AN AUTOMATIC PROCEDURE TO DETERMINE GROUPS OF NONPARAMETRIC REGRESSION CURVES

A PREPRINT

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January 1, 2021

ABSTRACT

In many situations it could be interesting to ascertain whether nonparametric regression curves can be grouped, especially when confronted with a considerable number of curves. The proposed testing procedure allows to determine groups with an automatic selection of their number. A simulation study is presented in order to investigate the finite sample properties of the proposed methods when compared to existing alternative procedures. Finally, the applicability of the procedure to study the geometry of a tunnel by analysing a set of cross-sections is demonstrated. The results obtained show the existence of some heterogeneity in the tunnel geometry.

Keywords multiple regression curves · nonparametric regression · testing equality · number of groups · clustering · tunnel profile

1 Introduction

One of the main goals of statistical modelling is to understand the dependence of a response variable, \(Y\), with respect to another explanatory variable, \(X\). This type of dependence can be studied through nonparametric regression models, where the relationship between \(Y\) and \(X\) is modelled without specifying in advance the function that links them. Within this framework, the study of the regression curves can be useful in the comparison of two or more groups, which is an important problem associated with statistical inference. In particular, the topic of hypothesis testing the equality of mean functions has been widely investigated in the literature, see, for instance, the review that González-Manteiga and Crujeiras (2013) offers about this topic. Relevant papers on this topic are Hall and Hart (1990), King et al. (1991), Delgado (1993), Kulasekera (1995), Young and Bowman (1995), Dette and Neumeyer (2001), Pardo-Fernández et al. (2007), Srihera and Stute (2010), among others. Furthermore, in order to compare the values of a response variable across several groups in the presence of a covariate effect, nonparametric analysis of covariance or factor-by-curve interaction test can be used. Young and Bowman (1995) generalized the one-way analysis of variance test to the nonparametric regression setting, and Dette and Neumeyer (2001) proposed to use Young and Bowman’s test also in the situation of a heteroscedastic error. In addition, Park and Kang (2008) developed a SiZer tool based on an analysis of variance type test statistic that is capable of comparing multiple curves based on the residuals. The evolution of this procedure is based on the comparison using the original regression curves Park et al. (2014). More recently, the
possibility of comparing curves as well as their derivatives has been proposed by Sestelo and Roca-Pardiñas [2019] using factor-by-curve interactions in a nonparametric framework.

When the null hypothesis of equality of curves is rejected, leading to the clear conclusion that at least one curve is different, it can be interesting to ascertain whether groups of curves can exist or, by contrast, that all these curves are different from each other. In this setting, one naïve approach would be to perform pairwise comparisons. Following the ideas of Rosenblatt [1975], González-Manteiga and Cao [1993], Härdle and Mammen [1993a], an alternative test based on the estimators of the regression functions was proposed by Dette and Neumeyer [2001], to check the null hypothesis of equality of curves. A similar statistic was considered by King et al. [1991]. However, such approaches lead to difficult interpretation of results because as the number of curves increases so does the number of comparisons. For example, considering 50 curves, the number of all pairwise comparisons that need to be conducted is 1225. One could make it but without the possibility of determining groups with similar regression curves.

With this focus but in time-to-event framework, Villanueva et al. [2019] have described a new procedure to determine groups of nonparametric regression curves in multiple survival curves. Some approaches have been developed also in functional data context Abraham et al. [2003], García-escudero and Gordaliza [2005], Tarpey [2007] and in longitudinal one Vogt and Linton [2017, 2020]. However, to the best of our knowledge the problem of determining groups of regression functions in a standard nonparametric framework (cross-sectional data) has not been considered explicitly in the literature.

Based on the above, and taking into account situations with a considerable number of curves, we introduce an approach that allows us to group multiple regression curves. Briefly, our procedure is described as follows. Firstly, the regression curves are estimated by kernel smoothers. Secondly, given a number of $K$ groups, the optimal possible assignment of $J$ curves into $K$ groups is chosen by means of a heuristic algorithm. Finally, the optimal number of groups is determined using an automatic bootstrap-based testing procedure.

The proposed methodology is used to study the geometry of a tunnel by analysing a set of cross-sections along it. These sections were obtained by adjusting a surface to a point cloud measured with a terrestrial laser scanning. The existence of different groups of cross-sections indicates that the tunnel has a heterogeneous geometry. This heterogeneity could be due to bad construction or to deformations in the tunnel.

The remainder of this paper is organized as follows. In Section 2.1 the notation and the methodological background are explained. In Section 3 the performance of our and existing procedures is shown through simulation studies. The results of the analysis of a real dataset are provided in Section 4. Finally, the main conclusions of this work are exposed in Section 5.

2 Methodology

2.1 Notation and technical details

Let $(X_j, Y_j)$ be $J$ independent random vectors, and assume that they satisfy the following nonparametric regression models, for $j = 1, \ldots, J$,

$$Y_j = m_j(X_j) + \varepsilon_j$$

(1)

where $m_j$ is a nonparametric smooth function and $\varepsilon_j$ is the regression error, which is assumed independent of the covariate $X_j$. Note that, by construction, $E(\varepsilon_j) = 0$ and $\text{Var}(\varepsilon_j) = \sigma_j^2$, which means that $m_j(X_j)$ represents the conditional mean, while $\sigma_j^2$ equals the residuals variance, i.e., $\sigma_j^2 = \text{Var}(Y_j - m_j(X_j))$. Throughout this paper, we will not require any assumptions on the error distributions.

