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FANOVA models in rectangular and circular domains

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Abstract. *FANOVA models on rectangles, circular disks and circular sectors are analyzed. Dirichlet boundary conditions are imposed to define the corresponding covariance operators of the Hilbert-valued components of the vector error term. Minimal conditions on the design matrix are imposed to derive a generalized least squares estimator of the Hilbert-valued vector of fixed effects.*

Keywords. *Generalized least-squares functional estimation; FANOVA models; Reproducing kernel Hilbert space; Hilbert-valued multivariate fixed effect model; Linear functional tests.*

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1 Introduction.

The functional analysis of variance is implemented, after suitable transformation of the functional data model, in the geometry of the Reproducing Kernel Hilbert Space (RKHS). A finite-dimensional chi-squared hypothesis testing is implemented in terms of vectorial projections for the significance analysis of the functional fixed effects. A simulation study is undertaken to illustrate the performance of the proposed methodology, and the the influence of the functional form of the fixed effect parameters, of the geometry of the domain, and of the truncation order is analyzed.

2 FANOVA on rectangular and circular domains.

2.1 The model.

In the following, H will denote a separable Hilbert space, D a Dirichlet regular bounded open domain, $-\Delta_D$ the negative Laplace operator on D, and $Y(\cdot)$ represents H^n-valued variables. In [4], the following model is introduced:

$$Y(\cdot) = [Y_1(\cdot),\dots,Y_n(\cdot)]^T = X\beta(\cdot)+\varepsilon(\cdot), \qquad E[Y]=X\beta, \qquad E[\varepsilon]=E[\varepsilon_1(\cdot),\dots,\varepsilon_n(\cdot)]^T=\overrightarrow{0}, \quad (1)$$

where $X \in \mathbb{R}^{n\times p}$ such that $X^TX = Id_p$, $\beta(\cdot)=[\beta_1(\cdot),\dots,\beta_p(\cdot)]^T \in H^p$, and $\varepsilon(\cdot)$ is a correlated H^n-valued standard Gaussian random variable, which covariance operator matrix is given by

$$\mathbb{R}_{\varepsilon\varepsilon} = \begin{pmatrix} \mathbb{R}_{\varepsilon_1\varepsilon_1} & \dots & \dots & \mathbb{R}_{\varepsilon_1\varepsilon_n} \\ \dots & \dots & \dots & \dots \\ \mathbb{R}_{\varepsilon_n\varepsilon_1} & \dots & \dots & \mathbb{R}_{\varepsilon_n\varepsilon_n} \end{pmatrix}, \text{ with } \mathbb{R}_{\varepsilon_i\varepsilon_j} = E[\varepsilon_i \otimes \varepsilon_j],\ \forall i,j=1,\dots,n,$$

under assumption that $\mathbb{R}_{\varepsilon_i\varepsilon_i} = f_i(-\Delta_D)$, $\forall i = 1,\dots,n$, is strictly positive and compact self-adjoint, in the trace class on $H = L^2_0(D)$, we have (see [1])

$$\lambda_{ki} \;=\; f_i(\lambda_k) \text{ eigenvalues of } \mathbb{R}_{\varepsilon_i\varepsilon_i}, \quad \mathbb{R}_{\varepsilon_i\varepsilon_i}\phi_k = \lambda_{ki}\phi_k,\ k\geq 1,\ i=1,\dots,n, \quad (2)$$

$$\varepsilon_i = \sum_{k=1}^{\infty} \sqrt{\lambda_{ki}}\eta_{ki}\phi_k, \quad E[\eta_{ki}\eta_{pj}] = \delta_{k,p}\left((1-\delta_{i,j})\frac{e^{-\frac{|i-j|}{\lambda_{ki}+\lambda_{pj}}}}{\sqrt{\lambda_{ki}\lambda_{pj}}} + \delta_{i,j}\sqrt{\lambda_{ki}\lambda_{pj}}\right), \tag{3}$$

$$\mathbb{R}_{\varepsilon_i\varepsilon_j} = \sum_{k=1}^{\infty}\left(\delta^*_{i,j} e^{-\frac{|i-j|}{\lambda_{ki}+\lambda_{kj}}} + \delta_{i,j}\sqrt{\lambda_{ki}\lambda_{kj}}\right)\phi_k \otimes \phi_k, \tag{4}$$

