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An exploratory penalized regression to identify combined effects of functional variables - Application to agri-environmental issues

Girault Gnanguenon Guesse^a, Patrice Loisel^a, Bénédicte Fontez^{a,*}, Thierry Simonneau^b, Nadine Hilgert^a

^aMISTEA, Université Montpellier, INRAE, Institut Agro, Montpellier, France

^bLEPSE, Université Montpellier, INRAE, Institut Agro, Montpellier, France

Abstract

Crop production is affected by a complex combination of agri-environmental dynamics, as temperature, irradiance, for example. To learn on these complex influences, the development of sensors in agriculture opens new avenues. This requires renewing statistical approaches to take into account the joint variations of these dynamic variables, which are considered here as functional variables. The objective of the paper is to infer an interpretable model to study the joint influence of two functional inputs on a scalar output. We propose a Sparse and Structured Procedure to Identify Combined Effects of Functional Predictors, denoted SPICEFP. It is based on a transformation of both functional variables into categorical variables by defining joint modalities, from which we derived a collection of multiple regression models, where the regressors are the frequencies associated to the joint class intervals. Selection of class intervals and related regression coefficients are performed through a Generalized Fused Lasso. SPICEFP is a generic and exploratory approach. Simulations performed show that it is flexible enough to select the true ranges of values. A use case in agronomy is also presented.

Keywords: joint distribution, penalized linear regression, information criteria, Generalized Fused Lasso, interpretable coefficient

1. Introduction

Nowadays, several fields of activity and in particular, agriculture, are being revolutionized by the emergence of sensor data. With regard to crops, the setting up of harvest can now be monitored with the aim of including/modeling the influence of multiple environmental conditions. Specifically, water scarcity and temperature increase are two major features which have long been analyzed as determining huge variation in crop yield. Their influences are increasing with climate change and are becoming a major concern for the sustainability of agriculture in many parts of the world. However, relationships between climatic conditions and quality of the harvest are still poorly understood and modeling approaches are still lacking. To better use newly available data from sensors, there is a need for methods able to explore which combination of climatic variables influences harvest quality and at which stage of plant development. Such data sets

*Corresponding author

Email addresses: girault.gnanguenon@gmail.com (Girault Gnanguenon Guesse), patrice.loisel@inrae.fr (Patrice Loisel), benedicte.fontez@supagro.fr (Bénédicte Fontez), thierry.simonneau@inrae.fr (Thierry Simonneau), nadine.hilgert@inrae.fr (Nadine Hilgert)

involve multivariate, longitudinal or temporal data which are handled in various ways, including the large family of functional data analysis [7].

One of the main lines of research on functional data concerns their treatment in regression problems. The regression toolbox is used to extract knowledge from input variables (functional data in our context) to predict and/or explain a scalar output or a continuous variable of interest. Applying directly machine learning and/or supervised learning with its usual black box tools (support-vector machine [5], random forest [22], neural networks [29], etc.) is not indicated in our context: all these black-box tools are based on complex combinations of the regressors whose individual effects are difficult to interpret. In [28, 26], the regression models are usually classified into 3 categories according to the role played by functional data. A distinction is made between the "scalar-on-function", "function-on-scalar" and "function-on-function" regressions. In this paper we will focus on the "scalar-on-function" regression where the response variable is a scalar and the regressors are functions. More precisely, regressors are two functions that jointly influence the response variable.

Various methods exist to solve "scalar-on-function" regressions and the reader can refer to [27] for a review. Regression with functional data often uses pre-treatment of the data like interpolation and/or projection on a basis [26]. This kind of regression is easily implemented (see R-package FDA), but again makes the influence of regressors not easy to interpret. By contrast, the work on "*functional linear regression that's interpretable*" [15] and its Bayesian version [12] open a new research area for functional regressions where interpretation is of major interest. Unfortunately, these models do not take into account a possible combined effect of explanatory variables.

