Multivariate Functional Regression for Classification With an Application to Geology

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Abstract–**The functional structure of data not necessarily requires using complex classification techniques such as support vector machines. In some applications extending common multivariate methods to functional data suffices not only in regard to classification error but also and mainly to reduce time for training and testing and to keep software as sparse as possible. The present analysis demonstrates this by a classification problem in the aggregates industry. Multivariate functional regression to identify 12 different rock types from reflectance spectra beats support vector machines not only in regard to classification error but also with respect to time requirements for training and testing.**

Keywords: Multivariate functional regression, support vector machines, margin tree, classification, geo-engineering

1 Introduction

In many real-life applications, such as geo-engineering, signal processing, speech recognition, chemical engineering, the data observed are naturally described as discretized functions or curves rather than vectors of feature values [26]. However, applying classic techniques of multivariate statistics directly to the functions observed might cause difficulties, since functions form high-dimensional and highly correlated data. This yields ill-posed problems, and in particular a substantial deterioration in the classification performance as well as highly imprecise parameter estimates [10] [13]. Techniques of functional data analysis can help to overcome these problems of multicollinearity and diminish spurious effects.

For classification problems different approaches exist to address the functional structure of the data. First, high-dimensional classifiers such as penalized or regularized discriminant analysis [13] or support vector machines [15] [3] [14] might be applied directy to the observed data. Second, after transforming the data approprietly, common classification methods might be used [27]. Most notably, approximating a function by a sum of basis functions aids further analysis. A basis expansion not only allows for representing the data as continous curves and though capturing the infinite dimension by using a few basis coefficients to represent the data, but it also yields some smoothing. Further analysis such as classification might be based on these coefficients or on scores from additional functional dimension reduction.

Third, common classification methods have been adapted to the specific structure of functional data such as linear functional discriminant analysis [13], functional logistic regression [28] [21], functional multinomial regression [1], functional penalized optimal scoring [2], a functional version of knn [10], functional support vector machines [27], or functional neural networks [30] [29] [23]. Even ensemble techniques that are based on the idea of constructing multiple function predictions from the data by means of a "weak" base procedure and using a convex combination of them for final aggregated prediction [6] [24] [4] [5] have been extended to functional data [11]. Basically, adapting common methods to functional data makes use of the theory of Hilbert spaces. Assuming that the functions considered are from the Hilbert space $L^2(\mathbb{R})$, the inner products and distances a method relys on may be replaced by the inner product for functions and its induced metrics, respectively.

In many applications support vector machines are used for classification of functional data due to their flexibility in determining nonlinear bounderies by constructing a linear boundery in a large, transformed version of the feature space [14]. Yet, they avoid overfitting by controlling the margin between classes and sparsely representing the margin by the support vectors. However, disadvantes are the choice of parameters (cost, kernel and kernel parameters), training time, extensive memory requirements, and the problem of how to cope with multi-class problems [7] [20].

Due to the overwhelming results in classification many researcher tend to use support vector machines by default ignoring the complexity of this method. However, a rule of thumb such as "the more complex the method the better the results" does not hold. Occasionally, simple methods such as multivariate functional regression yield not only surprisingly good or even better results than a complex technique but also require less resources, which is particularly important for time-critical applications. Below this is shown by a classification problem that

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ISBN: 978-988-18210-8-9
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

one of world's major industries, the aggregates industry, is faced with.

The question of what extent aggregates (sand, gravel, crushed rock) resist physical and chemical loads, is of great importance for their practical use. In general, petrological composition influences engineering properties of rocks such as mechanical or thermal characteristics [12] [16] [25]. Thus, a reliable method for classification of rock types and rock variants can support an appropriate choice of material [17] [18].

Due to the need for faster and more beneficial process and quality control, the aggregates industry has become interested in finding automatic means for identifying suitable rock characteristics. Such a device was developed in a project called PETROSCOPE, which started in 2001 [8] [9], leading to a patent pending process [32]. Today most of the testing of aggregates is performed after production rather than at the source of the rock or sediment extraction. With a more efficient test method, as promised by PETROSCOPE, it is expected that testing would increasingly being used for the analysis of the raw material, as well as for the end product [17] [18].