Several approaches can be used to estimated the regression models in (1), such as, methods based on regression splines de Boor [2001], Bayesian approaches Lang and Brezger [2004] or local polynomial kernel smoothers Wand and Jones [1995], Fan and Gijbels [1996]. In this work, local linear kernel smoothers, as implemented in the npregfast R package Sestelo et al. [2016, 2017], are used. Explicitly, given $J$ independent random samples, say

$$\{S_1 = \{(X_{i1}, Y_{i1})\}_{i=1}^{n_1}, \ldots, S_J = \{(X_{iJ}, Y_{iJ})\}_{i=1}^{n_J}\}$$

where the random variables $(X_{ij}, Y_{ij}), \ldots, (X_{nj}, Y_{nj})$ are i.i.d. for each $j = 1, \ldots, J$ and with a total sample size $n = \sum_{j=1}^{J} n_j$, the local linear kernel estimator

$$\hat{m}_j(x) = \Psi(x, S_j, h_j)$$

(2)
at a location \( x \) is given by \( \hat{m}_j(x) = \hat{\alpha}_{0j}(x) \), where \( \hat{\alpha}_{0j}(x) \) is the first element of the vector \( (\hat{\alpha}_{0j}(x), \hat{\alpha}_{1j}(x)) \) which is the minimiser of

\[
\sum_{i=1}^{n_j} \left( Y_{ij} - \alpha_{0j}(x) - \alpha_{1j}(x)(X_{ij} - x) \right)^2 \cdot \kappa \left( \frac{X_{ij} - x}{h_j} \right),
\]

(3)

where \( \kappa \) denotes a kernel function (normally, a symmetric density), and \( h_j > 0 \) is the smoothing parameter or bandwidth. Taking into account that nonparametric estimates depend heavily on the bandwidth \( h_j \), various methods for an optimal selection have been suggested, such as Generalised Cross-Validation [Golub et al., 1979] or plug-in methods, see e.g., [Ruppert et al., 1995]. See [Wand and Jones, 1995] for a good overview of this topic. However, optimal bandwidth selection is still a challenging problem. As a practical solution, and based on the simulation results, the bandwidths \( h_j \) can be selected automatically by minimising the following cross-validation criterion

\[
CV(h_j) = \sum_{i=1}^{n_j} \left( Y_{ij} - \hat{m}_j^{-i}(X_{ij}) \right)^2,
\]

(4)

where \( \hat{m}_j^{-i}(X_{ij}) \) indicates the fit at \( X_{ij} \) leaving out the \( i \)-th data point based on the smoothing parameter \( h_j \).

Additionally, it is well-known that bootstrap resampling techniques are time-consuming processes because the estimation of the model is carried out many times. Moreover, the use of cross-validation for selecting the bandwidth implies a high computational cost because it is necessary to repeat the estimation procedure several times to select the optimal estimate. Accordingly, to apply some computational acceleration technique is fundamental to ensure that the problem can be addressed adequately in practical situations. Thus, in this paper we use binning techniques to speed up the process. A detailed explanation of this technique can be found in [Fan and Marron, 1994].

### 2.2 The algorithm for determining groups

As pointed out in the Introduction, several nonparametric methods have been proposed in the literature in order to test the equality of regression curves, i.e., to test the null hypothesis \( H_0 : m_1 = \ldots = m_J \). If the test is statistical significant and this hypothesis is thus rejected, then determining groups of regression curves becomes of interest, that is, assessing if the levels \( \{1, \ldots, J\} \) can be grouped in \( K \) groups \( G_1, \ldots, G_K \) with \( K < J \) such that for each \( k = 1, \ldots, K \), \( m_i = m_j \) for all \( i, j \in G_k \). Note that \( (G_1, \ldots, G_K) \) must be a partition of \( \{1, \ldots, J\} \), and therefore must satisfy \( G_1 \cup \ldots \cup G_K = \{1, \ldots, J\} \) and \( C_i \cap G_j = \emptyset \), for all \( i \neq j \in \{1, \ldots, K\} \).

Let \( (X_{ij}, Y_{ij}), i = 1, \ldots, n_j \), be an i.i.d. sample from the distribution of \( (X_j, Y_j) \), for each \( j = 1, \ldots, J \), and with the total sample size \( n = \sum_{j=1}^J n_j \), we propose a procedure to test, for a given a number \( K \), the null hypothesis \( H_0(K) \) that at least one partition exists \( (G_1, \ldots, G_K) \) so that all the conditions above are satisfied. The alternative hypothesis \( H_1(K) \) is that for any \( (G_1, \ldots, G_K) \), exists at least a group \( G_k \) in which \( m_i \neq m_j \) for some \( i, j \in G_k \).

The testing procedure is based on the \( J \)-dimensional process

\[
\hat{V}(z) = (\hat{V}_1(z), \hat{V}_2(z), \ldots, \hat{V}_J(z))^t,
\]

where, for \( j = 1, \ldots, J \),

\[
\hat{V}_j(z) = \sum_{k=1}^K [\hat{m}_j(z) - \hat{f}_k(z)] \text{I}_{\{j \in G_k\}}
\]

and \( \hat{f}_k \) is the pooled local linear kernel estimate based on the combined \( G_k \)-partition sample, i.e.,

\[
\hat{f}_k(z) = \Psi(z, S_k, h_k)
\]

where

\[
S_k = \sum_{j \in G_k} S_j.
\]

The following test statistics were considered in order to test \( H_0(K) \): a Cramer-von Mises type test statistic

\[
D_{CM} = \min_{G_1, \ldots, G_K} \sum_{j=1}^J \int_{R_X} \hat{V}_j^2(z) \text{I}_{\{j \in G_k\}} dz
\]
and a modification of it based on the \(L_1\) norm proposed in the Kolmogorov-Smirnov test statistic

\[
D_{KS} = \min_{g_1, \ldots, g_K} \sum_{j=1}^{J} \int_{R_X} |\hat{V}_j(z)|dz I_{\{j \in G_k\}}.
\]

