

General tests for functional data

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- There exist several inferential methods for analyzing functional data in factorial designs.
- There is a lack of statistical tests that are valid:
 - ① in general designs,
 - ② under non-restrictive assumptions on the data generating process,
 - ③ allow for coherent post-hoc analyses.

- Let $\mathcal{L}_2(\mathcal{T})$ be the set of all squared integrable functions over closed finite interval \mathcal{T} , e.g., $\mathcal{T} = [0, 1]$.
- We consider the following FANOVA model given by $k \in \mathbb{N}$ independent groups of random processes

$$x_{i1}, \dots, x_{in_i} \sim \text{SP}(\eta_i, \gamma_i) \text{ i.i.d.} \quad \text{for each } i \in \{1, \dots, k\}, \quad (1)$$

which take values in $\mathcal{L}_2(\mathcal{T})$.

- $n = \sum_{i=1}^k n_i$ is the total sample size.
- The covariance functions of the different groups may differ from each other.
- A more general factorial structure can be incorporated easily by splitting up the indices.

- Assume that $r \in \mathbb{N}$ and $\mathbf{H} \in \mathbb{R}^{r \times k}$ is a known matrix.
- For example, \mathbf{H} can be a contrast matrix: $\mathbf{H}\mathbf{1}_k = \mathbf{0}_r$.
- Let $\boldsymbol{\eta} := (\eta_1, \dots, \eta_k)^\top$.
- We consider the following hypotheses

$$\mathcal{H}_0 : \mathbf{H}\boldsymbol{\eta}(t) = \mathbf{0}_r \text{ for all } t \in \mathcal{T} \quad \text{vs.} \quad \mathcal{H}_1 : \mathbf{H}\boldsymbol{\eta}(t) \neq \mathbf{0}_r \text{ for some } t \in \mathcal{T}. \quad (2)$$

- This general formulation contains many special cases like the one-way FANOVA problem of equal mean functions across groups: $\mathcal{H}_0 : \eta_1(t) = \dots = \eta_k(t)$ for all $t \in \mathcal{T}$ is equivalent to choosing

$$\mathbf{H} = \mathbf{P}_k := \mathbf{I}_k - \mathbf{J}_k/k.$$

Dunnett-type contrasts

$$\mathbf{H} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \\ -1 & 0 & 0 & \cdots & 1 \end{bmatrix} \in \mathbb{R}^{(k-1) \times k}$$

Tukey-type contrasts

$$\mathbf{H} = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & \cdots & \cdots & 1 \\ 0 & -1 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & -1 & 0 & 1 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \in \mathbb{R}^{k(k-1)/2 \times k}$$

- To illustrate that we can also treat higher way layouts we consider a two-way design with factors A (a levels) and B (b levels).
- We set $k := ab$ and split up the group index i in two subindices

$$(i_1, i_2) \in \{1, \dots, a\} \times \{1, \dots, b\}.$$

- We can test the following hypotheses:
 - $\mathcal{H}_0^A : \mathbf{H}_A \boldsymbol{\eta}(t) = \mathbf{0}_a$ for all $t \in \mathcal{T}$ with $\mathbf{H}_A := \mathbf{P}_a \otimes (\mathbf{1}_b^\top / b)$ (no main effect of A),
 - $\mathcal{H}_0^B : \mathbf{H}_B \boldsymbol{\eta}(t) = \mathbf{0}_b$ for all $t \in \mathcal{T}$ with $\mathbf{H}_B := (\mathbf{1}_a^\top / a) \otimes \mathbf{P}_b$ (no main effect of B),
 - $\mathcal{H}_0^{AB} : \mathbf{H}_{AB} \boldsymbol{\eta}(t) = \mathbf{0}_{ab}$ for all $t \in \mathcal{T}$ with $\mathbf{H}_{AB} := \mathbf{P}_a \otimes \mathbf{P}_b$ (no interaction effect).
- Here, \otimes denotes the Kronecker product.

- An unbiased estimator for the mean function is given by

$$\hat{\eta}_i(t) := \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij}(t)$$

and for the covariance function by

$$\hat{\gamma}_i(t, s) := \frac{1}{n_i - 1} \sum_{j=1}^{n_i} (x_{ij}(t) - \hat{\eta}_i(t)) (x_{ij}(s) - \hat{\eta}_i(s)) \quad (3)$$

for all $t, s \in \mathcal{T}, i \in \{1, \dots, k\}$.

