ANALYSIS OF VARIANCE WITH FUNCTIONAL DATA TO DETECT COLOR CHANGES IN GRANITE

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Keywords: Functional data, Anova, Spectral reflectance curve, Granite, Protective treatment.

Abstract: Analysis of spectral reflectance curves is useful in many application fields. Despite the functional nature of these curves, statistical methods used to date for analysing these curves (classification, analysis of variance, etc.) have tended to be scalar and do not fully take advantage of the information they contain as functional objects. In this article we applied functional analysis of variance to spectral reflectance curves in order to evaluate the impact of protective treatments on granite colour. The use of raw information on the spectrum means that significant changes are detected that might go unnoticed in models that use scalar values to measure colour. The application of the functional approach enables information to be obtained on changes whose intensity are statistically significant at each point of the spectrum without the need to perform different analyses for each area of the spectrum. Furthermore, the computational load is no greater than for classical multivariate models.

1 INTRODUCTION

Analysis of spectral reflectance curves is useful in several application fields, such as astronomy, agriculture, engineering, meteorology, environment, mining, geographical information systems, etc. (see for example, (Cho and Skidmore, 2006), (Stevens et al., 2006), (Ayala-Silva and Beyl, 2005), (Henry et al., 2004), (Iñigo et al., 2004), (Lacar et al., 2001), (Richardson et al., 2001), (Lebow et al., 1996) and references cited therein).

However, statistical methods currently used for this kind of analysis (classification, discrimination, regression, etc) has a basically scalar or, at best, multivariate, nature and so curves are considered merely as sets of observed points. When curves are considered under a functional view, the goal is not to implement a statistical analysis that handles them as such functional objects, but to implement a preliminary step to graphic or analytical studies (such as, for example, a functional approximation, the calculation of derivatives, or interpolation or extrapolation at some point of the spectrum, etc.), or statistical analysis of scalar indicators of some of their overall analytical properties (see the references given above).

In this article we describe a novel application of analysis of variance (e.g. (Montgomery, 1997)) with a functional approach (functional ANOVA or FANOVA) (Ramsay and Silverman, 1997), (Cuevas et al., 2004) to an analysis of spectral reflectance curves with a view to evaluating the impact of several protective treatments on granite rock colour.

In the architectural heritage preservation field, the colour of stone surfaces constitutes an element of the historical and artistic value of a monument, and, as such, should not undergo changes following cleaning, protection or consolidation processes (Lazzarini and Tabasso, 1986). It is therefore important to be aware of the potential impact of such treatments on ornamental rock so as to be able to avoid treatments that cause colour changes and choose treatments that are more suitable for preservation purposes.

Colour is quantitatively expressed using spectrophotometers which, based on measuring reflectance throughout the visible spectrum, define colour using colorimetric coordinates in the stimulus space of a standard observer. Coordinate systems widely used in this context include, for ex-
A functional linear regression model (Ramsey and Silverman, 1997) is an extension of the multivariate linear regression model to the case of infinite-dimensional or functional data. For each \( t \in \mathcal{T} \):

\[
E(Y(t)|X) = \alpha(t) + \langle X, \beta(t) \rangle
\]

with a parameter function \( \beta : \mathcal{T} \times \mathcal{T} \to \mathbb{R} \) and an overall mean response function \( \alpha : \mathcal{T} \to \mathbb{R} \). The data are a sample of pairs of random functions \((X, Y)\), with \(X\) the predictor and \(Y\) the response functions.

The above functional model can also be extended to the case of several functional predictors as follows:

\[
E(Y(t)|X) = \alpha(t) + \langle X, \beta(t) \rangle
\]

where \(X = (X_1, \ldots, X_d)\) are the functional predictors and \(Y\) is the response function.

Intermediate models between classical (1) and general (3) are models that produce a scalar response with functional predictors and models (like those used in this research) that produce a functional response with scalar predictors. The general model is as follows:

\[
E(Y(t)|X) = \alpha(t) + \langle X, \beta \rangle
\]

where \(X\) is the matrix \(n \times d\) of the design with elements \((X)_{ij} = X_{ij}\) (the \(i\)-th observation of the \(j\)-th covariable), \(\alpha\) is the overall functional mean and \(\beta\) is the functional vector of the \(d\) functional coefficients \(\beta_j\), with \(i = 1, \ldots, n, j = 1, \ldots, d\).