In order to solve the minimisation problem in each test statistic, all the different assignments of the \(J\) curves into \(K\) groups have to be evaluated. Because of the large number of calculations, this method is feasible only for small numbers of \(J\) and \(K\). Obviously, when confronted with a large number of \(J\) curves, the procedure requires an excessively high computational cost. To be more specific, we deal in our study of tunnel cross-sections with \(J = 66\) curves and \(K = 5\) groups and, taking into account the formula of Jain and Dubes [1988], the total number of different assignments is \(1e44\). This combinatorial explosion implies that the problem becomes intractable. Therefore, heuristic algorithms would be really appropriate to tackle much bigger problems. One the one hand, in the case of \(D_{C,M}\) test statistic which is defined in terms of the \(L_2\)-distance, we propose the use of the \(K\)-means [Macqueen 1967]. On the other hand, for the \(D_{KS}\) test statistic defined in terms of the \(L_1\)-norm, the \(K\)-medians [Macqueen 1967], Kaufman and Rousseeuw [1990] would be more suitable. In both cases, the carried out procedure is equivalent: the regression functions \(m_j\) and \(K\)-medians, and from these the “best” partition \((G_1, \ldots, G_K)\) is obtained.

Finally, the decision rule based on \(D\) consists of rejecting the null hypothesis if \(D\) is larger than \((1 - \alpha)\)-percentile obtained under the null hypothesis. To approximate the distributions of the test statistics, resampling methods such as the bootstrap introduced by Efron [1979] (see also Efron and Tibshirani [1993], Härdle and Mammen [1993b], Kauermann and Opsomer [2003]) can be applied instead. Here we use the wild bootstrap Wu [1986], Liu [1988], Mammen [1993] because this method is valid both for homoscedastic and for heteroscedastic models where the variance of the error is a function of the covariate.

The testing procedure used requires the following steps:

**Step 1.** Using the original sample, for \(j = 1, \ldots, J\) and \(i = 1, \ldots, n_j\), estimate in a common grid the regression functions \(m_j\) using each sample separately. Then, applying the proposed algorithms, obtain the “best” partition \((G_1, \ldots, G_K)\) and with it, obtain the estimated curves \(\hat{f}_k\) using a pooled local linear kernel estimator based on the combined partition samples.

**Step 2.** Obtain the \(D\) value as explained before, and the null errors under the \(H_0(k)\) as

\[
\hat{\varepsilon}_{ij} = \sum_{k=1}^{K} (Y_{ij} - \hat{f}_k(X_{ij})) I_{\{j \in G_k\}}.
\]

**Step 3.** Draw bootstrap samples as follows, for \(b = 1, \ldots, B\), and for each \(j \in G_k\), draw \(\{(X_{i1}, Y_{i1})\}_{i=1}^{n_j}, \ldots, \{(X_{iJ}, Y_{iJ})\}_{i=1}^{n_j}\) where

\[
Y_{ij}^{*b} = \sum_{k=1}^{K} \hat{f}_k(X_{ij}) I_{\{j \in G_k\}} + \varepsilon_{ij}^{*b}
\]

and

\[
\varepsilon_{ij}^{*b} = \hat{\varepsilon}_{ij} W_i
\]

being \(W_1, \ldots, W_n\) an i.i.d. random variables with mass \((5 + \sqrt{5})/10\) and \((5 - \sqrt{5})/10\) at the points \((1 - \sqrt{5})/2\) and \((1 + \sqrt{5})/2\). Note that this distribution satisfies \(E(W_i) = 0, E(W_i^2) = E(W_i^3) = 1\).

**Step 4.** Let \(D^{*b}\) be the test statistic obtained from the bootstrap samples \(\{(X_{ij}, Y_{ij}^{*b})\}_{i=1}^{n_j}, \ldots, \{(X_{ij}, Y_{ij}^{*b})\}_{i=1}^{n_j}\) after applying the steps 1 and 2 to the cited bootstrap sample.

As we mentioned, the decision rule consists of rejecting the null hypothesis if \(D > \hat{D}^{(1-\alpha)}\), where \(\hat{D}^{(1-\alpha)}\) is the empirical \((1 - \alpha)\)-percentile of the values \(D^{*1}, \ldots, D^{*B}\) obtained before.

It is important to note that the described procedure – testing \(H_0(K)\) – should be repeated from \(K = 1\) onwards until a certain null hypothesis is not rejected in order to determine automatically the number of \(K\) groups. Note, however, that unlike the previous test decision, this latter one is not statistically significant (strong evidences for rejecting the null hypothesis are not given). The whole procedure is briefly described step by step in Algorithm 1.
Algorithm 1 $k$-regression curves algorithm

1. With $(X_{ij}, Y_{ij})_{i=1}^{n_j}, i = 1, \ldots, n_j, j = 1, \ldots, J$, obtain $\hat{m}_j$.
2. Initialize with $K = 1$ and test $H_0(K)$:
   2.1 Obtain the “best” partition $G_1, \ldots, G_K$ by means of the $K$-means or $K$-medians algorithm.
   2.2 For $k = 1, \ldots, K$, estimate $\hat{f}_k$ and retrieve the test statistic $D$.
   2.3 Generate $B$ bootstrap samples and calculate $D^{*b}$, for $b = 1, \ldots, B$.
2.4 if $D > D^{*(1-\alpha)}$ then
   reject $H_0(K)$
   $K = K + 1$
   go back to 2.1
   else
   accept $H_0(K)$
   end
3. The number $K$ of groups of equal regression curves is determined.

3 Simulation study

Results of three Monte Carlo experiments settings conducted to evaluate the finite sample performance of the proposed methodology are reported in this section. Firstly, we show those ones related with testing one specific hypothesis $H_0(k)$, particularly, we start with $K = 1$. Note that testing $H_0(1)$ is equivalent to test the null hypothesis of no difference in nonparametric regression between two or more independent groups. Accordingly, we will compare our procedure with some other methods described in literature to this end, particularly with those ones used in [Pardo-Fernández et al. 2007] and [Park et al. 2014].