- Let $\hat{\boldsymbol{\eta}} := (\hat{\eta}_1, \dots, \hat{\eta}_k)^\top$.
- For $t, s \in \mathcal{T}$, let

$$\hat{\boldsymbol{\Sigma}}(t, s) := \text{diag} \left(\frac{n}{n_1} \hat{\gamma}_1(t, s), \dots, \frac{n}{n_k} \hat{\gamma}_k(t, s) \right)$$

be an estimator for

$$\boldsymbol{\Sigma}(t, s) := \text{diag} \left(\frac{1}{\tau_1} \gamma_1(t, s), \dots, \frac{1}{\tau_k} \gamma_k(t, s) \right) \in \mathbb{R}^{k \times k}.$$

- The point-wise Hotelling's T^2 -test statistic:

$$\text{TF}_{n,\mathbf{H}}(t) := n(\mathbf{H}\hat{\boldsymbol{\eta}}(t))^\top (\mathbf{H}\hat{\boldsymbol{\Sigma}}(t,t)\mathbf{H}^\top)^+(\mathbf{H}\hat{\boldsymbol{\eta}}(t)) \quad (4)$$

for all $t \in \mathcal{T}$, where \mathbf{A}^+ denotes the Moore-Penrose inverse of the matrix \mathbf{A} .

- Under the null hypothesis, we expect that the point-wise Hotelling's T^2 -test statistic is small since $\mathbf{H}\hat{\boldsymbol{\eta}}(t)$ is an estimator for $\mathbf{H}\boldsymbol{\eta}(t)$.
- The term $\mathbf{H}\hat{\boldsymbol{\Sigma}}(t,t)\mathbf{H}^\top$ approximates the covariance matrix of $\sqrt{n}\mathbf{H}\hat{\boldsymbol{\eta}}(t)$.
- The globalizing point-wise Hotelling's T^2 -test (GPH) statistic:

$$T_n(\mathbf{H}) := \int_{\mathcal{T}} \text{TF}_{n,\mathbf{H}}(t) dt.$$

- We reject the null hypothesis for large values of $T_n(\mathbf{H})$.

- Invariance under Orthogonal Transformations: Multiplying the left and right side of the null hypothesis in (2) with an orthogonal matrix $\mathbf{P} \in \mathbb{R}^{r \times r}$ leads to the same testing problem. The point-wise test statistic is invariant under orthogonal transformations, i.e., $\text{TF}_{n, \mathbf{P}\mathbf{H}}(t) = \text{TF}_{n, \mathbf{H}}(t)$.
- Scale-invariance: We have the scaled functional data $x_{ij}^h(t) := h(t)x_{ij}(t)$. Then, $\mathcal{H}_0 : \mathbf{H}\boldsymbol{\eta}^h(t) = \mathbf{0}_r$, where $\boldsymbol{\eta}^h(t) := h(t)\boldsymbol{\eta}(t)$. We have the scale-invariance of the point-wise Hotelling's T^2 -test statistic $\text{TF}_{n, \mathbf{H}}^h(t) = \text{TF}_{n, \mathbf{H}}(t)$.

Theorem 1

Let $\mathbf{z} \sim GP_r(\mathbf{0}_r, \mathbf{H}\boldsymbol{\Sigma}\mathbf{H}^\top)$. Under appropriate assumptions and the null hypothesis in (2), we have

$$T_n(\mathbf{H}) \xrightarrow{d} \int_{\mathcal{T}} \mathbf{z}^\top(t) (\mathbf{H}\boldsymbol{\Sigma}(t, t)\mathbf{H}^\top)^+ \mathbf{z}(t) dt \text{ as } n \rightarrow \infty, \quad (5)$$

where \xrightarrow{d} denotes convergence in distribution in the sense of van der Vaart and Wellner (1996).