2 FUNCTIONAL ANOVA

2.1 Introduction to Functional Linear Models

The linear regression model for a single input variable \(X\) and a response variable \(Y\) takes the form:

\[
E(Y|X) = \alpha + \beta X
\]

where \(\alpha, \beta\) are the regression coefficients. This model is easily generalized to \(d\) regression variables \(X = (X_1, \ldots, X_d)^T\) by means of

\[
E(Y|X) = \mu + \sum_{i=1}^{d} \beta_i X_i = \alpha + \langle X, \beta \rangle
\]

where \(\alpha\) and \(\beta = (\beta_1, \ldots, \beta_d)^T\) are now the regression coefficients.

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E(Y(t)|X) = \alpha(t) + \langle X, \beta(t) \rangle
\]

with a parameter function \( \beta : \mathcal{T} \times \mathcal{T} \to \mathbb{R} \) and an overall mean response function \( \alpha : \mathcal{T} \to \mathbb{R} \). The data are a sample of pairs of random functions \((X, Y)\), with \(X\) the predictor and \(Y\) the response functions.

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span\{\phi_1, ..., \phi_m\} with \{\phi_k\} sets of basis functions (Ramsay and Silverman, 1997). For our research, we chose a family of B-splines as the set of basis functions, given their good local behaviour. If, for the sake of simplicity, we represent as \( y \) any of the functions \( y_i \), \( i = 1, ..., n \) in the sample, we have:

\[
y(t) = \sum_{k=1}^{m} c_k \phi_k(t) = c^T \Phi(t)
\]

where \( \Phi(t) = (\phi_1(t), ..., \phi_m(t))^T \).

Hence, the smoothing problem consists in determining the solution \( y \) to the following regularization problem:

\[
\min_{x \in \mathcal{X}} \sum_{i=1}^{n} (z_i - y(t_i))^2 + \lambda \Gamma(y)
\]

where \( z_i = y(t_i) + e_i \) is the result of observing \( y \) at the point \( t_i \), \( \Gamma \) is an operator that penalizes the complexity of the solution, and \( \lambda \) is a regularization parameter that regulates the intensity of this penalization. In our case, we used the operator \( \Gamma(y) = \int_\mathcal{X} \{D^2y(t)\}^2 dt \), where \( \mathcal{X} = [t_{\min}, t_{\max}] \) and \( D^2 \) is the second-order differential operator.

Bearing in mind the expansion (5), the above problem (6) may be written as:

\[
\min \left\{ (z - \Phi c)^T (z - \Phi c) + \lambda \mathbf{c}^T \mathbf{R} \mathbf{c} \right\}
\]

where \( z = (z_1, ..., z_n)^T \), \( \mathbf{c} = (c_1, ..., c_n)^T \), \( \Phi \) is the \( n_p \times n_b \) matrix with elements \( \Phi_{jk} = \phi_k(t_j) \) and \( \mathbf{R} \) is the \( n_b \times n_b \) matrix with elements \( R_{kl} = \{D^2 \phi_k, D^2 \phi_l\}_{L^2(\mathcal{X})} \).

The solution to this problem is given by \( \hat{c} = (\Phi^T \Phi + \lambda \mathbf{R})^{-1} \Phi^T z \), such that the estimated values of the true function \( y \) at the observation points are obtained by means of \( \hat{y} = S \hat{c} \), where \( S = \Phi (\Phi^T \Phi + \lambda \mathbf{R})^{-1} \Phi^T \) and \( \hat{y} = (\hat{y}(t_1), ..., \hat{y}(t_n))^T \).

The selection of the \( \lambda \) forms part of the model selection problem and is usually performed using cross validation.