Based on these two publications, the following scenarios (with models and variance functions) are proposed in order to carry out the simulation:

(R1) $m_1(x) = m_2(x) = m_3(x) = x$
(R2) $m_1(x) = x, m_2(x) = x + 0.25, m_3(x) = x + 0.5$
(R3) $m_1(x) = x, m_2(x) = 0.5, m_3(x) = 1 - x$
(R4) $m_1(x) = m_2(x) = x, m_3(x) = 1 - 48x + 218x^2 - 315x^3 + 145x^4$

(V1) $\sigma_1^2(x) = \sigma_2^2(x) = \sigma_3^2(x) = 0.5$
(V2) $\sigma_1^2(x) = \sigma_2^2(x) = \sigma_3^2(x) = 0.5(0.5 + 2x)$
(V3) $\sigma_1^2(x) = x, \sigma_2^2(x) = 0.5, \sigma_3^2(x) = 0.5(2.5 - 2x)$
(V4) $\sigma_1^2(x) = \sigma_2^2(x) = x, \sigma_3^2(x) = 0.5(-4x^2 + 4x + 0.5)$.

Note that, all the above scenarios were considered in the simulation section described by [Park et al. 2014] while only (R1), (R2), (R3) models with variance function (V1) were considered in [Pardo-Fernández et al. 2007].

The simulated data were generated from equation in [1], with the covariate $X_j$ drawn from a uniform distribution on the interval [0, 1] and with independent model errors $\varepsilon_j$ drawn from a standard normal distribution with mean 0 and variance $\sigma_j^2(x)$, for $j = 1, 2, 3$. In each case, to determine the critical values of the test statistics we applied bootstrap method, specifically using $B = 500$ bootstrap samples. In order to perform an unbalanced study we used unequal sample sizes for each $j$ curve, with $n_{ij} = 300, 400, 500$. Both type I error rates and power values were calculated on the basis of 1000 simulation runs at the significance levels of $\alpha = 0.05$ and $\alpha = 0.10$. Finally, note that bandwidths are selected automatically by minimising the cross-validation criterion defined in Section [2].

Table [1] shows the results under the null hypothesis –(R1) model– and under the alternative –(R2), (R3), and (R4) models– of the tests based on $D_{CM}$ and $D_{KS}$. Note that errors are homoscedastic when variance function (V1) is chosen and heteroscedastic when we select the variance functions (V2)-(V4).
The two test statistics of our procedure control type I error rate very close to the nominal level and this approximation is much better than the obtained by Pardo-Fernández et al. [2007] –from (R1) with the level being held or coming fairly close to the nominal size in most cases, especially with large sample sizes.

As in the previous simulated scenario, Type I errors are registered by using the test statistics (R2)– very similar behaviours both in type I errors and powers were found. If minor differences are appreciated in terms of power these could be due to sample size. The highest sample size used by these authors was \( n_1 = 100 \) against size of \( n_j = 500 \) used in this simulation.

The second simulation setting was designed to assess the performance of the procedure testing one specific hypothesis \( H_0(K) \), using in this case \( K = 5 \). Note that, in this case, we are dealing with testing if the \( J \) regression curves can be grouped in five groups. Accordingly, a new scenario is proposed. The regression model given in (1) is considered for \( j = 1, \ldots, 30 \), with

\[
\begin{align*}
m_j(X_j) &= \begin{cases} 
X_j + 2 & \text{if } j \leq 5 \\
X_j^2 + 3 & \text{if } 5 < j \leq 10 \\
2 \sin(2X_j) - 2 & \text{if } 10 < j \leq 15 \\
2 \sin(X_j) & \text{if } 15 < j \leq 20 \\
2 \sin(X_j) + a \varepsilon_j & \text{if } 20 < j \leq 25 \\
1 & \text{if } j > 25,
\end{cases}
\end{align*}
\]

where \( a \) is a real constant, \( X_j \) is the explanatory covariate drawn from a uniform distribution on the interval \([-2,2]\], and \( \varepsilon_j \) is the error distributed in accordance to a \( N(0, \sigma_j^2(x)) \). We have also considered a homoscedastic and a heteroscedastic situation. In the homoscedastic case, the variance functions are given by \( \sigma_j^2(x) = 0.5 \), while in the heteroscedastic case, the variance functions are given by \( \sigma_j^2(x) = 0.5 + 0.05m_j(x) \).

As in the previous simulated scenario, \( B = 500 \) bootstrap samples were generated in order to know the distribution of the test statistic. Type I error rates and power values are calculated as the proportions of rejections in 1000 simulation for different significance levels (\( \alpha = 0.05, 0.10 \)). We have also considered unequal sample sizes for each \( j \) curve, particularly, \( (n_1, n_2, \ldots, n_J) \sim \text{Multinomial}(n; p_1, p_2, \ldots, p_J) \) being \( p_j = p_j^* / \sum_{j=1}^J p_j^* \), with \( p_j^* \) randomly drawn from \( \{1, 1.5, 2, 2.5, 3\} \). We used \( n = 1000, 3000 \) and 6000.

Different values of \( a \) were considered, ranging from 0 to 0.4. It should be noted that the value \( a = 0 \) corresponds to the null hypothesis (the thirty regression curves can be classified in five groups), and as the value of \( a \) increases, so does the difference between the curves leading to six groups.

