a_m\right). \end{aligned} \tag{S.2}$$

PROOF. Assumptions (A1) and (T1) imply $E\|X\|_2^2 < \infty$, so the first line in (S.1) follows from Theorems 3.9 and 4.2 in [9]. The second line in (S.1) follows from Corollaries 2.3(b) and 3.5(b) in [33]. We will show the argument for the mean estimate in (S.2), and the covariance follows similarly.

Let M be as given in assumption (A1) and set $D_1 = 2M$. Define

$$E_n = \bigcap_{i=1}^{n} \left\{ d_\infty(f_i, \check{f}_i) \leq D_1^{-1} \right\}.$$

Then $P(E_n^c) \to 0$ by assumptions (D2) and (S1). Take C_1 as given in (T1) for D_1 as defined above. Also by (S1), there is $R > 0$ such that

$$P(\{d_\infty(\tilde{\nu}, \hat{\nu}) > R a_m\} \cap E_n) \leq n \max_{1 \leq i \leq n} P(d_\infty(f_i, \check{f}_i) > C_1^{-1} R a_m) \to 0$$

as $n \to \infty$, so $d_\infty(\tilde{\nu}, \hat{\nu}) = O_p(a_m)$. Thus, by the triangle inequality, $d_\infty(\nu, \hat{\nu}) = O_p\left(\left(\frac{\log n}{n}\right)^{1/2} + a_m\right)$.

Next, letting $\widehat{X}_i = \psi(\check{f}_i)$,

$$\begin{aligned} P\left(\{d_2(\tilde{\nu},\hat{\nu}) > R\} \cap E_n\right) &\le P\left(\left\{\sum_{i=1}^n d_2(X_i, \widehat{X}_i) > Rn\right\} \cap E_n\right) \\ &\le P\left(\sum_{i=1}^n d_2(f_i, \check{f}_i) > C_1^{-1}Rn\right) \\ &\le C_1 R^{-1} n^{-1} \sum_{i=1}^n \sqrt{E(d_2(f_i,\check{f}_i)^2)} = R^{-1}O(b_m), \end{aligned}$$

which shows that $d_2(\tilde{\nu},\hat{\nu}) = O_p(b_m)$, so the result holds by the triangle inequality. □

COROLLARY 1. *Under assumption (A1) and (T1), letting* $A_k = \|\rho_k\|_\infty$, *with* δ_k *as in (5.1),*

$$\begin{aligned} |\tau_k - \tilde{\tau}_k| &= O_p(n^{-1/2}), \\ d_2(\rho_k, \tilde{\rho}_k) &= \delta_k^{-1} O_p(n^{-1/2}), \ \textit{and} \\ d_\infty(\rho_k, \tilde{\rho}_k) &= \tilde{\tau}_k^{-1} O_p\left(\frac{(\log n)^{1/2} + \delta_k^{-1} + A_k}{n^{1/2}}\right), \end{aligned} \tag{S.3}$$

where all O_p *terms are uniform over* k*. If the additional assumptions (D1), (D2) and (S1) hold,*

$$\begin{aligned} |\tau_k - \hat{\tau}_k| &= O_p(n^{-1/2} + b_m), \\ d_2(\rho_k, \hat{\rho}_k) &= \delta_k^{-1} O_p(n^{-1/2} + b_m), \ \textit{and} \\ d_\infty(\rho_k, \hat{\rho}_k) &= \hat{\tau}_k^{-1} O_p\left(\frac{(\log n)^{1/2} + \delta_k^{-1} + A_k}{n^{1/2}} + a_m + b_m[\delta_k^{-1} + A_k]\right), \end{aligned} \tag{S.4}$$

where again all O_p *terms are uniform over* k*.*

PROOF. First, observe that (A1) and (T1) together imply that X satisfies the assumptions of Lemma 2. The first two lines of both (S.3) and (S.4) follow by applying Lemmas 4.2 and 4.3 of [9] with the rates given in Lemma 3, above. For the uniform metric on the eigenfunctions, we follow the argument given in the proof of Lemma 1 in [36] to find that

$$d_\infty(\tau_k\rho_k, \tilde{\tau}_k\tilde{\rho}_k) \le |\mathcal{T}|^{1/2}\left[d_\infty(H,\widetilde{H}) + \|H\|_\infty d_2(\rho_k,\tilde{\rho}_k)\right] = O_p\left(\frac{(\log n)^{1/2} + \delta_k^{-1}}{n^{1/2}}\right).$$

It follows that

$$
\begin{aligned}
|\rho_k(s) - \tilde\rho_k(s)| &\le \tilde\tau_k^{-1}\left(|\tau_k\rho_k(s) - \tilde\tau_k\rho_k(s)| + |\rho_k(s)|\,|\tau_k - \tilde\tau_k|\right)\\
&= \tilde\tau_k^{-1} O_p\left(\frac{(\log n)^{1/2} + \delta_k^{-1} + A_k}{n^{1/2}}\right).
\end{aligned}
$$

Since this last expression is independent of s, this proves the third line of (S.3). The third line of (S.4) is proven in a similar manner. □