The objective of the present paper is to infer an interpretable model to study the joint influence of two functional inputs on a scalar output. Our approach is based on a transformation of the functional data that implies a change from "scalar-on-function" regression to "scalar-on-image" regression, where the "image" is a bivariate representation of both functional datasets. Scalar-on-image regression models aim to control the smoothness of non-zero estimated coefficients. Different approaches are used to solve scalar-on-image regressions, among which Bayesian approaches [18, 11], total variation penalizing approaches [40], neighborhood taken into account in the selection of variables [19] inspired by the Fused Lasso, etc. [17] proposed an approach based on the Gaussian process and compared it to the Fused Lasso. Other studies on scalar-on-image regressions are inspired, used or compared to models involving different L_1 regularization. Following this trend, we chose to use the fused lasso, and more specifically its implementation via the genlasso package [3], for identifying parsimonious and structured coefficients. The selection of the coefficients is performed using information criteria instead of cross-validation, as proposed in [42].

In the following, we present a Sparse and Structured Procedure to Identify Combined Effects of Functional Predictors, denoted SPICEFP, and its theory. Simulations and a use case based on a real question in agri-environment are also provided.

2. The SPICEFP approach

This section describes the main steps of the approach; first in §2.1, the originality of our approach was to transform both functional variables into categorical variables by defining joint modalities using class intervals (with bins of equal size). Several candidate partitions are defined this way, depending on the choice of the bin size. The functional model is presented in §2.2, from which we derived a linear multiple regression model where the regressors are the frequencies associated to the joint class intervals. As explained in [8], when faced to a high number of discretization points of functional data, the naive approach would be to consider these data as a classical multi-

57 variate sample having as dimension the number of discretization points of the functional variables.
58 In this case, multivariate statistics meets limits, among which its failure to take into account the
59 very strong colinearity existing between discretized variables. By contrast, colinearity can be con-
60 sidered in the Fused Lasso penalized regression which was therefore retained in our approach. We
61 followed a "scalar on image" regression model, where the "image" is a contingency table of the
62 joint class intervals, for a fixed candidate partition, to which we associated a graph of contiguity
63 constraints defined in subsection §2.3. Identification was performed through a Generalized Fused
64 Lasso (see §2.4) using each candidate contingency table as input variables. The selection of the
65 best candidate and of its relative regression coefficients was achieved by minimizing an information
66 criteria. To combine our exploratory objectives with technical constraints (such as potentially a
67 small amount of data, for example), we have favored an iterative approach (see §2.5) which explores
68 a larger space of solutions, while keeping aware of possible slight overestimation.

69 2.1. Transformation of both functional variables

70 Let us consider the samples $(\mathcal{A}_i)_{i=1,\dots,n}$ and $(\mathcal{B}_i)_{i=1,\dots,n}$ of two explanatory functional variables
71 \mathcal{A} and \mathcal{B} , associated to a scalar response variable y with samples $(y_i)_{i=1,\dots,n}$, where n is the number
72 of statistical individuals. Both \mathcal{A} and \mathcal{B} are observed on the same set T containing equidistant
73 observation times. It is assumed that they have no missing values. These practical conditions
74 of use can be released with some pre-treatment of the data (like interpolation, smoothing and
75 imputation), see Section 6 for more details.

76 The requirement for variable transformation is intrinsically linked to the goal of the approach:
77 identify joint class intervals of the explanatory variables that influence the response. The trans-
78 formation requires the definition of joint class intervals which can be used as linear regressors to
79 predict the response. The steps to achieve this transformation are shown in the Figure 2.1.

80

81 *Contingency table of the joint class intervals*

82

83 Let's partition the first explanatory variable \mathcal{A} in $n_{\mathcal{A}}$ class intervals according to a linear scale.
84 This partition generates $n_{\mathcal{A}} + 1$ breaks denoted $L_{\mathcal{A}}(v)$, $v = 1, \dots, n_{\mathcal{A}} + 1$. We chose to have
85 equidistant breaks, as defined in equation (2.1) :

$$L_{\mathcal{A}}(v) = \underline{\mathcal{A}} + \frac{v-1}{n_{\mathcal{A}}} (\bar{\mathcal{A}} - \underline{\mathcal{A}}), \quad v = 1, \dots, n_{\mathcal{A}} + 1 \quad (2.1)$$