Type I errors are registered by using the test statistics \( D_{CM} \) and \( D_{KS} \) for different significance levels and sample sizes in Table 1. Results reported in this Table 1 reveal that the the two test statistics perform similarly and reasonably well, with the level being held or coming fairly close to the nominal size in most cases, especially with large sample sizes. Some test performance results in terms of power are shown in Table 2 and Figure 1. Both in the homoscedastic and in
Table 2: Estimated type I error of testing $H_0(5)$ based on the test statistics $D_{CM}$ and $D_{KS}$, for different sample sizes and nominal levels. Results given for the homoscedastic and the heteroscedastic situation.

| Scenario       | $\alpha$: | $n = 1000$ |        | $n = 3000$ |        | $n = 6000$ |        |
|----------------|-----------|------------|--------|------------|--------|------------|--------|
|                |           | $\alpha$:  | 0.050  | 0.100  | 0.050  | 0.100  | 0.050  | 0.100 |
| Homoscedastic  | $D_{CM}$  | 0.034      | 0.067  | 0.041  | 0.080  | 0.033  | 0.071  |        |
|                | $D_{KS}$  | 0.051      | 0.104  | 0.057  | 0.104  | 0.039  | 0.088  |        |
| Heteroscedastic| $D_{CM}$  | 0.032      | 0.083  | 0.037  | 0.079  | 0.026  | 0.076  |        |
|                | $D_{KS}$  | 0.053      | 0.113  | 0.051  | 0.109  | 0.045  | 0.108  |        |

Table 3: Rejections probabilities of testing $H_0(5)$ based on the test statistic $D_{CM}$ and $D_{KS}$ for different $\alpha$ values and different sample sizes. The significance level is $\alpha = 0.05, 0.10$. Results given for the homoscedastic and heteroscedastic scenario.

| $n$  | $\alpha$: | Homoscedastic | Heteroscedastic |
|------|-----------|---------------|-----------------|
|      | $\alpha$: | $\alpha$: 0.050 | $\alpha$: 0.100 | $\alpha$: 0.050 | $\alpha$: 0.100 |
| 1000 | 0.1       | $D_{CM}$ 0.056 | $D_{KS}$ 0.091  | $D_{CM}$ 0.056 | $D_{KS}$ 0.091  |
|      |           | 0.129       | 0.191           | 0.129       | 0.191           |
| 0.2  |           | $D_{CM}$ 0.231 | $D_{KS}$ 0.324  | $D_{CM}$ 0.231 | $D_{KS}$ 0.324  |
|      |           | 0.359       | 0.457           | 0.359       | 0.457           |
| 0.3  |           | $D_{CM}$ 0.529 | $D_{KS}$ 0.638  | $D_{CM}$ 0.529 | $D_{KS}$ 0.638  |
|      |           | 0.630       | 0.746           | 0.630       | 0.746           |
| 0.4  |           | $D_{CM}$ 0.743 | $D_{KS}$ 0.837  | $D_{CM}$ 0.743 | $D_{KS}$ 0.837  |
|      |           | 0.813       | 0.887           | 0.813       | 0.887           |
| 3000 | 0.1       | $D_{CM}$ 0.587 | $D_{KS}$ 0.539  | $D_{CM}$ 0.587 | $D_{KS}$ 0.539  |
|      |           | 0.719       | 0.682           | 0.719       | 0.682           |
| 0.2  |           | $D_{CM}$ 1.000 | $D_{KS}$ 0.996  | $D_{CM}$ 1.000 | $D_{KS}$ 0.996  |
|      |           | 1.000       | 0.999           | 1.000       | 0.999           |
| 0.3  |           | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  |
|      |           | 1.000       | 1.000           | 1.000       | 1.000           |
| 0.4  |           | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  |
|      |           | 1.000       | 1.000           | 1.000       | 1.000           |
| 6000 | 0.1       | $D_{CM}$ 0.993 | $D_{KS}$ 0.993  | $D_{CM}$ 0.993 | $D_{KS}$ 0.993  |
|      |           | 0.996       | 0.996           | 0.996       | 0.996           |
| 0.2  |           | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  |
|      |           | 1.000       | 1.000           | 1.000       | 1.000           |
| 0.3  |           | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  |
|      |           | 1.000       | 1.000           | 1.000       | 1.000           |
| 0.4  |           | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  | $D_{CM}$ 1.000 | $D_{KS}$ 1.000  |
|      |           | 1.000       | 1.000           | 1.000       | 1.000           |

Finally, note that in order to obtain the results of the simulations, we have used wild bootstrap and we have selected the bandwidth (both in the original samples and in the bootstrap replicates) by means of cross-validation. However, although the whole results are not shown, we have also evaluated both the selected bootstrap procedure and the effect of the smoothing parameter. Regarding to the resampling technique, the simple bootstrap was also used; and two new situations were considered for the bandwidth: (i) to use cross-validation for obtaining the bandwidth for the original samples and then to fix these in the bootstrap replicates, (ii) to fix some bandwidths a priori. In all cases, poor results were obtained (lower powers and poorer approximations of type I error, especially with small sample sizes) when compared to those based on the approximation exposed here.
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Figure 1: Power curves. Rejection probabilities of the proposed tests for nominal level 5% (red line), for $n = 1000$, 3000 and 6000 (upper, middle and lower panels, respectively) and for both scenarios (left and right panels, respectively)
Table 4: Number of times in % (of 1000 repetitions) that the Algorithm selects the number of groups using a nominal level of 5%.

| $n_j$ | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-------|---|---|---|---|---|---|----|
| 100   | 0.2| 94.3| 4.1| 1.1| 0.1| 0.1| 0.1|
| 150   | 0.0| 94.5| 4.4| 0.9| 0.1| 0.1| 0.0|
| 200   | 0.0| 95.2| 3.7| 0.7| 0.4| 0.0| 0.0|

The last conducted simulation aims to assess the performance of the Algorithm, i.e., the whole procedure. We compare our method with the procedure recently developed by [Vogt and Linton 2017]. The method aims to classify nonparametric functions in the longitudinal data framework. We have kept exactly the scenario described in Section 5 of the above mentioned paper. Then, for $j = 1, \ldots, 120$, the regression model given in (1) is considered with

$$m_j(x_j) = \begin{cases} 
0 & \text{if } j \leq 50, \\
1 - 2x_j & \text{if } 51 < j \leq 80, \\
0.75 \tan^{-1} 10 (X_j - 0.6) & \text{if } 81 < j \leq 100, \\
2.5 (1 - X_j^2)^3 \mathbb{1}(|X_j| \leq 1) & \text{if } 101 < j \leq 110, \\
1.75 \tan^{-1} 5(X_j - 0.6) + 0.75 & \text{if } 111 < j \leq 120,
\end{cases}$$

being $X_j$ the explanatory covariate drawn from a uniform distribution on the interval $[0, 1]$, and $\varepsilon_j$ the error distributed in accordance to a normal distribution $N(0, 1.3)$. The simulation study was carried out under different samples sizes $n_j = 100, 150, 200$ taking into account the test statistic $D_{CM}$. The remainder parameters of the simulation (number of simulation runs and number of bootstrap replicates) were kept as in the previous two scenarios.