where $\delta^*_{i,j} = 1-\delta_{i,j}$, $\{\eta_{ki}\}_{k\geq 1,\ i=1,\dots,n} \sim N(0,1)$, $\{\Phi_k\}_{k\geq 1}$ and $\{\lambda_k\}_{k\geq 1}$ eigenfunctions and eigenvalues of $-\Delta_D$ respectively, and $\{f_i\}_{i=1\dots,n}$ are continuous decreasing functions. Given an orthonormal set of eigenfunctions $\{\Phi_k\}_{k\geq 1}$ of H, we denote Φ^* as $\Phi^*(f) = \{\Phi^*_k(f)\}_{k\geq 1} = \left\{(\langle f_1,\phi_k\rangle,\dots,\langle f_n,\phi_k\rangle)^T\right\}_{k\geq 1}$, that represents the projection of f on $\{\Phi_k\}_{k\geq 1}$. The inverse operator Φ is given by $\Phi\left(\{f_k^T\}_{k\geq 1}\right) = \left(\sum_{k=1}^{\infty} f_{k1}\phi_k,\dots,\sum_{k=1}^{\infty} f_{kn}\phi_k\right)^T$. Also we get $\Phi^*\mathbb{R}_{\varepsilon\varepsilon}\Phi = \{\Lambda_k\}_{k\geq 1}$ and

$$\langle f,g\rangle_{\mathbb{R}^{-1}_{\varepsilon\varepsilon}} = \mathbb{R}^{-1}_{\varepsilon\varepsilon}(f,g) = \sum_{k=1}^{\infty} f_k^T\Lambda_k^{-1}g_k,\ \forall f,\ g\in\mathbb{R}^{1/2}_{\varepsilon\varepsilon}(H^n),\ \Lambda_{kij} = e^{-\frac{|i-j|}{\lambda_{ki}+\lambda_{kj}}}\ (i\neq j),\ \Lambda_{kii} = \lambda_{ki}. \tag{5}$$

2.2 Negative Laplacian operator on Dirichlet regular bounded open domains: rectangle, disk and circular sector.

Explicit formulae of the eigenfunctions and eigenvalues of the negative Laplacian operator on rectangular and circular domains are given in [2] for different type of boundary conditions. Here, Dirichlet boundary conditions are considered. That is,

$$-\Delta_D = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}, \quad -\Delta_D\phi_k(x) = \lambda_k\phi_k(x)\ \left(x\in D\subseteq\mathbb{R}^2\right), \quad \phi_k(x) = 0\ (x\in\partial D). \tag{6}$$

According to [6], in rectangular domains $D = \prod_{i=1}^{2}[a_i,b_i]$, we get the asymptotics $\lambda_k^{-\gamma} = \mathcal{O}\left(k^{-\frac{2\gamma}{d}}\right)$, $k\to\infty$. From [2],

$$\phi_k(x) = \phi^{(1)}_{k_1}(x_1)\phi^{(2)}_{k_2}(x_2),\ \lambda_k = \lambda^{(1)}_{k_1} + \lambda^{(2)}_{k_2}, \quad \lambda^{(i)}_{k_i} = \frac{\pi^2(k_i+1)^2}{l_i^2}, \tag{7}$$

$$\phi^{(i)}_{k_i}(x_i) = \sin\left(\frac{\pi(k_i+1)(b_i-x_i)}{l_i}\right),\ \forall x_i\in[a_i,b_i],\ l_i = b_i - a_i,\ 1\leq k_i\leq k,\ \forall i = 1,2, \tag{8}$$

where $k = 1,\dots,trunc$, with $trunc$ denoting the truncation parameter, that in the case of rectangle domains is $trunc = TR\times TR$, with TR being one-dimensional truncation order at each coordinate. In the case of $D = \left\{x\in\mathbb{R}^2:\ 0<\|x\|<R\right\}$, its rotation symmetry allows us to define $-\Delta_D$ in polar coordinates as

$$-\Delta_D = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}, \quad \lambda_{kh} = \frac{\alpha^2_{kh}}{R^2}, \tag{9}$$