86 with $\underline{\mathcal{A}} \in \mathbb{R}$ and $\bar{\mathcal{A}} \in \mathbb{R}$ the minimum and maximum scalar values in \mathcal{A} . The bins used for
87 partitioning all $(\mathcal{A}_i)_{i=1,\dots,n}$ are $I_{\mathcal{A}}(v) = [L_{\mathcal{A}}(v), L_{\mathcal{A}}(v+1)[, v = 1, \dots, n_{\mathcal{A}}$. The partition is the same
88 for all $i, i = 1, \dots, n$. Using the same approach for partitioning the second explanatory variable \mathcal{B} ,
89 we obtain $n_{\mathcal{B}} + 1$ breaks $L_{\mathcal{B}}(w)$. $\underline{\mathcal{B}} \in \mathbb{R}$ and $\bar{\mathcal{B}} \in \mathbb{R}$ are the minimum and maximum scalar values
90 in \mathcal{B} . The bins used for partitioning all $(\mathcal{B}_i)_{i=1,\dots,n}$ are $I_{\mathcal{B}}(w) = [L_{\mathcal{B}}(w), L_{\mathcal{B}}(w+1)[, w = 1, \dots, n_{\mathcal{B}}$.
91 The numbers of class intervals $n_{\mathcal{A}}$ and $n_{\mathcal{B}}$ have to be set to compute the breaks $L_{\mathcal{A}}(v)$ and $L_{\mathcal{B}}(w)$,
92 $v = 1, \dots, n_{\mathcal{A}}, w = 1, \dots, n_{\mathcal{B}}$.

93 Let's define a partition vector $u = (n_{\mathcal{A}}, n_{\mathcal{B}})$. For all i , it is then possible to obtain the frequency
94 bivariate histogram of $(\mathcal{A}_i, \mathcal{B}_i)$ as a contingency table C_i^u , of dimension $n_{\mathcal{A}} \times n_{\mathcal{B}}$, whose components
95 $C_{i,(v,w)}^u$ are obtained through (2.2). The new variables are the joint class intervals, noted $I_{\mathcal{A}}^u(v) \times$
96 $I_{\mathcal{B}}^u(w)$, $v = 1, \dots, n_{\mathcal{A}}, w = 1, \dots, n_{\mathcal{B}}$. They are called joint modalities.

$$C_{i,(v,w)}^u = \sum_{t \in T} \mathbf{1}_{\mathcal{A}_i(t) \in I_{\mathcal{A}}^u(v), \mathcal{B}_i(t) \in I_{\mathcal{B}}^u(w)} = \text{Card} \{t \in T | \mathcal{A}_i(t) \in I_{\mathcal{A}}^u(v), \mathcal{B}_i(t) \in I_{\mathcal{B}}^u(w)\}, \quad (2.2)$$

97 for all $v = 1, \dots, n_A$, $w = 1, \dots, n_B$ and each $u = (n_A, n_B)$, with: $\sum_{v=1}^{n_A} \sum_{w=1}^{n_B} C_{i,(v,w)}^u = \text{Card}(T)$.

98 $C_{i,(v,w)}^u$ is the number of times that the observations of \mathcal{A}_i and \mathcal{B}_i are at the same time in
 99 $I_{\mathcal{A}}^u(v) \times I_{\mathcal{B}}^u(w)$. $C_{i,(v,w)}^u$ can also be interpreted as a discrete approximation of the density of the
 100 time spent by the individual i with variable \mathcal{A} around $L_{\mathcal{A}}(v)$ and variable \mathcal{B} around $L_{\mathcal{B}}(w)$.

101 Part 1 of Figure 2.1 shows the transformation of the functional explanatory variables \mathcal{A} and
 102 \mathcal{B} for the fixed $u = (4, 3)$. Note that, for a fixed u , the $(I_{\mathcal{A}}^u(v) \times I_{\mathcal{B}}^u(w))_{v,w}$ is a collection of 2D
 103 intervals in which the pairs $(\mathcal{A}_i, \mathcal{B}_i)$ will be projected. This is detailed in the following subsection.