In order to perform correctly, the Algorithm must reject the first null hypothesis, $H_0(1)$, continues, rejects again the second one, $H_0(2)$, and so on until it accepts $H_0(5)$. Results of this simulation are shown in Table 4 which refers to the number of times that the procedure works well (in %) selecting the number of groups $K$ and using a nominal level of 5%.

Results reported in Table 4 reveal a good behaviour of the proposed Algorithm 1, with rates of success around 95%, coming quite close to the $(1 - \alpha)$ established. Already for the smallest samples size $n_j = 100$, our procedure selects the true number of groups $K = 5$ in 94.3\% of the times unlike the results obtained by the method proposed in [Vogt and Linton 2017] that show the 75\% of the times. Moreover, there is a slight improvement on the proportion of success as the sample size increases.

To measure how well the procedure assigns each curve $(J = 120)$ to their correct group $(G_1, \ldots, G_5)$, the number of curves wrongly classified was analysed. Figure 2 shows the distribution of this variable for the different sample size $(n_j = 100, 150, 200)$. Particularly, it is shown the number of times in which a certain number of wrong assignments is obtained. Note that as the sample size increases, so does the number of correctly classified curves. For $n_j = 100$ our procedure gives satisfactory results taking into account that at most five curves are wrongly classified in 90\% of cases. At a sample size of $n_j = 150$ our procedure is able to classify correctly all the curves in about 70\% of the cases. Finally, for the biggest sample size, all the curves are correctly classified in 91\% of the cases and most of the wrong classifications are due to the error in only one single curve out of a total of 120. It should be mentioned that these results are quite better regarding to those ones obtained by [Vogt and Linton 2017] in which, considering the best scenario $(n_j = 200)$, all the curves are correctly classified about 80\% of cases.

4 Application to real data

Our methodology is applied to the study of the geometry of a tunnel through the analysis of a set of cross-sections. These sections were obtained by adjusting a point cloud collected with a RIEGL LMS.Z390 time of flight terrestrial laser scanner (TLS). It has a maximum range of about 400 m for objects with reflectance greater than 80\% and 6 mm nominal accuracy for a single point to a distance of 50 m. The capture rate is 8000 data points/second.

Terrestrial laser scanning is a ground based technique to measure the position and dimension of objects in a three dimensional space. Thereby, a laser beam is emitted from a laser light source and used to scan the surface of surrounding objects. The distance between the scanner and the object is determined by the time of flight principle. The laser range
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Figure 2: Simulation results for the estimation of the groups $G_1, \ldots, G_5$. (a)–(c) distributions of the number of wrong assignments for the Algorithm 1 (without Holm’s correction) and sample sizes $n_j = 100, 150, 200$, respectively.

finder sends a laser pulse towards the object and measures the time taken by the pulse to be reflected from the target and returned to the sender. Also horizontal and vertical angles from the center of the scanner to the point are measured. Then the coordinates of the points are calculated using polar coordinates.

The tunnel was made by drilling and blasting. It is approximately circular and its theoretical diameter is 9 m. The cross-section of the tunnel should be constant throughout the tunnel but, in drill and blast, there can be over-break amounting to 10 to 20% of the excavated cross-sectional area, which must be removed and possibly refilled. In the case of an insufficient excavation, the cross-section must be expanded by mechanical or manual methods. This represents a significant increase in the cost of the work.

Figure 3 shows the point cloud of the tunnel obtained with the TLS. Although the irregularities of its surface can be visually appreciated, it is of interest to know if the tunnel section is, in general terms, homogeneous or if, on the contrary, there are different areas of homogeneous section. The engineers could take advantage of this information to plan activities to rebuild the tunnel. Thus, it is very interesting to distinguish between areas of the tunnel that need to be refilled from those that are under-excavated and, consequently, need to be widened. It also can provide useful information regarding the mechanical characteristics of the materials. Moreover, our methodology allows taking into account the fact that some differences between the profiles could be due to the noise associated to the point cloud. Then small differences between the profiles that could have their origin in the measuring system are not computed as real differences in the tunnel.

In order to determine the homogeneity of the tunnel, a data set of $n = 16\,075$ coordinates constituted by 66 cross-sections were obtained from the point cloud in Cartesian coordinates. The cross-sections were obtained by the intersection of the plane perpendicular to the axis of the tunnel and the 3D model created from the point cloud. For $j = 1, \ldots, 66$ sections, the point cloud measured with the TLS provides $(X_j, Y_j)$ coordinates. As the cross-sections given in Cartesian coordinates are not univariate functions, we first perform a transformation of the coordinates. The Cartesian coordinates $(X_j, Y_j)$ can be converted to polar coordinates $(r_j, \alpha_j)$ given by

$$( r_j, \alpha_j ) = \left( \sqrt{X_j^2 + Y_j^2}, \arctan \left( \frac{Y_j}{X_j} \right) \right)$$

being $r$ the distance to each point and $\alpha$ the polar angle. Then, we use our proposed approach in the following regression models

$$r_j = m_j(\alpha_j) + \varepsilon_j \quad \text{for} \quad j = 1, \ldots, 66.$$
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The application of the proposed methodology —using the test statistics $D_{CM}$— indicates that, for a nominal level of 5%, the null hypothesis is rejected (with p-values lower than 0.01) until $K = 5$ (with a p-value of 0.45) and therefore the cross-section $m_1, \ldots, m_{66}$ can be grouped in five groups.