- First, we estimate $\gamma_1, \dots, \gamma_k$ by $\hat{\gamma}_1, \dots, \hat{\gamma}_k$.
- Second, we generate parametric bootstrap samples via

$$x_{i1}^{\mathcal{P}}, \dots, x_{in_i}^{\mathcal{P}} \sim GP(0, \hat{\gamma}_i), \quad \text{for each } i \in \{1, \dots, k\}.$$

- Using a Gaussian process for generating the parametric bootstrap sample seems natural regarding the limiting distribution in Theorem 1 since the mean function estimators are asymptotically Gaussian anyway.
- Moreover, using the estimators of sample covariance functions, we mimic the covariance structure of the given functional data.

- The parametric bootstrap point-wise Hotelling's T^2 -test statistic at t is defined by

$$\text{TF}_{n,\mathbf{H}}^{\mathcal{P}}(t) := n \left(\mathbf{H} \hat{\boldsymbol{\eta}}^{\mathcal{P}}(t) \right)^{\top} \left(\mathbf{H} \hat{\boldsymbol{\Sigma}}^{\mathcal{P}}(t, t) \mathbf{H}^{\top} \right)^+ \mathbf{H} \hat{\boldsymbol{\eta}}^{\mathcal{P}}(t).$$

- The parametric bootstrap globalizing point-wise Hotelling's T^2 -test statistic:

$$T_n^{\mathcal{P}}(\mathbf{H}) := \int_{\mathcal{T}} \text{TF}_{n,\mathbf{H}}^{\mathcal{P}}(t) dt. \quad (6)$$

Theorem 2

Let $\mathbf{z} \sim GP_r(\mathbf{0}_r, \mathbf{H}\boldsymbol{\Sigma}\mathbf{H}^{\top})$. Under appropriate assumptions, it holds that

$$T_n^{\mathcal{P}}(\mathbf{H}) \xrightarrow{d^*} \int_{\mathcal{T}} \mathbf{z}^{\top}(t) (\mathbf{H}\boldsymbol{\Sigma}(t, t)\mathbf{H}^{\top})^+ \mathbf{z}(t) dt \text{ as } n \rightarrow \infty, \quad (7)$$

where here and throughout $\xrightarrow{d^*}$ denotes conditional convergence in distribution given the data $(x_{i1}, x_{i2}, \dots)_{i \in \{1, \dots, k\}}$.

- Let $\alpha \in (0, 1)$ be the significance level and $B \in \mathbb{N}$ sufficiently large.
 - ① Calculate $\hat{\gamma}_1, \dots, \hat{\gamma}_k$ in (3).
 - ② Simulate B times n independent Gaussian processes $x_{i1;b}^{\mathcal{P}}, \dots, x_{ini;b}^{\mathcal{P}} \sim GP(0, \hat{\gamma}_i)$, $i \in \{1, \dots, k\}$, $b \in \{1, \dots, B\}$.
 - ③ Compute the parametric bootstrap GPH statistic $T_{n;b}^{\mathcal{P}}(\mathbf{H})$ as in (6) for all $b \in \{1, \dots, B\}$.
 - ④ Determine the empirical $(1 - \alpha)$ -quantile $Q_{n,1-\alpha}^{\mathcal{P}}$ of the computed values.
 - ⑤ Reject the null hypothesis in (2) if and only if $T_n(\mathbf{H}) > Q_{n,1-\alpha}^{\mathcal{P}}$.

- We interpret \mathbf{H} as follows:

$$\mathbf{H} = [\mathbf{h}_1^\top, \dots, \mathbf{h}_r^\top]^\top$$

for matrices $\mathbf{h}_\ell \in \mathbb{R}^{1 \times k}$, where $\ell \in \{1, \dots, r\}$.

- The main idea of multiple tests is to split up the global null hypothesis in (2) with $\mathbf{H} = [\mathbf{h}_1^\top, \dots, \mathbf{h}_r^\top]^\top$ into r single tests with hypothesis matrices $\mathbf{h}_1, \dots, \mathbf{h}_r$.
- This leads to the multiple testing problem

$$\mathcal{H}_{0,\ell} : \mathbf{h}_\ell \boldsymbol{\eta}(t) = 0 \text{ for all } t \in \mathcal{T}, \quad \text{for } \ell \in \{1, \dots, r\}. \quad (8)$$

- This general formulation of the multiple testing problem covers the post-hoc testing problem.