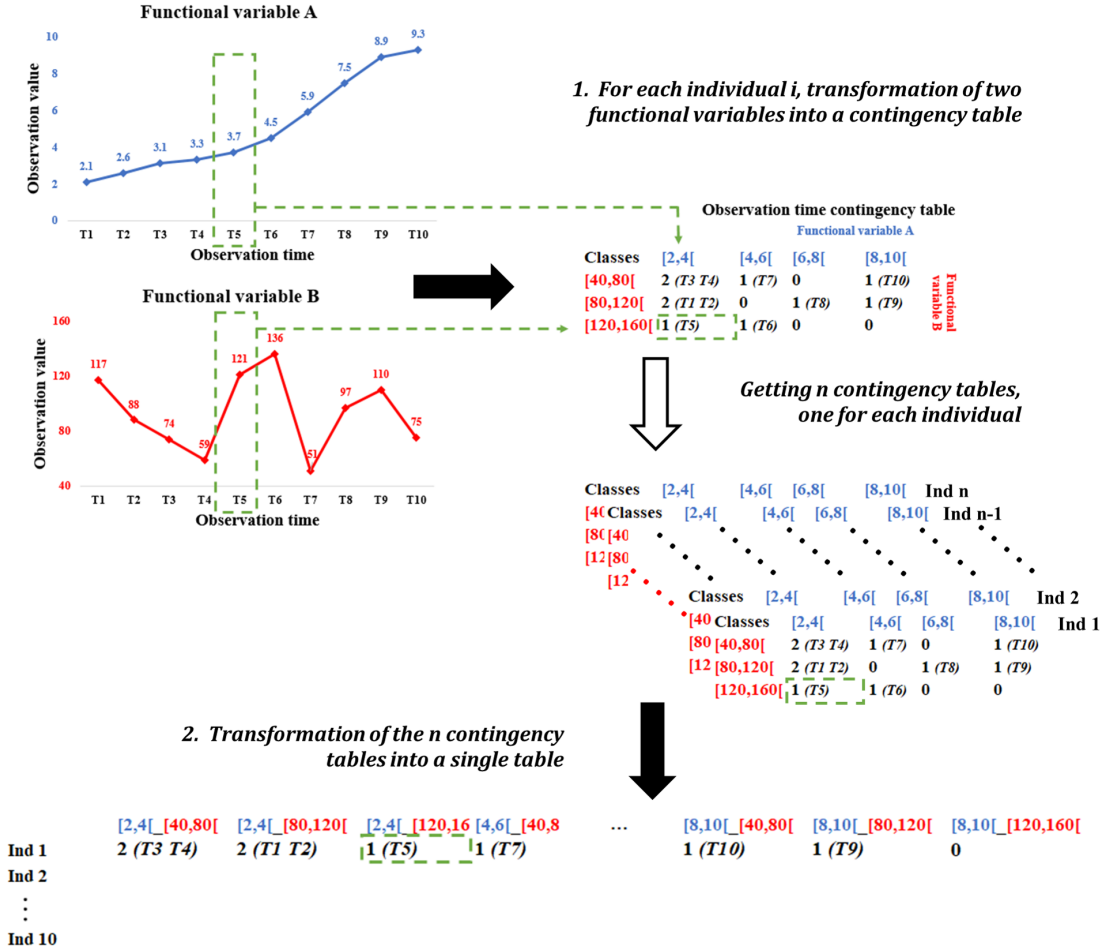


Figure 2.1: Transformation of both functional explanatory variables for the SPICEFP approach

104 2.2. Functional model

The functional model used in the present work can be formulated as follows:

$$y = \int F_{u,\beta}(\mathcal{A}(t), \mathcal{B}(t))dt + \varepsilon \quad (2.3)$$

105 where $F_{u,\beta} = \mathcal{I}^u \cdot \beta$ (scalar product of two vectors), \mathcal{I}^u is a vector of components functions $\mathcal{I}_{v,w}^u$
 106 defined by $\mathcal{I}_{v,w}^u(a, b) = \mathbb{1}_{a \in I_{\mathcal{A}}^u(v), b \in I_{\mathcal{B}}^u(w)}$ for $a \in [\underline{\mathcal{A}}, \bar{\mathcal{A}}]$ and $b \in [\underline{\mathcal{B}}, \bar{\mathcal{B}}]$, and $\beta = (\beta_{(v,w)})_{v,w}$ is the

107 vector of unknown coefficients to estimate. ε is an i.i.d. Gaussian error. Through (2.3), we note
 108 that the relationship between the variable to be explained y and the predictors $\mathcal{A}(\cdot)$ and $\mathcal{B}(\cdot)$ is
 109 stable over time: the function $F_{u,\beta}$ (and thus β) is not time-dependent. It is hence assumed that
 110 certain ranges of cross-values have an influence and that only the time spent in these ranges is
 111 important.