Using data from the PETROSCOPE project [19], the present investigation deals with classifying 12 different rock types or varieties of the same type with different textural properties, different porosity, and different stages of alteration and surface weathering by means of their reflectance of visible and near infrared light using multivariate functional regression (compare [23]). The spectra serve as predictors for multivariate responses that are found from class membership by a dummy variable approach. Classification performance of multivariate functional regression, measured as classifiction error as well as time complexity, is compared to that of support vector machines.

2 Multivariate Functional Regression

2.1 Functional Regression

Let be a sample consisting of a scalar response y_i and a . In a functional regression model

$$y_i = \beta_0 + \int \beta(t)\, x_i(t) dt, \tag{1}$$

a function $\beta(t)$ and a scalar $\beta_0 \in \mathbb{R}$ ought to be determined from functional predictors $x_i(t)$, $i = 1, \ldots, n$ to estimate the scalar y_i. Calculations simplify on representing the functions involved by basis functions $\phi_k \in L^2(\mathbb{R})$, $k = 1, \ldots, K$ [26, p. 43]. $x_i(t)$ and $\beta(t)$ need not be represented by the same basis functions.

Let $\phi_k(t)$, $k = 1, \ldots, K$ be a basis for $x_i(t)$, $i = 1, \ldots, n$ such that

$$x_i(t) = \sum_{k=1}^{K} \alpha_{ik}\, \phi_k(t) = \boldsymbol{\phi}' \boldsymbol{\alpha}_i$$

with $\boldsymbol{\phi} = (\phi_1(t), \ldots, \phi_K(t))'$ and $\boldsymbol{\alpha}_i = (\alpha_{i1}, \ldots, \alpha_{iK})'$. Let $\psi_l(t)$, $l = 1, \ldots, L$ be a basis for $\beta(t)$ such that

$$\beta(t) = \sum_{l=1}^{L} \gamma_l\, \psi_l(t) = \boldsymbol{\psi}' \boldsymbol{\gamma}$$

with $\boldsymbol{\psi} = (\psi_1(t), \ldots, \psi_L(t))'$ and $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_L)'$. Thus,

$$\begin{aligned} \int \beta(t)\, x(t)\, dt &= \int \boldsymbol{\gamma}' \boldsymbol{\psi}\, \boldsymbol{\phi}' \boldsymbol{\alpha}_i\, dt = \\ &= \boldsymbol{\gamma}' \left(\int \boldsymbol{\psi}\, \boldsymbol{\phi}' dt \right) \boldsymbol{\alpha}_i = \boldsymbol{\gamma}'\, \mathbf{B}\, \boldsymbol{\alpha}_i\,, \end{aligned}$$

where $\mathbf{B} = (b_{ij})_{L \times K}$ and $b_{ij} = \int \psi_i(t)\, \phi_j(t)\, dt$. Thus, regression model (1) turns to

$$y_i = \beta_0 + \boldsymbol{\alpha}_i' \mathbf{B}' \boldsymbol{\gamma}\,. \tag{2}$$

This yields classic linear regression with design matrix $\mathbf{X} = (\mathbf{1}\ \mathbf{AB}')$, where the ith row of $\mathbf{A}$ is $\boldsymbol{\alpha}_i'$ and $\mathbf{1}$ is a vector of ones to account for the intercept. The solution of (2) is $(\beta_0, \boldsymbol{\gamma}')' = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$, where $\mathbf{y} = (y_1, \ldots, y_n)$.