$$\phi_{kh}(r,\varphi) = J_k(\alpha_{kh}r/R)(cos(k\varphi)+sin(k\varphi)),\ 0<r<R,\ \varphi\in[0,2\pi], \tag{10}$$

where $k = 1,\dots,trunc$ and α_{kh} are the $trunc_k$ positive roots of $J_k(z)$, $z\in[0,R]$, with $h = 1,\dots,trunc_k$. The following asymptotic formulae hold:

$$\begin{aligned} j_{kh} &= k+\delta_h k^{1/3} + \mathcal{O}\left(k^{-1/3}\right) \\ j_{kh} &= \pi(h+k/2-1/4) + \mathcal{O}\left(k^{-1}\right) \end{aligned}$$

for the zeros of Bessel functions $J_k(z)$ of the first kind and order k on circular domains (see [3]; [5]). In particular, for the circular sector of radius R and angle $\pi\theta$, $\phi_{kh}(r,\varphi) = J_{k/\theta}(\alpha_{kh}r/R)\sin(k\varphi/\theta),\ 0<r<R,\ 0<\varphi<\pi\theta, \qquad \lambda_{kh} = \frac{\alpha^2_{kh}}{R^2}$.

3 Generalized least-squares estimator and FANOVA statistics

From [4], considering the geometry of the RKHS,

$$\|Y - X\beta\|^2_{\mathbb{R}^{-1}_{\varepsilon\varepsilon}} = \mathbb{R}^{-1}_{\varepsilon\varepsilon}(\varepsilon,\varepsilon)\,,\ \widehat{\beta} = \left(\sum_{k=1}^{\infty}\widehat{\beta_{k1}}\phi_k, \ldots, \sum_{k=1}^{\infty}\widehat{\beta_{kp}}\phi_k\right)^T,\ \varepsilon = \Phi\left(\{M_k Y_k\}_{k\geq 1}\right), \tag{11}$$

$\widehat{\beta}_k = \left(X^T\Lambda_k^{-1}X\right)^{-1}\Lambda_k^{-1}X^T Y_k$, $M_k = Id_n - X\left(X^T\Lambda_k^{-1}X\right)^{-1}X^T\Lambda_k^{-1}$ and $\sum_{k=1}^{\infty} trace\left(X^T\Lambda_k^{-1}X\right)^{-1} < \infty$. For the FANOVA analysis, we consider the transformation of our functional data model (1) by a suitable matrix operator $\mathbf{W}$ satisfying the conditions formulated in [4], in order to ensure almost surely finiteness of the functional components of variance. The residual variance, the total sum of squares and the explained functional variability are respectively given by:

$$\begin{aligned}
\widetilde{SSE} &= \sum_{k=1}^{\infty}\left(M_k W_k Y_k\right)^T \Lambda_k^{-1} M_k W_k Y_k, \quad \widetilde{SST} = \sum_{k=1}^{\infty} Y_k^T W_k^T \Lambda_k^{-1} W_k Y_k, \qquad (12)\\
\Lambda_k &= \Psi_k \Omega\left(\Lambda_k\right)\Psi_k^T,\ W_k = \Psi_k\Omega_k\left(W_k\right)\Psi_k^T,\ \Omega\left(\Lambda_k\right) = diag\left(\omega_1\left(\Lambda_k\right), \ldots, \omega_n\left(\Lambda_k\right)\right),\ \forall k \geq 1,
\end{aligned}$$

and $\widetilde{SSR} = \widetilde{SST} - \widetilde{SSE}$, where $\{\psi_{ki}\}_{k\geq 1,\ i=1,\ldots,n}$ and $\{\omega_i\left(\Lambda_k\right)\}_{k\geq 1,\ i=1,\ldots,n}$ are the eigenvectors and eigenvalues of Λ_k respectively, and $\Omega\left(W_k\right) = diag\left(w_{k11}, \ldots, w_{knn}\right)$ is given by $w_{kii} = \omega_i\left(\Lambda_k\right) + \frac{1}{a_k}$, under $\sum_{k=1}^{\infty}\frac{1}{a_k} < \infty$. We get $a_k = k^2$. Lastly, the significance of functional fixed effects is tested as follows: For for $k = 1, \ldots, trunc_k$,