A discrete version of the model (2.3) can be written as follows (up to a constant), for each i :

$$y_i = \sum_{t \in T} F_{u,\beta}(\mathcal{A}_i(t), \mathcal{B}_i(t)) + \varepsilon_i = \sum_{t \in T} \mathcal{I}^u(\mathcal{A}_i(t), \mathcal{B}_i(t)) \cdot \beta + \varepsilon_i,$$

112 which, combined with (2.2), yields $C_{i,(v,w)}^u = \sum_{t \in T} \mathcal{I}_{v,w}^u(\mathcal{A}_i(t), \mathcal{B}_i(t))$ and:

$$y_i = \sum_{v=1}^{n_A} \sum_{w=1}^{n_B} C_{i,(v,w)}^u \beta_{(v,w)}^u + \varepsilon_i \quad (2.4)$$

113 This model is a linear multiple regression model where the regressors are the frequencies associated
 114 to the joint class intervals $(I_{\mathcal{A}}^u(v) \times I_{\mathcal{B}}^u(w))_{v,w}$. The indicator functions $(\mathcal{I}_{v,w}^u)_{v,w}$ define a functional
 115 basis.

116 From the contingency tables C_i^u , we construct the design matrix X^u associated to model (2.4)
 117 as follows. After vectorization (stacking column by column) and transposition of the contingency
 118 table C_i^u (see part 2 of Figure 2.1), we obtain, for a fixed partition vector $u = (n_A, n_B)$, a row
 119 vector of length $n_A \cdot n_B$:

$$X_i^u = {}^t \text{Vect}(C_i^u), \quad X_i^u \in \mathbb{R}^{n_A n_B} \quad (2.5)$$

120 which represents the number of time observations t during which an individual i has been
 121 observed in each of the $n_A \times n_B$ levels described by the joint class intervals. The n stacked row
 122 vectors form the matrix $X^u = {}^t(X_1^u, X_2^u, \dots, X_n^u) \in \mathbb{R}^{n \times n_A n_B}$.

123 2.3. Creation of a graph of contiguity constraints

124 To each matrix X^u corresponds a graph $G^u(V^u, E^u)$, which contains the contiguity constraints
 125 between modalities of the contingency table. V^u represents the columns (new variables) of the
 126 candidate matrix X^u and E^u all the edges connecting two close joint modalities. We used the
 127 Rook's case contiguity rule [24] where two joint modalities are said to be close if the bins following
 128 the variable \mathcal{A} (indexed by v) or (exclusive) the bins following the variable \mathcal{B} (indexed by w) are
 129 consecutive.

130 2.4. Selection of class intervals and related regression coefficients

131 The Fused Lasso is a variant of the Lasso introduced in 2005 by [35], in order to take into
 132 account the existence of a structure in the variables. In its original form, the Fused Lasso aims not
 133 only at parsimony of coefficients but also at parsimony of differences in consecutive coefficients.
 134 This version of the Fused Lasso can be interpreted as a one-dimensional Fused Lasso (1D-Fused
 135 Lasso). The Generalized Fused Lasso (GFL) [41] aims to promote smoothness over neighboring
 136 variables on a general graph $G = (V, E)$ made of V knots and E edges. Each explanatory variable
 137 corresponds to a node on the graph and an edge symbolizes the link between a pair of separate
 138 nodes in G .