2.2 Data Representation

The functions $x_i(t)$, $i = 1, \ldots, n$, are known only for a given set of arguments, $t_j \in \mathbb{R}$, $j = 1, \ldots, p$. These arguments need not be equal for all functions. Similar to [23], the observed values are assumed to be $z_{ij} = x_i(t_j) + \varepsilon_{ij}$, i.e. the function values contain some noise ε_{ij} with $\mathrm{E}(\varepsilon_{ij}) = 0$, $i = 1, \ldots, n; j = 1, \ldots, p$. Using a basis representation $x_i(t) = \sum_{k=1}^{K} \alpha_{ik}\phi_k(t)$, the functions $x_i(t)$ can easily be determined by least squares estimation, i.e. the coefficients α_{ik} are found from minimizing

$$\sum_{j=1}^{m} \left(z_{ij} - \sum_{k=1}^{K} \alpha_{ik}\phi_k(t_j) \right)^2 = (\mathbf{z}_i - \Phi\boldsymbol{\alpha}_i)'(\mathbf{z}_i - \Phi\boldsymbol{\alpha}_i),$$

where $\Phi = (\Phi_{jk})$ is a $p \times K$ matrix with $\Phi_{jk} = \phi_k(t_j)$, $\mathbf{z}_i = (z_{i1}, \ldots, z_{ip})'$. To avoid overfitting penalized regression might be carried out. For further reading cf [26, p. 86]. The estimated functions then are

$$x_i(t) = \sum_{k=1}^{K} \hat{\alpha}_{ik}\phi_k(t) = \boldsymbol{\phi}'\hat{\boldsymbol{\alpha}}_i, \tag{3}$$

where $\hat{\boldsymbol{\alpha}}_i = (\Phi'\Phi)^{-1}\Phi'\mathbf{z}_i$, and $\boldsymbol{\phi} = (\phi_1(t), \ldots, \phi_K(t))'$.

2.3 Basis

The choice of an appropriate basis is crucial. The basis should allow approximating the functions observed arbitrarily well [26, p. 43]. In particular, they should be able

ISBN: 978-988-18210-8-9
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

to mirror local behaviour of the functions and not require too many resources. Moreover, an easy handling is highly desirable. Wavelets are well appropriate to model local behaviour, but they are very complex and transforms require much time. B-splines have convenient local properties due to their finite support, but they are not orthonormal like wavelets. However, they can be calculated easily and rapidly. Calculation of the basis transform is also less time-consuming than that of a wavelet transform. Derivatives and integrals of B-splines can easily be obtained due to their polynomial structure. Thus, the spectra are represented by means of B-splines in the present analysis.

2.4 Multivariate Functional Regression

Using a basis representation, model (2) can easily be extended to multivariate responses $\mathbf{y}_i = (y_{i1}, \ldots, y_{iq})$ such that

$$y_{is} = \beta_{0s} + \int \beta_s(t)\, x_i(t)\, dt = \boldsymbol{\gamma_s}'\mathbf{B}\,\boldsymbol{\alpha}_i\,,$$

where $\mathbf{B}$ and $\boldsymbol{\alpha}_i$ are defined as in section 2.1, and $\boldsymbol{\gamma}_s = (\gamma_{s1}, \ldots, \gamma_{sL})$, $s = 1, \ldots, q$ are the coefficients of the basis representation of the regression functions $\beta_s(t)$, i.e. $\beta_s(t) = \sum_{l=1}^{L} \gamma_{sl}\, \psi_l(t) = \boldsymbol{\psi}'\boldsymbol{\gamma}_s$. The coefficients are found from

$$\mathbf{G} = (\boldsymbol{\beta}_0, \boldsymbol{\Gamma}')' = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}\,, \qquad (4)$$

where $\boldsymbol{\beta}_0 = (\beta_{01}, \ldots, \beta_{0q})'$, the design matrix is defined as in section 2.1, and $\boldsymbol{\Gamma}$ is an $L \times q$ matrix whose columns are $\boldsymbol{\gamma}_s$, $s = 1, \ldots, q$. $\mathbf{Y}$ is the $n \times q$ response matrix whose ith row is $\mathbf{y}_i = (y_{i1}, \ldots, y_{iq})$,

For classification problems the response vector is obtained from the vector of class labels by means of a dummy variable approach. The ith response vector $\mathbf{y}_i$ consists of zeros except at position s if the ith sample belongs to class s.