### 2.3 Fitting the Functional Response – Scalar Predictor Linear Model

Below we focus on the functional response model with scalar covariables (4) as used in this research. So as to avoid the independent term \( \alpha(t) \), below, we propose assuming that the vector of covariables includes a first constant covariable equal to 1 whose functional coefficient is \( \beta_1 = \alpha \). We can thus reformulate the model (4) as:

\[
E(Y(t)|X) = X \beta(t) = \sum_{j=1}^{d} X_j \beta_j(t)
\]

Within this framework, we assume that the above smoothing process on the example functions produces the expansions \( y_i(t) = c_i^T \Phi(t), \ i = 1, ..., n \) which may be jointly written by means of \( y(t) = \mathbf{C} \Phi(t) \) where \( \mathbf{C} \) is a matrix \( n \times m \) with rows \( c_i^T \).

We likewise assume that each of the functional coefficient \( \beta_j \) admits an expansion in terms of the aforementioned bases:

\[
\beta_j(t) = \sum_{k=1}^{m} b_{jk} \eta_k(t) = b_j^T \eta(t)
\]

where \( b_j = (b_{j1}, ..., b_{jm})^T \). This may be written in functional form as: \( \hat{\beta}_j = b_j^T \Phi \). Using this expression for all the coefficients \( \hat{\beta}_j \) jointly, we obtain:

\[
\beta = (\beta_1, ..., \beta_d)^T = \mathbf{B} \eta
\]

where \( \mathbf{B} = (\mathbf{b}_1, ..., \mathbf{b}_m)^T \).

From all the above, for each observation \( i = 1, ..., n \), the model (7) becomes: \( \hat{y}_i(t) = x_i \hat{\beta}(t) = \mathbf{x}_i \mathbf{B} \eta(t) \) or equivalently, in compact functional form: \( \hat{y}_i(t) = \mathbf{x}_i \eta \). Applying the above to all the example observations, we obtain the following functional-type vectorial expression:

\[
\hat{y} = \mathbf{X} \mathbf{B} \eta
\]

The fit is carried out using the criterion of regularized minimum squared errors:

\[
\sum_{i=1}^{n} \| y_i - \hat{y}_i \|^2_{L^2(\mathcal{X})} + \lambda \Gamma(\beta)
\]

where \( \mathbf{J}_{\eta \eta} = \int \eta(t) \eta(t)^T dt \), \( \mathbf{J}_{\phi \eta} = \int \Phi(t) \eta(t)^T dt \), and \( \mathbf{J}_{\phi \phi} = \int \Phi(t) \Phi(t)^T dt \) and \( \Gamma = \lambda \mathbf{R} \).

Deriving the expression (8) with respect to \( \mathbf{B} \), the following normal equations are obtained (Ramsay and Silverman, 1997):

\[
\mathbf{X}^T \mathbf{X} \mathbf{J}_{\eta \eta} + \lambda \mathbf{R} = \mathbf{X}^T \mathbf{C} \mathbf{J}_{\phi \eta}
\]
and also the following expression of the solution in terms of the Kronecker product $\otimes$:

$$\text{vec}(B) = \left[(J_{m n} + \lambda R) \otimes (X^T X)\right]^{-1} \text{vec}(X^T C_{m n})$$

where $\text{vec}(B)$ is the column vector obtained by stacking the columns of the matrix $B$ on top of one another and where $\lambda$ can be selected using, for example, cross-validation.

### 3.4 ANOVA Table and F Test

The significance of the model can be evaluated using one of two possible approaches: by evaluating the significance of the functional model as a whole (e.g. (Cuevas et al., 2004), (Ramsay and Silverman, 1997)), or by performing an analysis of significance in any case, for each wavelengths where significant changes occur. Significance, in any case, for each $t \in \mathcal{T}$ logically provides overall significance for the functional model.

The significance of the model for each point can be determined using a functional version of Snedecor’s $F$ distribution, in which the statistic is also a function defined in the support $\mathcal{T}$ for the $\mathcal{F}$ functions (Ramsay and Silverman, 1997). This produces an $F$ distribution for each point of this support, enabling detection of possibly statistically significant changes in areas where changes occur. Given that the following expressions are functions of $t \in \mathcal{T}$:

$$SSE(t) = \sum_{i=1}^{n} (y_i(t) - \hat{y}_i(t))^2$$

$$SSY(t) = \sum_{i=1}^{n} (y_i(t) - \hat{\alpha}(t))^2$$

$$SSM(t) = SSY(t) - SSE(t)$$

the statistics of the ANOVA table also are functions of $t$:

<table>
<thead>
<tr>
<th>Source of Variation</th>
<th>$df$</th>
<th>$MS(t) = \frac{SS(t)}{df}$</th>
<th>$F(t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>$d-1$</td>
<td>$MS_M(t)$</td>
<td>$MS_M(t)$/$MS_E(t)$</td>
</tr>
<tr>
<td>Error</td>
<td>$n-d$</td>
<td>$MS_E(t)$</td>
<td>$MS_M(t)$/$MS_E(t)$</td>
</tr>
<tr>
<td>Total</td>
<td>$n-1$</td>
<td>$MS_E(t)$</td>
<td>$MS_M(t)$/$MS_E(t)$</td>
</tr>
</tbody>
</table>

Therefore, an $F$ test can be performed for each $t \in \mathcal{T}$.

## 3 DETECTING CHANGES IN REFLECTANCE CURVES USING FUNCTIONAL ANOVA

### 3.1 Data and Experiment Design

Used in the experiment was a medium-grained pre-Hercynian granite composed of quartz, mica (muscovite and biotite) and feldspar. This granite, brownish-yellow in colour, is widely used in architectural monuments in northwest Spain.

The rock was treated with water repellent products intended to prevent or slow down water entry in the rock and consequent deterioration. The products applied were BS29 (supplied by Wacker Chimie) and Tegosivin HL100 (supplied by Evonik). BS29 is a water thinnable mixture of silane, siloxane and synthetic resins and Tegosivin HL100 is an solvent organic methylethoxy polysiloxane. For each product, five prisms (5x5x1 cm) were selected. Colour was measured at eight points chosen at random prior to the application of each product. A 5% (w/w) solution of each product (using white spirit as a solvent in the case of Tegosivin HL100 and distilled water in the case of BS29) was applied to the samples via partial immersion for one minute. After 48 hours colour was measured at another eight points of the treated surface of the prism chosen at random.

Colour was measured using a Minolta CM710 spectrophotometer in SCI mode, using D65 as a light source, an 8 mm target area and an observer angle of 10$. Obtained for each point were values of the reflectance spectrum, expressing the percentage of reflectance of the object for every 10 nm of wavelength in the range between 400 and 720 nm (support for the functions was thus the wavelength interval $\mathcal{T} = [400, 720]$ nm).

Observations for each product totalled 40, whether as colorimetric coordinates and attributes or as spectral reflectance curves. The curves were smoothed and assumed to belong to a functional space $\mathcal{F} = \{\phi_1, ..., \phi_d\}$ generated by a set of order 6 B-splines with 12 knots, resulting in a total of $d = 16$ basis functions. (This number of basis functions, chosen in view of the complexity of the observed functions, does not produce significant changes in the results for a wide range of values). Hence, all the spectral functions are unambiguously determined by their coefficients in terms of the expression:

$$y = \sum_{i=1}^{m} c_i \phi_i$$

Changes in colour were evaluated by means of the application of FANOVA to the reflectance curves.
obtained. For each protective treatment used (BS29 or HL100), a full factorial design for treatment factors (no/yes), prism (1, 2, 3, 4 and 5) and interaction was postulated, with the following functional linear model:

\[ y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \]

\[ i = 1, \ldots, p, \ j = 1, \ldots, q, \ k = 1, \ldots, r, \]

with \( p = 2 \) levels of treatment (treated or untreated), \( q = 5 \) different test prisms and \( r = 8 \) replications, subject to restrictions as follows:

\[ \sum_{i=1}^{2} \alpha_i = 0; \sum_{j=1}^{5} \beta_j = 0; \sum_{i=1}^{2} (\alpha\beta)_{ij} = 0; \sum_{ij} (\alpha\beta)_{ij} = 0 \]

(9)

where \( y_{ijk}, \epsilon \) was the spectral reflectance curve obtained from the spectrophotometer for the observation \( ijk, \mu \) was the global mean, \( \alpha_i \) the main effect corresponding to level \( i \) of the treatment factor (treated or untreated), \( \beta_j \) the main effect corresponding to level \( j \) of the prism factor (prism \( j \)), \( (\alpha\beta)_{ij} \) was the interaction effect between level \( i \) and prism \( j \) and where \( \varepsilon_{ijk} \) was a residual function accounting for the unexplained variation specific to the \( k \)-th observation for prism \( j \) with treatment \( i \).