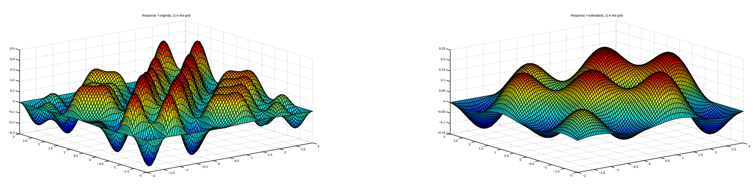
$$\begin{aligned}
H_{0k} &: \quad K_k\beta_k = C_k, \quad C_k = (0,0,\ldots,0)^T \in \mathbb{R}^{(p-1)\times 1},\ \forall k = 1, \ldots, trunc_k, \qquad (13)\\
T_k &= \left(K_k\widehat{\beta}_k - C_k\right)^T\left(K_k X_{\Lambda_k} K_k^T\right)^{-1}\left(K_k\widehat{\beta}_k - C_k\right) \sim \chi^2_{p-1}, \qquad (14)
\end{aligned}$$

$$p-value_k = 1 - P\left(\chi^2_{p-1} \leq T_k\right), \quad K_k = \Phi_k^* K \Phi_k = \begin{pmatrix} 1 & -1 & 0 & \ldots & 0\\ 1 & 0 & -1 & \ldots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & 0 & 0 & \ldots & -1 \end{pmatrix} \in \mathbb{R}^{(p-1)\times p}.$$

3.1 Results

The numerical simulations performed are shown in Figures 1 and 2. We have considered the square-integrable space, $H = L_0^2(D) = \overline{C(D)}^{L^2\left(\mathbb{R}^2\right)}$, with compact support. The following empirical least-squares errors have been computed, additionally to the F-statistics for the truncated FANOVA analysis (see Table 3), to illustrate the performance of the proposed rectangular and circular analysis of variance:

$$FMSE_{\beta_s}(\cdot) = \|\beta_s(\cdot) - \widehat{\beta}_s(\cdot)\|^2,\ \forall s = 1, \ldots, p, \quad FMSE_Y(\cdot) = \sum_{i=1}^{n}\frac{\|Y_i(\cdot) - \widehat{Y}_i(\cdot)\|^2}{n}. \tag{15}$$



(a) Simulated response with rectangle domain. (b) Estimated response with rectangle domain.

Figure 1: Responses with rectangle domain.

(a) Simulated response with disk domain. (b) Estimated response with disk domain.

Figure 2: Responses with disk domain.

n	p	TR	$a_1 = a_2$	$b_1 = b_2$	$h_x = h_y$	γ_i $\left(\lambda_{ki} = \lambda_k^{-\frac{\gamma_i}{2}}\right)$	$\beta_s(x,y),\ s = 1,\ldots,p$
200	4	4	-2	3	0.05	$1 + \frac{i}{n}$	$\beta_s(x,y) = \sin\left(\frac{\pi s x_{b_1}}{l_1}\right)\sin\left(\frac{\pi s y_{b_2}}{l_2}\right)$

Table 1: Parameters in the rectangle domain.

n	p	R	TR	h_R	h_ϕ	C	γ_i $\left(\lambda_{ki} = C\lambda_k^{-\frac{\gamma_i}{2}}\right)$	$\beta = \boldsymbol{Comb} * \Phi,\ s = 1,\ldots,p$
200	9	100	1	$\frac{R}{145}$	$\frac{2\pi}{135}$	R^2	$4 + \frac{2i}{n}$	$Comb_{sk} = \frac{1}{R}e^{\frac{s+\frac{k}{R}}{n}} + k\cos\left((-1)^k 2\pi\frac{R}{k}\right)$

Table 2: Parameters in the disk domain.

Case	$\Vert FMSE_Y\Vert_\infty$	$\max_{s=1,\ldots,p} \Vert FMSE_{\beta_s}\Vert_\infty$	F statistics
Rectangle	0.0014	0.0015	1.9263
Disk	0.0007	0.0027	$(1.4)10^7$

Table 3: Results.

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