Several steps are necessary to estimate the class label c of a new sample $x_N(t)$: First, the basis coefficients $\hat{\boldsymbol{\alpha}}_s$ are determined by least squares estimation from the discretized function $\mathbf{z}_N = (z_{N1}, \ldots, z_{Np})'$ similar to (3) by $\hat{\boldsymbol{\alpha}}_N = (\Phi'\Phi)^{-1}\Phi'\mathbf{z}_N$. Second, the predictor is found from $\mathbf{x} = (1\ \hat{\boldsymbol{\alpha}}_N n'\mathbf{B}')$, which yields $\hat{\mathbf{y}} = \mathbf{x}\,\mathbf{G}$ using (4). Finally, the class label is predicted from $\hat{c} = \arg\max \hat{\mathbf{y}}$.

3 Support Vector Machines

Support vector classification is based on finding a separating hyperplane such that the margin between two groups is a maximum. In the two-group linear classification problem with class labels $y \in \{-1, 1\}$, a function $f(\boldsymbol{x}) = \beta_0 + \boldsymbol{\beta}'\boldsymbol{x}$ with the associated classifier $c(\boldsymbol{x}) = \text{sign}[f(\boldsymbol{x})]$ is to be estimated from n training pairs $(\boldsymbol{x}_i, y_i) \in \mathbb{R}^p \times \{-1, 1\}$ by solving

$$\min_{\beta_0, \boldsymbol{\beta}} \frac{1}{2}||\boldsymbol{\beta}\,||^2 + C\sum_{i=1}^{n}\xi_i$$
$$\text{s.t. } y_i(\beta_0 + \boldsymbol{\beta}'\,\boldsymbol{x}_i) \geq 1 - \xi_i, \quad (i = 1, \ldots, n)$$

where C is a cost parameter chosen by the user. The larger the values of C, the higher the penalty to errors.

Different approaches exist to address the multiple class problem: margin tree support vector machines [31] or a one-against-one approach combined with majority voting [22]. Based on the margin $M(i,j) = 2||\boldsymbol{\beta}||^{-1}$ between the classes i and j, the classes are partitioned into two groups, G_1 and G_2. The classifier is designed to separate these two groups. Various ways exist to find the partition of the classes. Complete linkage clustering chooses the partition $P = \{G_1, G_2\}$ with the largest margin M_0, i.e.

$$\max M(i,j) \leq M_0 \text{ for } i,j \in G_k,\ k = 1,2$$
$$\max M(i,j) \geq M_0 \text{ for } i \in G_1, j \in G_2$$

It yields more balanced trees than single linkage clustering [31, p. 640].

4 Description of the Data

For 12 different rock types and varients that are of worldwide economic importance ten particles per class were selected and irradiated with visible and near infrared light. Depending on the sample size, 1 to 3 measurements were carried out from different postitions. Altogether, 313 spectra were collected. The measurements were made in reflectance mode from 338 nm to 1100 nm. In the present analysis only the region from 385 nm to 981 nm is considered. The measurements were done with regard to control of optical geometries to attain both reproducibility and optimal inclusion of the variations of the rock surface. Table 1 gives an overview of the rock types and variants, their origin and some of their properties.

5 Results

In the present analysis the B-spline basis for the spectra consists of 200 basis functions of order 4. The regression functions are represented by 50 B-spline basis functions of order 4. Order and number of the bases as well as the cost parameter and the kernel for support vector classification are selected by 5-fold cross-validation to minimize classification error. Thus, support vector machines use a linear kernel. Classification performance is assessed by the level of classification error and by the time required for training and testing using 5-fold cross validation and 50 runs.