139 For a fixed partition vector $u = (n_{\mathcal{A}}, n_{\mathcal{B}})$, the GFL criterion to minimize is written:

$$\frac{1}{2} \sum_{i=1}^n (y_i - X_i^u \beta)^2 + \lambda_p \sum_{j \in V^u} |\beta_j| + \lambda_f \sum_{(j,j') \in E^u} |\beta_j - \beta_{j'}| \quad (2.6)$$

140 with respect to β , where:

- 141 • $\beta = {}^t(\beta_{(1,1)}, \beta_{(2,1)}, \dots, \beta_{(1,2)}, \dots, \beta_{(n_{\mathcal{A}}, n_{\mathcal{B}})}) \in \mathbb{R}^{n_{\mathcal{A}} n_{\mathcal{B}}}$ the unknown coefficients,
- 142 • $\lambda_p \geq 0$ and $\lambda_f > 0$ the regularization parameters (of parsimony and fusion) to be optimized,
- 143 • for $j = (v, w)$ fixed, the couples (j, j') relative to j and contained in E^u are $(j, j')_1 =$
 144 $((v, w), (v + 1, w))$ and $(j, j')_2 = ((v, w), (v, w + 1))$. In the following and depending on the
 145 context, the index j will refer either to the pair (v, w) , or to the j^{th} element of the vector
 146 obtained from the matrix stored by columns.

147 The argmin solution of (2.6), denoted $\widehat{\beta}^u$, is computed as a function of the regularization
 148 parameters λ_p and λ_f , for a fixed value of u .

149 2.4.1. The Generalized Fused Lasso in the Generalized Lasso framework

150 If differences of contiguous coefficients were not penalized in (2.6) (i.e. if λ_f was zero), then the
 151 criterion would reduce to the Lasso criterion presented by [34]. The Lasso minimizes the residual
 152 sum of squares subject to the constraint that the sum of the absolute value of the coefficients
 153 is less than a constant. In this case, there is only one regularization parameter to estimate. [6]
 154 proposed the Least-Angle Regression (LARS) algorithm able to solve the problem for all $\lambda \in [0, \infty[$,
 155 producing a full piece-wise linear solution path. The result of the path algorithm is the finite set of
 156 increasing λ values, where each λ delimits a model reduction dimension (the number of non-zero
 157 β components). Criterion (2.6) has two regularization parameters λ_p and λ_f to be optimized. The
 158 path algorithm is no longer suitable to identify them.

159 Our proposal is to parameterize (2.6) with the ratio:

$$\gamma = \frac{\lambda_p}{\lambda_f} \quad (2.7)$$

160 (choice made in the R package `genlasso` [3] used for implementing `SPICEFP`). This ratio represents
 161 a balance between parsimony and fusion. Then, for a fixed value of γ , criterion (2.6) can be
 162 equivalently rewritten as:

$$\frac{1}{2} \|y - X^u \beta\|_2^2 + \lambda \|D^{u,\gamma} \beta\|_1, \quad (2.8)$$

163 where $y = {}^t(y_1, y_2, \dots, y_n) \in \mathbb{R}^n$ is the response vector and $D^{u,\gamma}$ is a specified penalty matrix
 164 (see below). This model corresponds to the Generalized Lasso model, introduced by [36] as an
 165 encapsulation of statistical models using the L_1 norm to impose additional constraints. Through
 166 this new parametrization, the value of $\lambda = \lambda_f$ can be optimized with the path algorithm and a
 167 corresponding $\widehat{\beta}^{u,\gamma}(\lambda)$ can be estimated. Finally, there are as many pairs $(\lambda, \widehat{\beta}^{u,\gamma}(\lambda))$ solutions as
 168 there are u and γ parameters set. So, several models are available and we have to select one of
 169 them in order to deduce the optimal pair. Selection of the best model is done with an information
 170 criteria which requires an estimation of the degree of freedom for each model. Parameter λ_p will
 171 be deduced from γ through $\lambda_p = \gamma \lambda_f$.