- We adopt the idea for the construction of simultaneous confidence bands proposed by Bühlmann (1998) *Sieve bootstrap for smoothing in nonstationary time series*, Annals of Statistics.
- Let $T_n^{1,\mathcal{P}}(\mathbf{h}_\ell), \dots, T_n^{B,\mathcal{P}}(\mathbf{h}_\ell)$ denote B parametric bootstrap counterparts of the GPH statistic based on \mathbf{h}_ℓ , $\ell \in \{1, \dots, r\}$.
- For each $b \in \{1, \dots, B\}$, the same bootstrap sample is used for $T_n^{b,\mathcal{P}}(\mathbf{h}_1), \dots, T_n^{b,\mathcal{P}}(\mathbf{h}_r)$.
- Let $q_{\ell,\beta}^{\mathcal{P}}$ denote the empirical $(1 - \beta)$ -quantile of $T_n^{1,\mathcal{P}}(\mathbf{h}_\ell), \dots, T_n^{B,\mathcal{P}}(\mathbf{h}_\ell)$.
- Let

$$\tilde{\beta} := \max \left\{ \beta \in \left\{ 0, \frac{1}{B}, \dots, \frac{B-1}{B} \right\} \mid \frac{1}{B} \sum_{b=1}^B \mathbf{1} \left\{ \exists \ell \in \{1, \dots, r\} : T_n^{b,\mathcal{P}}(\mathbf{h}_\ell) > q_{\ell,\beta}^{\mathcal{P}} \right\} \leq \alpha \right\}$$

be the largest $\beta \in \{0, 1/B, \dots, (B-1)/B\}$ such that the approximated family-wise type I error rate (FWER) is bounded by the significance level α .

- For each $\ell \in \{1, \dots, r\}$, we reject $\mathcal{H}_{0,\ell}$ if and only if $T_n(\mathbf{h}_\ell) > q_{\ell, \tilde{\beta}}^{\mathcal{P}}$ ($0/0 := 1$).
- We reject the global null hypothesis \mathcal{H}_0 whenever at least one of $\mathcal{H}_{0,1}, \dots, \mathcal{H}_{0,r}$ is rejected, i.e.,

$$\max_{\ell \in \{1, \dots, r\}} \frac{T_n(\mathbf{h}_\ell)}{q_{\ell, \tilde{\beta}}^{\mathcal{P}}} > 1.$$

- Each test statistic $T_n(\mathbf{h}_\ell), \ell \in \{1, \dots, r\}$, is treated in the same way and has the same impact since we use the same $\tilde{\beta}$ for each linear combination.
- The definition of $\tilde{\beta}$ ensures that the level of significance for the global test and the FWER for the multiple testing problem is controlled asymptotically.
- Simultaneous asymptotic confidence regions for the linear combinations $\mathbf{h}_1\boldsymbol{\eta}, \dots, \mathbf{h}_r\boldsymbol{\eta}$ are $CR_\ell := \left\{ \boldsymbol{\xi} \in \mathcal{L}_2(\mathcal{T}) \mid n(\mathbf{H}\hat{\boldsymbol{\eta}}(t) - \boldsymbol{\xi}(t))^\top (\mathbf{H}\hat{\boldsymbol{\Sigma}}(t, t)\mathbf{H}^\top)^+ (\mathbf{H}\hat{\boldsymbol{\eta}}(t) - \boldsymbol{\xi}(t)) \leq q_{\ell, \tilde{\beta}}^{\mathcal{P}} \right\}, \ell \in \{1, \dots, r\}$.

- We take into account the type I error control and power of the new and competing statistical tests.
- Since multiple tests for functional data are not tackled in the literature up until now, we compared our multiple test (mGPH) with the following global tests by using the Bonferroni correction:
 - the Fmax- and GPF-test by Smaga and Zhang (2019, Technometrics) with nonparametric bootstrap approach,
 - the bootstrap L^2 -norm-based (L2b) and F-type (Fb) test by Zhang (2013),
 - the projection test (CAFB) by Cuesta-Albertos and Febrero-Bande (2010, Test),
 - the parametric bootstrap globalizing point-wise Hotelling's T^2 -test (GPH) for the global testing problem.
- The Bonferroni correction is used since it is directly related to the construction of confidence regions in contrast to a stepwise procedure as, e.g., the Holm correction.