LEMMA 4. *Assume (A1), (T1) and (T2) hold. Let $A_k = \|\rho_k\|_\infty$, M as in (A1), δ_k as in (5.1), and C_1 as in (T1) with $D_1 = M$. Let $K^*(n) \to \infty$ be any sequence which satisfies $\tau_{K^*} n^{1/2} \to \infty$ and*

$$
\sum_{k=1}^{K^*}\left[(\log n)^{1/2} + \delta_k^{-1} + A_k + \tau_{K^*}\delta_k^{-1}A_k\right] = O(\tau_{K^*} n^{1/2}).
$$

Let C_2 be as in (T2), $X_{i,K} = \nu + \sum_{k=1}^{K}\eta_{ik}\rho_k$, $\widetilde{X}_{i,K} = \tilde\nu + \sum_{k=1}^{K}\tilde\eta_{ik}\tilde\rho_k$, and set

$$
S_{K^*} = \max_{1\le K\le K^*}\max_{1\le i\le n} C_2(\|X_{i,K}\|_\infty, \|X'_{i,K}\|_\infty).
$$

Then

$$
\max_{1\le K\le K^*}\max_{1\le i\le n} d(f_i(\cdot,K,\psi), \tilde f_i(\cdot,K,\psi)) = O_p\left(\frac{S_{K^*}\sum_{k=1}^{K^*}\delta_k^{-1}}{n^{1/2}}\right).
$$

PROOF. First, observe that $f_i(\cdot,K,\psi) = \psi^{-1}(X_{i,K})$ and $\tilde f_i(\cdot,K,\psi) = \psi^{-1}(\widetilde{X}_{i,K})$. Recall that $|\eta_{ik}| \le 2C_1|\mathcal{T}|^{1/2}$ for all i and k (see (4.13). Then, by (A1) and Corollary 1,

$$
|\eta_{ik} - \tilde\eta_{ik}| \le d_2(X_i,\nu)d_2(\rho_k,\tilde\rho_k) + d_2(\nu,\tilde\nu) = \delta_k^{-1}O_p(n^{-1/2}),
$$

where the O_p term is uniform over i and k. Next, using Lemma 3 and Corollary 1, along with the requirement that $\tau_{K^*}n^{1/2}\to\infty$, for $K \le K^*$

$$
\begin{aligned}
d_\infty(X_{i,K}, \widetilde{X}_{i,K}) &\le d_\infty(\nu,\tilde\nu) + \sum_{k=1}^{K} d_\infty(\eta_{ik}\rho_k, \tilde\eta_{ik}\tilde\rho_k)\\
&\le d_\infty(\nu,\tilde\nu) + \sum_{k=1}^{K}|\eta_{ik}|d_\infty(\rho_k,\tilde\rho_k) + \sum_{k=1}^{K}\|\rho_k\|_\infty|\eta_{ik} - \tilde\eta_{ik}|\\
&= O_p\left(\frac{\sum_{k=1}^{K}\left[(\log n)^{1/2} + \delta_k^{-1} + A_k + \tau_K\delta_k^{-1}A_k\right]}{\tau_K n^{1/2}}\right).
\end{aligned}
$$

Since the O_p term does not depend on i or K, by the first assumption in the statement of the Lemma, we have

$$\max_{1\le K\le K^*}\max_{1\le i\le n} d_\infty(X_{i,K},\widetilde{X}_{i,K}) = O_p(1).$$

For $C_{3,K,i} = C_3(d_\infty(X_{i,K},\widetilde{X}_{i,K}))$ as in (T2),

$$\max_{1\le K\le K^*}\max_{1\le i\le n} C_{3,K,i} = O_p(1),$$

whence

$$\begin{aligned} d_2(X_{i,K},\widetilde{X}_{i,K}) &\le d_2(\nu,\tilde\nu) + \sum_{k=1}^{K} d_2(\eta_{ik}\rho_k,\tilde\eta_{ik}\tilde\rho_k) \\ &\le d_2(\nu,\tilde\nu) + \sum_{k=1}^{K} |\eta_{ik}| d_2(\rho_k,\tilde\rho_k) + \sum_{k=1}^{K} |\eta_{ik} - \tilde\eta_{ik}| \\ &= O_p\left(n^{-1/2}\sum_{k=1}^{K}\delta_k^{-1}\right). \end{aligned}$$

Again, this O_p term does not depend on i or K, so

$$\max_{1\le K\le K^*}\max_{1\le i\le n} d_2(X_{i,K},\widetilde{X}_{i,K}) = O_p\left(n^{-1/2}\sum_{k=1}^{K^*}\delta_k^{-1}\right),$$

leading to

$$\begin{aligned} \max_{1\le K\le K^*}\max_{1\le i\le n} d(f_i(\cdot,K,\psi),\tilde f_i(\cdot,K,\psi)) &\le S_{K^*}\max_{1\le K\le K^*}\max_{1\le i\le n} C_{3,K,i}\, d_2(X_{i,K},\widetilde{X}_{i,K}) \\ &= O_p\left(\frac{S_{K^*}\sum_{k=1}^{K^*}\delta_k^{-1}}{n^{1/2}}\right). \end{aligned}$$

□