Note that the restrictions (9) imply sum zero in such a way that each main effect represents the mean alteration of the global mean for each treatment, and each interaction effect indicates the mean alteration for each main effect caused by each combination of levels of the factors.

3.2 Results

Figure 1 shows for BS29 the overall mean and the effect of no treatment and the effect of treatment. As can be observed, the effect of treatment was negative, indicating a reduction in the intensity of the spectral reflectance curves which should indicate that colour of the rock becomes darker.

The significance of these effects are analysed in Figure 2 (BS29) and 3. The last one shows (left to right) the curves for the FANOVA table and the functional \( F \) statistics corresponding to the treatment factor, the prism and the crossed treatment \( \times \) prism factor. In these figures, the broken line indicates the value of \( F \) that corresponds to 5% significance for each \( t \) in \( T \); values below this level should be considered less significant or non-significant. The content of each FANOVA table responds to Table 1, with \( p = 2 \) (levels of treatment), \( q = 5 \) (prisms), \( r = 8 \) (replications) and \( n = pqr = 80 \) observations, and where (e.g. (Montgomery, 1997)):

\[ SS_T = \frac{\sum_{i=1}^{p} \sum_{j=1}^{q} \sum_{k=1}^{r} y_{ijk}^2}{kpr} - \frac{y_{ijk}^2}{kpr} \]

\[ SS_P = \frac{1}{pr} \sum_{j=1}^{q} y_{ij}^2 - \frac{y_{ijk}^2}{kpr} \]

\[ SS_Q = \frac{1}{pq} \sum_{i=1}^{p} y_{ij}^2 - \frac{y_{ijk}^2}{kpr} \]

\[ SS_{PQ} = \frac{1}{r} \sum_{i=1}^{p} \sum_{j=1}^{q} y_{ijk}^2 - \frac{y_{ijk}^2}{kpr} - SS_P - SS_Q \]

\[ SS_E = SS_T - SS_P - SS_Q - SS_{PQ} \]

are the different ANOVA decomposition functions.

Figure 1: For BS29, overall mean, effect of level 1 treatment (No) and level 2 treatment (Yes).

Table 1: ANOVA table corresponding to the full factorial design used.

<table>
<thead>
<tr>
<th>Variation</th>
<th>df</th>
<th>( MS(t) = \frac{SS(t)}{df} )</th>
<th>( F(t) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Treat.</td>
<td>( p - 1 )</td>
<td>( MS_T(t) )</td>
<td>( MSp(t) )</td>
</tr>
<tr>
<td>Prism</td>
<td>( q - 1 )</td>
<td>( MS_P(t) )</td>
<td>( MSq(t) )</td>
</tr>
<tr>
<td>Treat. ( \times ) Prism</td>
<td>( (p - 1) \times (q - 1) )</td>
<td>( MS_{PQ}(t) )</td>
<td>( MS_{PQ}(t) )</td>
</tr>
<tr>
<td>Error</td>
<td>( pq(r - 1) )</td>
<td>( MS_E(t) )</td>
<td>( MS_E(t) )</td>
</tr>
<tr>
<td>Total</td>
<td>( n - 1 )</td>
<td>( \overline{MS_E(t)} )</td>
<td>( \overline{MS_E(t)} )</td>
</tr>
</tbody>
</table>

As can be observed in Figures 2 and 3, the application of BS29 produces significant changes in the reflectance curve as a consequence of the three factors, namely, application of the treatment, prism and treatment \( \times \) prism. For the last two of these factors, this change is significant for the entire spectrum considered, whereas in regard to the treatment factor, the change is not significant above 600nm (orange-red reflectance).

Combining these results with the sign of the effect (Figure 1) it can be concluded that treatment with
BS29 produces a reduction in colour reflectance in the entire spectrum except for the orange-red part.