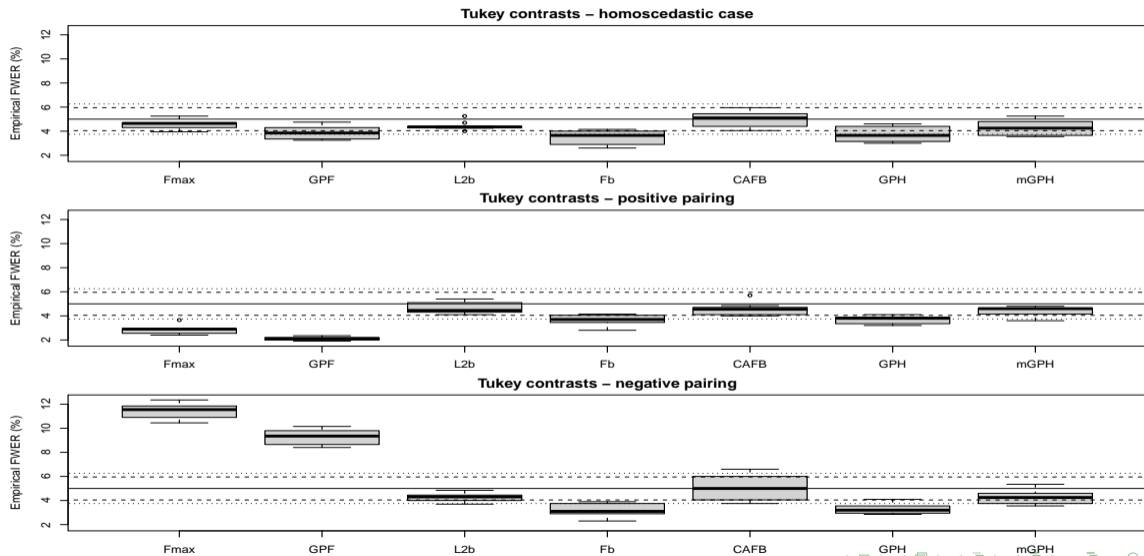
- The simulation setup is based on the simulations in Paparoditis and Sapatinas (2016) *Bootstrap-based testing of equality of mean functions or equality of covariance operators for functional data*, Biometrika.
- We simulated $k = 4$ samples with sample sizes $(n_1, n_2, n_3, n_4) = K \cdot (15, 20, 25, 30)$, where $K \in \{1, 2, 4\}$, by

$$v_{ij}(t) = h(t)\lambda_i \sum_{q=1}^{10} \left(\sqrt{\frac{2}{q}} \sin(\pi qt) Y_{ijq} + \sqrt{\frac{1}{q}} \cos(\pi qt) Z_{ijq} \right), \quad t \in \mathcal{T} = [0, 1].$$

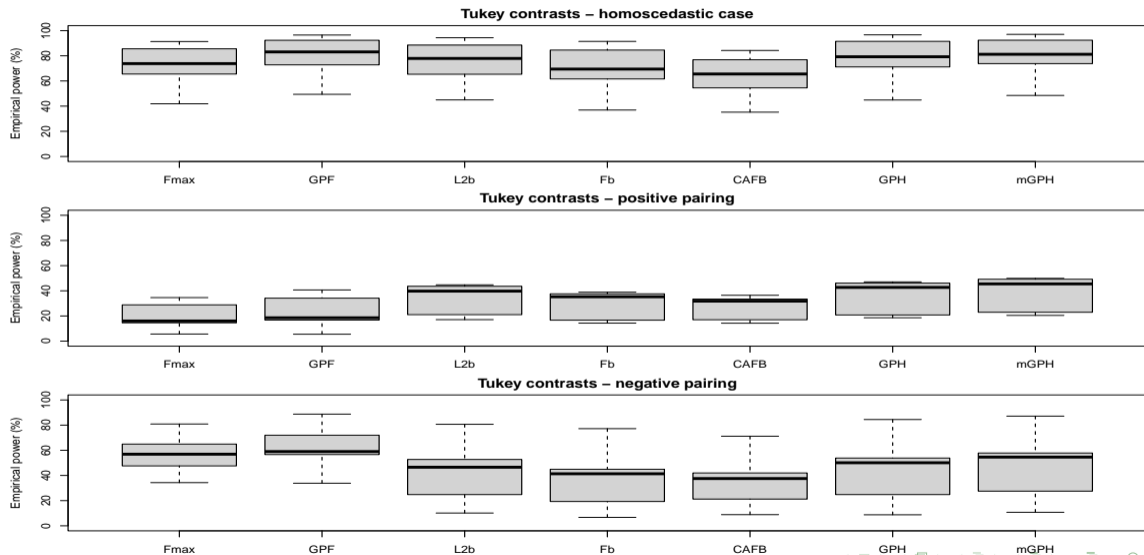
- $Y_{ijq}, Z_{ijq}, j \in \{1, \dots, n_i\}, i \in \{1, 2, 3, 4\}, q \in \{1, \dots, 10\}$ are generated independently using standardized normal, t_5 - and χ_5^2 -distributed random variables.