The estimated regression curves in polar coordinates given by $(\alpha_j, \hat{m}_j(\alpha_j))$ for $j = 1, \ldots, 66$ are drawn in the left panel of Figure 4. Curves assigned to each group are plotted with the same color. The differences between groups are almost visually appreciable. Additionally, in order to graphically assess the analysis, the curves are shown in Cartesian coordinates using the transformation $(\hat{m}_j(\alpha_j) \cos(\alpha_j), \hat{m}_j(\alpha_j) \sin(\alpha_j))$ (see right panel of Figure 4).

Finally, Figure 5 depicts the spatial distribution of the cross-sections along the tunnel. A specific color is assigned for each section according to the group in which it belongs. As can be appreciated, there are two non-consecutive areas that belong to the same group (printed in black). It is also clear that three of the five groups (magenta, blue and green profiles) correspond to areas of the tunnel with a big over-excavation. The differences between them tell us that different coatings of shotcrete are needed for each of the three areas.

The good performance of the proposed procedure in terms of spatial distribution should be highlighted. The cross-sections which are spatially close belong to the same group, and accordingly, this provides an easy interpretation of results. Therefore, the identification of homogeneous areas allows a better planning of the work to build the final section of the tunnel, which should fit with the theoretical one.

5 Conclusion

Several nonparametric procedures have been proposed for the comparison of regression functions, however they are no fully informative when the null hypothesis is rejected. This is especially important in practice and in situations where the number of $J$ curves is large enough. In order to solve this situation, we proposed a new procedure that let us not only testing the equality of nonparametric regression curves but also grouping them if they are not equal. Insofar as our comprehensive simulation studies are concerned, we have shown that the results are satisfactory (both in terms of type I error and power) and indicate similar or even better performance than other procedures used in the literature.

Figure 3: Tunnel point cloud. Tunnel measured with the terrestrial laser scanner
Figure 4: Estimated tunnel regression curves. The curves are colored according to the groups to which they belong. Upper, middle and lower panels correspond to these curves assigned into three ($K = 3$), four ($K = 4$) and five groups ($K = 5$), respectively. Left and right panels are the estimates in polar and Cartesian coordinates, respectively.
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The methodology has been applied to a tunnel inspection work addressed to determine heterogeneities in the tunnel geometry. By grouping a set of cross-sections of the tunnel surface it has been possible to identify five areas with significant differences in their geometry.

It is worth mentioning that software in the form of an R package named clustcurv [Villanueva et al. 2020], [Villanueva and Sestelo 2020] was developed implementing the proposed method which seems to be stable and computational efficient. clustcurv is available from the Comprehensive R Archive Network (CRAN) at https://cran.r-project.org/web/packages/clustcurv and can be called to group multiple nonparametric curves both in the regression and in the survival framework.

Even though two different clustering techniques have been implemented in the methodology for determining groups of regression curves, it might expand the reach of this work allowing more arbitrary clustering techniques such as $K$-medoids [Kaufman and Rousseeuw 1990] or Mean-Shift algorithms [Keinosuke and Hostetler 1975].

Furthermore, although the proposed test is designed for detecting groups of regression curves with continuous response, it can be extended without much difficulty to determine groups of logistic regression curves, or other parametric families such as Poisson. Our methodology suffers from the limitation of solely being able to address a single continuous covariate; few further work is nevertheless needed to extend the proposed methodology to the case of multiple covariates. Performing inference in complex analysis is a worthwhile goal, so a more challenging target, however, is to consider the application of these methods to a Big Data environment where the classical bootstrap techniques can be prohibitively demanding.

References

Wenceslao González-Manteiga and Rosa M. Crujeiras. An updated review of Goodness-of-Fit tests for regression models. Test, 22:361–411, 2013.

Peter Hall and Jeffrey D. Hart. Bootstrap test for difference between means in nonparametric regression. Journal of the American Statistical Association, 85(412):1039–1049, December 1990.
Eileen King, Jeffrey D. Hart, and Thomas E. Wehrly. Testing the equality of two regression curves using linear smoothers. *Statistics and Probability Letters*, 12(3):239–247, 1991. ISSN 0167-7152.

M. A. Delgado. Testing the equality of nonparametric regression curves. *Statistics and Probability Letters*, 17:199–204, June 1993.

K. B. Kulasekera. Comparison of regression curves using quasi-residuals. *Journal of the American Statistical Association*, 90(431):1085–1093, 1995. ISSN 01621459.

S. G. Young and A. W. Bowman. Nonparametric analysis of covariance. *Biometrics*, 51:920–931, 1995.

D. Dette and N. Neumeyer. Nonparametric analysis of covariance. *The Annals of Statistics*, 29:1361–1400, 2001.

Juan Carlos Pardo-Fernández, Ingrid Van Keilegom, and Wenceslao González-Manteiga. Testing for the equality of k regression curves. *Statistica Sinica*, 17:1115–1137, 2007.

Ramidha Srihera and Winfried Stute. Nonparametric comparison of regression functions. *Journal of Multivariate Analysis*, 101:2039–2059, October 2009. ISSN 0047-259X.

Cheolwoo Park and Kee-Hoon Kang. Sizer analysis for the comparison of regression curves. *Computational Statistics and Data Analysis*, 52(8):3954–3970, 2008. ISSN 0167-9473. doi:10.1016/j.csda.2008.01.006

Cheolwoo Park, Jan Hannig, and Kee-Hoon Kang. Nonparametric comparison of multiple regression curves in scale-space. *Journal of Computational and Graphical Statistics*, 23(3):657–677, 2014. doi:10.1080/10618600.2013.822816

M. Sestelo and J. Roca-Pardiñas. Testing critical points of non-parametric regression curves: application to the management of stalked barnacles. *Journal of the Royal Statistical Society C*, 68(4):1051–1070, 2019.