172 In our context, the penalty matrix $D^{u,\gamma}$ is a row-binding of two sub-matrices, namely:

- 173 • $D^{u,\gamma,p} \in \mathbb{R}^{n_{\mathcal{A}}n_{\mathcal{B}} \times n_{\mathcal{A}}n_{\mathcal{B}}}$: the penalty sub-matrix associated to the regularization of parsimony
174 $\left(\lambda_p \sum_{j \in V^u} |\beta_j| \right)$
- 175 • $D^{u,f} \in \mathbb{R}^{2n_{\mathcal{A}}n_{\mathcal{B}} \times n_{\mathcal{A}}n_{\mathcal{B}}}$: the sub-matrix associated to the regularization of the fusion according
176 to the two dimensions $\left(\lambda_f \sum_{(j,j') \in E^u} |\beta_j - \beta_{j'}| \right)$. Affecting two dimensions, $D^{u,f}$ can be
177 subdivided into $D^{u,f1}$ and $D^{u,f2}$.

178 Hence $D^{u,\gamma} = \begin{pmatrix} D^{u,f1} \\ D^{u,f2} \\ D^{u,\gamma,p} \end{pmatrix} \in \mathbb{R}^{3n_{\mathcal{A}}n_{\mathcal{B}} \times n_{\mathcal{A}}n_{\mathcal{B}}}$ with:

$$D^{u,f1}_{(v,w)(v',w')} = \begin{cases} 1 & \text{if } (v', w') = (v + 1, w) \\ -1 & \text{if } (v', w') = (v, w) \text{ and } v < n_{\mathcal{A}} \\ 0 & \text{if not} \end{cases}$$

$$D^{u,f2}_{(v,w)(v',w')} = \begin{cases} 1 & \text{if } (v', w') = (v, w + 1) \\ -1 & \text{if } (v', w') = (v, w) \text{ and } w < n_{\mathcal{B}} \\ 0 & \text{if not} \end{cases} \quad (2.9)$$

$$D^{u,\gamma,p} = \gamma \cdot \mathbb{I}_{n_{\mathcal{A}}n_{\mathcal{B}}}$$

179 where $\gamma \geq 0$ and $\mathbb{I}_{n_{\mathcal{A}}n_{\mathcal{B}}}$ is an identity matrix.

180 The Generalized Fused Lasso presented in criterion (2.6) is a 2 Dimensional - Sparse Fused
181 Lasso (2d-SFL).

182 2.4.2. Degrees of freedom of the Generalized Fused Lasso fit

183 Our approach follows that of [37], who established the calculation of the degree of freedom for
184 any Lasso-type regression written as a generalized Lasso problem as presented in (2.8).

We first introduce some notations. For any penalty matrix $D \in \mathbb{R}^{m \times p}$ involved in a generalized Lasso problem of type (2.8), let \mathcal{S} be the active set corresponding to a particular solution $\hat{\beta}$, it is defined as:

$$\mathcal{S} = \{r \in \{1, \dots, m\} : (D\hat{\beta})_r \neq 0\} = \text{support}(D\hat{\beta}).$$

185 Let $D_{-\mathcal{S}}$ be the matrix D from which were removed the rows indexed by \mathcal{S} . And let $\text{null}(D_{-\mathcal{S}})$ be
186 the null space or kernel of $D_{-\mathcal{S}}$.

187 The calculation of the degrees of freedom of the generalized Lasso fit is stated in [37, Theorem
188 3] and reminded here :

189 **Theorem (Generalized lasso degrees of freedom - Tibshirani and Taylor (2012))**
190 Assume that $y \in \mathbb{R}^n$ follows a normal distribution ($y \sim N(\mu, \sigma^2 I)$ with given (unknown) mean
191 vector $\mu \in \mathbb{R}^n$ and marginal variance σ^2). For any fixed and nonrandom predictor matrix $X \in$
192 $\mathbb{R}^{n \times p}$, penalty matrix $D \in \mathbb{R}^{m \times p}$ and $\lambda \geq 0$, the degree of freedom of the generalized Lasso fit can
193 be expressed as

$$df(X\hat{\beta}) = E[\dim(X(\text{null}(D_{-\mathcal{S}})))] \quad (2.10)$$

194 with $\mathcal{S} = \mathcal{S}(y)$ the active set corresponding to any generalized Lasso solution $\hat{\beta}(y)$ at y .