- The factors λ_i are determined by:
 - ① 1 for the homoscedastic case,
 - ② $\lambda_i = 0.75 + 0.25i$ for a positive pairing (i.e., the variability increases with sample size),
 - ③ $\lambda_i = 2 - 0.25i$ for a negative pairing (i.s., the variability decreases with sample size)for all $i \in \{1, 2, 3, 4\}$.
- A scaling function h is multiplied, where
 - ① $h(t) = 1$ for all $t \in [0, 1]$ for a scenario without scaling function,
 - ② $h(t) = 1/(t + 1/J)$ for all $t \in [0, 1]$ for a scenario with scaling function.

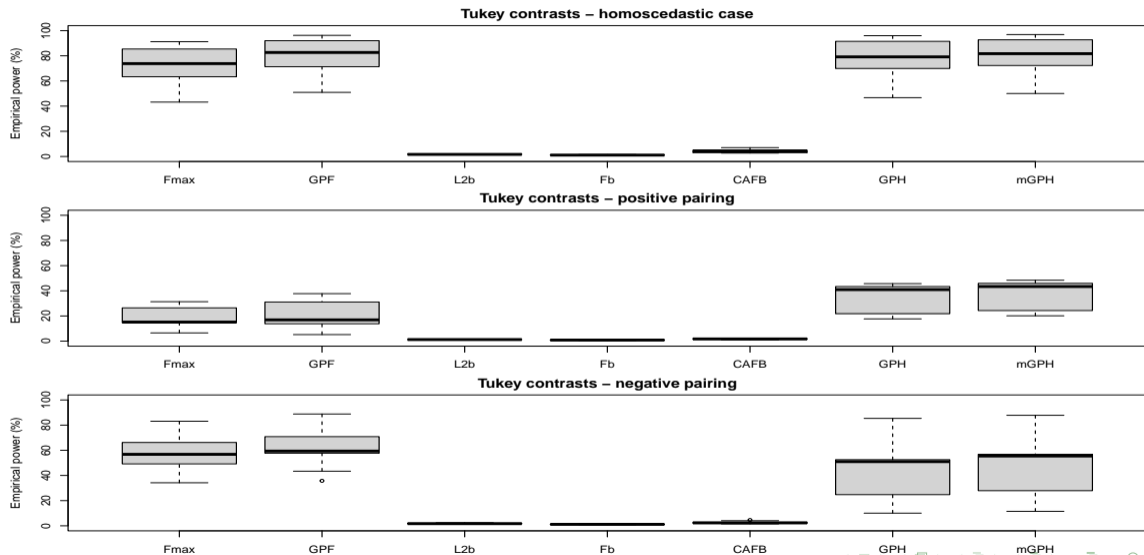
Simulation studies - empirical FWER



Simulation studies - empirical power

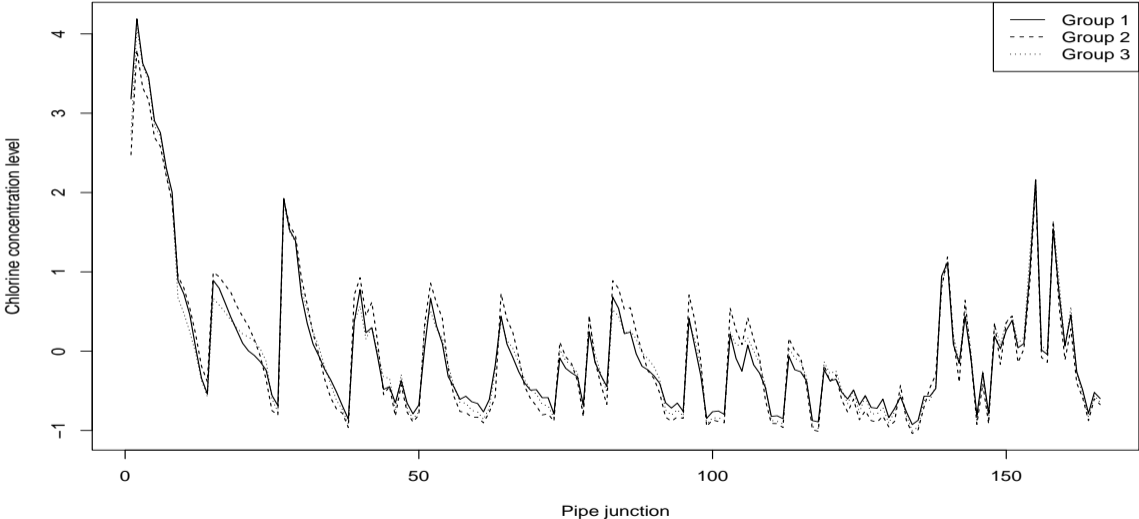


Simulation studies - empirical power



- Chen, Keogh, Hu, Begum, Bagnall, Mueen, Batista, The UCR time series classification archive, 2015 www.cs.ucr.edu/~eamonn/time_series_data/.
- The data set was produced by the simulation tool EPANET, which models the hydraulic and water quality behavior of water distribution piping systems, allowing for the tracking of water levels and pressures in tanks, water flow in pipes, and the concentration of chemical species throughout a given network over a simulated period of time. Here, simulated Chlorine concentration levels were measured at 166 pipe junctions over a period of 15 days.
- The final data set contains functional observations measured in 166 design time points (pipe junctions).
- It is divided into three classes (groups). We consider three samples of 25 functional observations each taken from the groups in the training data set.