M. Rosenblatt. A quadratic measure of deviation of two-dimensional density estimates and a test of independence. *The Annals of Statistics*, 3(1):1–14, 01 1975.

Wenceslao González-Manteiga and Ricardo Cao. Testing the hypothesis of a general linear model using nonparametric regression estimation. *Test*, 2(1):223–249, 1993.

W. Härdle and E. Mammen. Testing parametric versus nonparametric regression. *Annals of Statistics*, 21:1926–1947, 1993a.

Nora M. Villanueva, Marta Sestelo, and Luí’s Meira-Machado. A Method for Determining Groups in Multiple Survival Curves. *Statistics in Medicine*, 38:366–377, 2019.

C. Abraham, P. A. Cornillon, E. Matzner-Løber, and N. Molinari. Unsupervised curve clustering using b-splines. *Scandinavian Journal of Statistics*, 30(3):581–595, 2003. ISSN 1467-9469. doi:10.1111/1467-9469.00350

Luis Angel García-Escudero and Alfonso Gordaliza. A proposal for robust curve clustering. *Journal of Classification*, 22(2):185–201, 2005.

Thaddeus Tarpey. Linear transformations and the k-means clustering algorithm. *The American Statistician*, 61(1):34–40, 2007. doi:10.1198/000313007X171016

Michael Vogt and Oliver Linton. Classification of non-parametric regression functions in longitudinal data models. *Journal of the Royal Statistical Society Series B*, 79(1):5–27, 2017.

Michael Vogt and Oliver Linton. Multiscale clustering of nonparametric regression curves. *Journal of Econometrics*, 216(1):305–325, 2020.

Carl A. de Boor. *A Practical Guide to Splines*. Springer Verlag, New York, 2001.

Stefan Lang and Andreas Brezger. Bayesian p-splines. *Journal of Computational and Graphical Statistics*, 13:183–212, 2004.

M. P. Wand and M. C. Jones. *Kernel Smoothing*. Chapman & Hall: London, 1995.

Jianqing Fan and Irène Gijbels. *Local polynomial modelling and its applications*. Number 66 in Monographs on statistics and applied probability series. Chapman & Hall, 1996.

Marta Sestelo, Nora M. Villanueva, and Javier Roca-Pardiñas. npregfast: Nonparametric Estimation of Regression Models with Factor-by-Curve Interactions. R package version 1.4.0, 2016. URL [http://CRAN.R-project.org/package= npregfast](http://CRAN.R-project.org/package= npregfast)

Marta Sestelo, Nora M. Villanueva, Luís Meira-Machado, and Javier Roca-Pardiñas. npregfast: An R Package for Nonparametric Estimation and Inference in Life Sciences. *Journal of Statistical Software*, 82(12):1–27, 2017. doi:10.18637/jss.v082.i12

G.H. Golub, M. Heath, and G. Wahba. Generalized cross-validation as a method for choosing a good ridge parameter. *Technometrics*, 21(2):215–223, 1979.
An automatic procedure to determine groups of nonparametric regression curves

D. Ruppert, S. J. Sheather, and M. P. Wand. An effective bandwidth selector for local least squares regression. *Journal of the American Statistical Association*, 90(432):1257–1270, 1995. ISSN 01621459.

J. Fan and J.S. Marron. Fast implementation of nonparametric curve estimators. *Journal of Computational and Graphical Statistics*, 3:35–56, 1994.

Anil K Jain and Richard C Dubes. *Algorithms for clustering data*. Prentice-Hall, Inc., Upper Saddle River, NJ, USA, 1988.

James B. Macqueen. *Some methods of classification and analysis of multivariate observations*, volume 1. Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability (Univ. of Calif. Press), 1967.

Leonard Kaufman and Peter J Rousseeuw. *Finding Groups in Data: An Introduction to Cluster Analysis*. John Wiley, 1990.

Bradley Efron. Bootstrap methods: another look at the jackknife. *The Annals of Statistics*, 7:1–26, 1979.

E. Efron and R. J. Tibshirani. *An introduction to the Bootstrap*. Chapman and Hall, London, 1993.

W. Härdle and E. Mammen. Comparing nonparametric versus parametric regression fits. *The Annals of Statistics*, 21(4):1926–1947, 1993b.

G. Kauermann and J.D. Opsomer. Local Likelihood Estimation in Generalized Additive Models. *Scandinavian Journal of Statistics*, 30:317–337, 2003.

C. F. J. Wu. Jackknife, Bootstrap and other resampling methods in regression analysis. *The Annals of Statistics*, 14(4):1261–1295, 1986. doi:10.2307/2241454

Regina Y. Liu. Bootstrap Procedures under some Non-I.I.D. Models. *The Annals of Statistics*, 16(4):1696–1708, 1988.

Enno Mammen. Bootstrap and Wild Bootstrap for High Dimensional Linear Models. *The Annals of Statistics*, 21(1):255–285, 1993.

Nora M. Villanueva, Marta Sestelo, Luís Meira-Machado, and Javier Roca-Pardiñas. clustcurv: An r package for determining groups in multiple curves. *Manuscript submitted for publication*, 2020.

Nora M. Villanueva and Marta Sestelo. clustcurv: Determining Groups in Multiple Curves. R package version 2.0.0, 2020. URL [http://cran.r-project.org/web/packages/clustcurv](http://cran.r-project.org/web/packages/clustcurv)

Fukunaga Keinosuke and Larry D. Hostetler. The estimation of the gradient of a density function, with applications in pattern recognition. *IEEE Transactions on Information Theory*, 21(1):32–40, 1975.