Figure 1 dipicts the data and classification results. Figure 1(a) shows the mean curves derived from 1 to 3 measurements of 10 particles per rock type. On average, multivariate functional regression yields smaller classification

ISBN: 978-988-18210-8-9
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)

Table 1: Rock type of samples and their characteristics

Rock type	Place name, country code	Grading [mm]	Porosity	Number
Igneous rocks				
Plutonic Rocks				
Granite	Ingå, FI	8/16	Dense	10
Gabbro	Dean, GB	6/10	Dense	31
Extrusive igneous rocks (volcanics)				
Rhyolite	Glera, IS	8/16	Dense	10
Andesite	Zagaj, SI	8/16	Dense	25
Dacite	Korce, AL	8/16	Dense	36
Basalt	Kloech, AT	8/16	5%	15
Sedimentary rocks				
Chemical and biogenic rocks				
Limestone	Griza, SI	8/16	Dense	31
Dolomite	Paka, SI	8/16	5%	30
Chert	Mirna, SI	8/16	Dense	34
Metamorphic rocks				
Amphibolite	Siilinjarvi, FI	8/16	Dense	30
Gneiss	Josidpol, SI	8/16	Dense	30
Serpentinite	Bistrica, SI	8/16	Dense	31

error than support verctor machines applied to the basis coefficients, which can be seen from Figure 1(b). Mean classification errors are 0.0452 and 0.0534 for multivariate functional regression and support vector classification, respectively. According to a sign test, classification error of multivariate functional regression is significantly smaller than of margin tree support vector machines (p-value $9.2477 \cdot 10^{-6}$).

Table 2: Classification error of 50 simulation for multivariate functional regression (FMreg). Pairwise SVM (pSVM), margin tree SVM (SVM) and multivariate Regression (Mreg) are applied to the coefficients of basis representation.

	pSVM	FMreg	SVM	Mreg
Mean	0.0873	0.0452	0.0534	0.1898
Std	0.0125	0.0063	0.0081	0.0196
Min	0.0607	0.0319	0.0319	0.1534
Max	0.1214	0.0575	0.0671	0.2492

Table 3: Average training and testing time of 50 simulation for multivariate functional regression (FMreg) and margin tree SVM (SVM) applied to the coefficients of basis representation.

	Training		Testing	
	FMreg	SVM	FMreg	SVM
Mean	0.0076	0.3154	0.0033	0.0907
Std	0.0100	0.0246	0.0063	0.0090
Min	0.0000	0.2726	0.0000	0.0728
Max	0.0377	0.3692	0.0260	0.1242

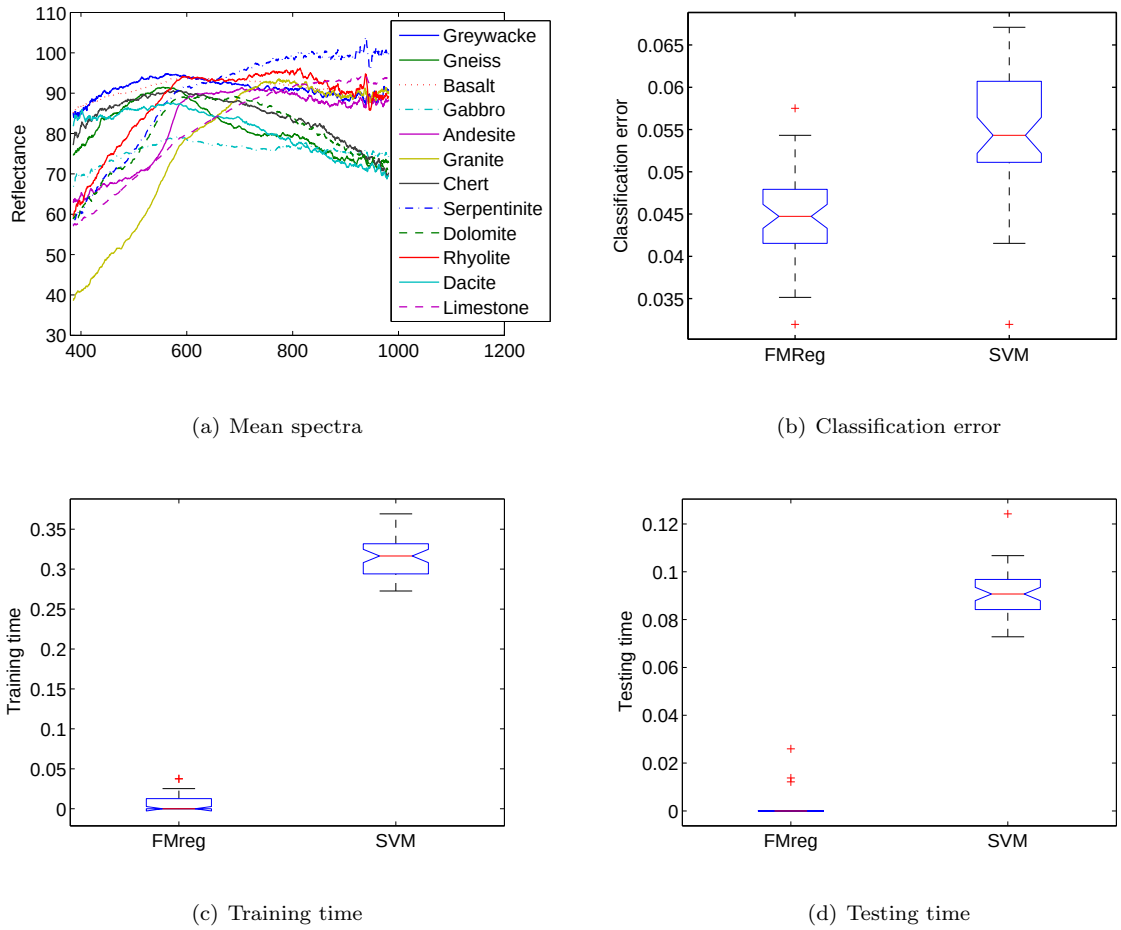
Table 2 summarizes statistics of classification error obtained from 50 runs of 5-fold cross validation. To show that multivariate regression need not yield low error rates, Table 2 also gives classification error for multivariate regression on the coefficients of the B-spline basis representation of the spectra. Also, it shows that the worse performance of margin tree support vector machines compared to multivariate functional regression is not caused by the decision tree since pairwise support vector machines yield even worse results.