Data example - Chlorine Concentration

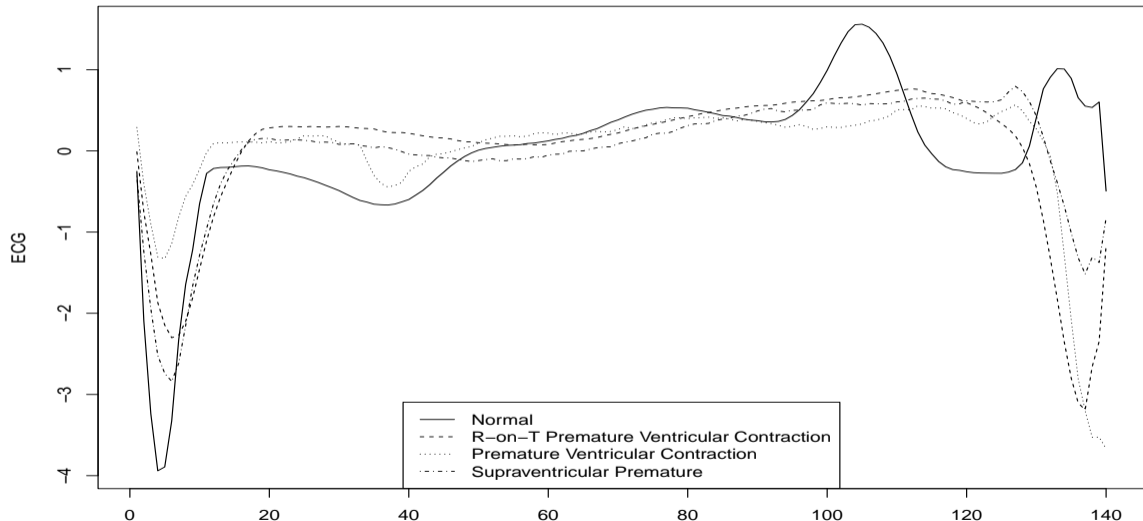


- Homoscedastic case

	Hypothesis	Fmax	GPF	L2b	Fb	CAFB	GPH	mGPH
	$\mathcal{H}_{0,1} : \eta_1 \equiv \eta_2$	12.9	4.8	13.5	16.2	7.8	1.5	1.7
	$\mathcal{H}_{0,2} : \eta_1 \equiv \eta_3$	100.0	90.0	100.0	100.0	100.0	83.1	53.4
	$\mathcal{H}_{0,3} : \eta_2 \equiv \eta_3$	90.6	37.2	31.2	35.1	73.6	38.1	28.7
FWER		4.95	4.95	6.35	5.15	4.20	4.80	5.35
Empirical powers	$\mathcal{H}_{0,1}$	70.20	66.10	40.70	35.00	54.30	65.95	67.10
	$\mathcal{H}_{0,2}$	26.90	16.65	10.25	7.60	17.50	15.90	17.35
	$\mathcal{H}_{0,3}$	30.10	26.95	28.55	25.10	21.00	27.65	28.75

- Goldberger, Amaral, Glass, Hausdorff, Ivanov, Mark, Mietus, Moody, Peng, Stanley (2000) *PhysioBank, PhysioToolkit, and PhysioNet*, Circulation.
- It is a 20-hour long electrocardiogram (ECG) obtained from Physionet.
- The data set underwent pre-processing consisting of two steps. Firstly, each heartbeat was extracted from the ECG and, secondly, the heartbeat lengths were adjusted using interpolation.
- The patient has severe congestive heart failure (pol. *ciężką zastoinową niewydolność serca*) and annotation was used to obtain class values.
- Groups: (1) Normal, (2) R-on-T Premature Ventricular Contraction, (3) Premature Ventricular Contraction, (4) Supraventricular premature or ectopic beat
- There are four samples of functional data measured in 141 design time points.
- The sample sizes are equal to 292, 177, 10, and 19 respectively.