As for application of THL100, the FANOVA results (not shown) indicate that the prism and treatment × prism factors are equally significant in the entire spectrum considered, whereas the treatment factor is only significant for smaller wavelengths, corresponding to reflectance in the lower green part and in all the blue and purple parts. It can be concluded that treatment with THL100 also produces a reduction in colour reflectance, but only conclusively below 500 nm (the lower green part and all the blue and purple parts). This reduction is also more intense for smaller wavelengths.

Finally, it should be noted that for both products there was high standard deviation in the upper part of the spectrum, from the wavelength value above which there was no significance for the treatment factor for THL100 and low significance for the treatment factor for BS29. This would appear to indicate that some factor exists, not associated with the presence of the treatments, whose dispersion in a part of the spectrum prevents the model from capturing the variability associated with the presence of the product.

The indications are that this factor arises in the chromatic variability existing in the rock, with standard deviation higher in the range of the spectrum covering the colours yellow, orange and red. The colour of the rock is yellow-reddish, resulting, on the one hand, from cream-yellow feldspars (less intense colours for albite-anortite compositions and yellow for potassium compositions) and, on the other hand, from brownish-reddish iron oxyhydroxide patinas distributed unevenly throughout the rock.

Furthermore, since the rock is fine-grained hetero-granular granite, colour is strongly determined by textural unevenness in the rock. This is manifested in the great dispersion in the reflectance spectra in the range corresponding to the rock colour range, i.e., mainly above 600 nm (orange-red). This variablity prevents the model from detecting, in this particular range, the effects of the treatments, although it does not prevent it doing so in the range where dispersion is less—that is, below green and towards the blues. The significance in the entire spectrum for the prism and treatment prism factors is also a consequence of this chromatic variability and textural unevenness in the rock.

4 CONCLUSIONS

We described how we used FANOVA to evaluate changes in spectral reflectance curves resulting from the application of two commercial protective treatments to granite rock (BS29 and Tegosivin HL100). Methods used to date are scalar and have to be applied repeatedly at points or areas of the spectrum in order to determine the statistical significance of wavelength changes. The results obtained in our research demonstrate the usefulness of the functional approach when it is necessary to analyse changes in functional objects, such as reflectance curves. The application of the functional approach enables information to be obtained on changes whose intensity are statistically significant at each point of the spectrum (without having to perform analyses for each point of the spectrum) and changes that might go unnoticed in models that use scalar values to measure colour. Furthermore, the computational load is no greater than that required for multivariate ANOVA (except for the effort required to smooth the functions in the sample).

The method was applied to evaluating the changes in colour reflectance for granite rock following the application of two water repellent products (BS29 and
HL100). The results showed a reduction in colour reflectance in the rock, although, for the BS29, the reduction affected wavelengths below 650 nm (yellow) and for the HL100, the reduction was only significant in wavelengths below 500 nm.

For both products, a reduction in the luminosity of the rock can be anticipated, greater in the case of BS29. In upcoming research, we will analyse how detected reflectance changes influence changes in colour as perceived by a standard observer. In other words, we will apply this functional approach to the colour curves resulting from superimposing the source spectral curve, the object reflectance curve and the colour matching curves of the standard observer, so as to be able to measure the colour in the stimulus space. The results obtained will be compared with those that classical statistical methods (e.g. multivariate ANOVA) obtain in any normal space for measuring colour (e.g. CIE L∗a∗b∗).

Finally, the significance of the prism effect and of the interaction between the prism factor and the treatment factors suggest a design that reduces the variability produced by the experimental unit (prism) as far as possible. In regard to FANOVA, the lesser significance in the upper part of the spectrum may be a result of the greater variance in the curves in this part of the spectrum as a consequence of the granite’s own colour characteristics. One of our new lines of research is the design of new experiments that deal with this variability (e.g. paired designs or designs with additional random blocking factors).

ACKNOWLEDGEMENTS

We wish to express our gratitude to Professor J. O. Ramsay and his team for the functional data analysis software for Matlab that served as the nucleus for the developments that were necessary to carry out this study. The authors also thank to Evonik Industries and Wacker Chemie for supplying Tegosivin HL100 and BS29 respectively. J.M. Matás’s research is supported by the Spanish Ministry of Education and Science, Grant No. MTM2008-03010.

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