The boxplots in Figures 1(c) and 1(d) indicate that multivariate functional regression is not only much faster in training but also in testing than support vector classification, which is particularly important for time critical decision. Table 3 summarizes the statistics of training and testing time. A two-sided sign test confirms that training time (p-value $1.7764 \cdot 10^{-15}$) and testing time (p-value $1.7764 \cdot 10^{-15}$) are significantly smaller for multivariate functional regression than for support vector machines. However, it has to be mentioned that pairwise support vector machines even need significantly more time in training (p-value 0.0066) and testing (p-value $1.7764 \cdot 10^{-15}$) than margin tree support vector machines.

6 Conclusion

Functional data not automatically justify the use of complex classification techniques such as support vector machines. In some applications extending common multivariate methods to functional data suffices not only in regards to classification error but also and mainly to reduce training and testing time and keep software as sparse as possible. This is demonstrated impressivly using data from aggregates industry that wants for statistical classification of 12 different rock classes and variants by means of visible and near infrared reflectance spectra. The rock

ISBN: 978-988-18210-8-9
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)



(a) Mean spectra

(b) Classification error

(c) Training time

(d) Testing time

Figure 1: Mean spectra from 385 nm to 981 nm for 12 rock types.

samples cover rock types that are of worldwide economic importance and used for aggregates. Multivariate functional regression beats support vector machines not only in classification error but also in time requirements for training and testing. This facilitates the development of a simple and fast classification code.

7 Acknowledgements

Special thank goes to Throrgeir S. Helgason from Petromodel ehf. in Reykjavik, Iceland for his idea to analyse aggregates statistically, for lauching the EUREKA PETROSCOPE project and for managing sampling and providing the data. Thanks also goes to Ana Mladenovic at ZAG Ljubljana, Andrew Nevitt at RMC Materials Ltd (now CEMEX UK Operations Ltd), Hanna Järvenpää Lohja Rudus Oy, FI, Karsten Iversen at Linuhoennun hf, Iceland, for time consuming sampling and analyses of the samples. Finally, thank goes to John Knight at Knight Photonics Ltd., UK, for his useful comments at the final stage of the work.

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ISBN: 978-988-18210-8-9
ISSN: 2078-0958 (Print); ISSN: 2078-0966 (Online)