Data example - Electrocardiogram



- Heteroscedastic case

Hypothesis		Fmax	GPF	L2b	Fb	CAFB	GPH	mGPH
	$\mathcal{H}_{0,1} : \eta_1 \equiv \eta_2$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	$\mathcal{H}_{0,2} : \eta_1 \equiv \eta_3$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	$\mathcal{H}_{0,3} : \eta_1 \equiv \eta_4$	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	$\mathcal{H}_{0,4} : \eta_2 \equiv \eta_3$	0.0	0.0	1.8	39.0	0.0	5.4	3.8
	$\mathcal{H}_{0,5} : \eta_2 \equiv \eta_4$	0.0	0.0	1.2	3.0	4.9	7.2	4.9
	$\mathcal{H}_{0,6} : \eta_3 \equiv \eta_4$	0.0	7.8	3.0	4.8	0.0	15.0	9.6
FWER		57.50	35.80	6.90	3.40	5.20	3.75	5.45
Empirical powers	$\mathcal{H}_{0,1}$	100.00	100.00	100.00	100.00	100.00	100.00	100.00
	$\mathcal{H}_{0,2}$	100.00	100.00	100.00	99.65	100.00	99.30	99.90
	$\mathcal{H}_{0,3}$	100.00	100.00	100.00	99.60	100.00	100.00	100.00
	$\mathcal{H}_{0,4}$	100.00	100.00	85.00	45.05	97.25	55.30	65.75
	$\mathcal{H}_{0,5}$	93.90	89.60	71.15	60.00	69.20	55.60	62.15
	$\mathcal{H}_{0,6}$	99.85	57.50	76.25	53.55	96.50	40.85	49.45

- Ditzhaus M., Munko M., Pauly M., Smaga Ł., Zhang J.-T. (2023). multiFANOVA: Multiple Contrast Tests for Functional Data. R package version 0.1.0, <https://CRAN.R-project.org/package=multiFANOVA>.
- `multiFANOVA(`
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 `h,`
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Thank you for your attention!