195
 196 The notation $X(V)$ represents the image space of a subspace V by X . It is the space generated
 197 by the columns of the X matrix projected on V . The assumptions required for this Theorem are
 198 those usually made in regression estimations (Gaussian i.i.d. errors). No assumptions are made
 199 on matrix D nor on X . This result can thus be applied to the 2d-Sparse Fused Lasso constraint.
 200 To compute $df(X^u \hat{\beta}^{u,\gamma})$, we need $\beta^{u,\gamma}$, X^u , $D^{u,\gamma}$, λ defined in (2.8) and γ in (2.7). Note that, in
 201 our context, $m = 3n_{\mathcal{A}}n_{\mathcal{B}}$ the number of rows in $D^{u,\gamma}$ and $p = n_{\mathcal{A}}n_{\mathcal{B}}$ the number of columns in X^u .

202 With fused lasso constraints, we are interested in sets of parameters that share the same value.
 203 By this, we refer to connected components, which are illustrated on Figure 2.4.2 and defined as
 204 follows:

205 **Definition 2.1.** A **connected component** cc is a set of indexes of non zero coefficients $\beta_{v,w}^{u,\gamma}$ that
 206 are linked together via the $D^{u,\gamma}$ matrix (2.9) and that all share the same real value.

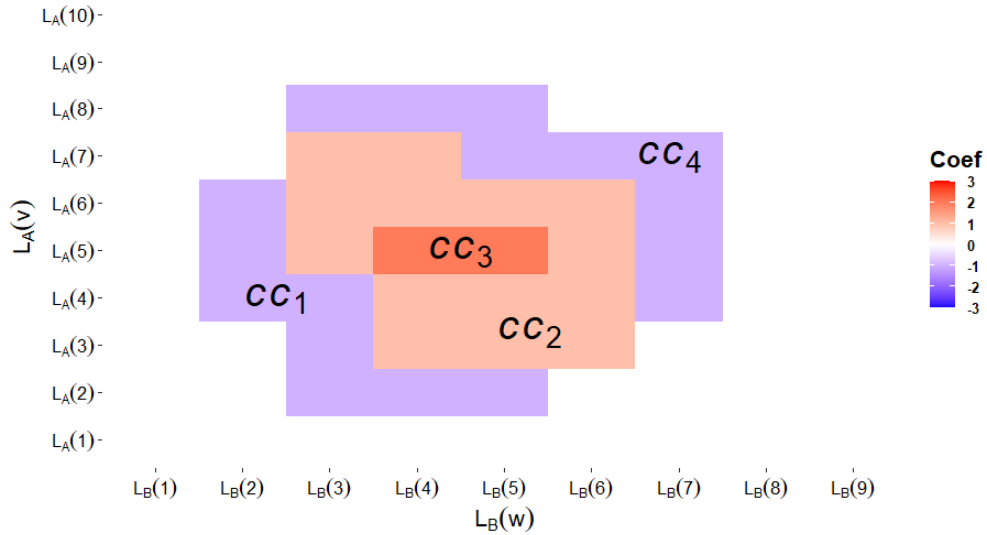


Figure 2.2: Example of $\beta^{u,\gamma}$ coefficient values with 4 connected components (here $u = (9, 8)$).

207 Two coefficients $\beta_{v,w}^{u,\gamma}$ and $\beta_{v',w'}^{u,\gamma}$ are linked via the $D^{u,\gamma}$ matrix if and only if $|v' - v| = 1$ or
 208 (exclusive) $|w' - w| = 1$ (i.e., if and only if $|v' - v| + |w' - w| = 1$). Let us consider that the
 209 estimated coefficient $\hat{\beta}^{u,\gamma}$ contains $Q^{u,\gamma}$ connected components denoted cc_q , $q = 1, 2, \dots, Q^{u,\gamma}$. In
 210 order to identify the respective coefficients involved in each non-zero connected component, we
 211 introduce the matrix Θ through Definition 2.2.

212 **Definition 2.2.** Let $(cc_q)_{q=1,\dots,Q}$ be a set of connected components. The **connected component**
 213 **membership matrix** is a binary matrix $\Theta \in \mathbb{R}^{n_{\mathcal{A}}n_{\mathcal{B}} \times Q}$ whose q -th column $\Theta^{(q)}$ indicates the
 214 membership or not of the $\hat{\beta}^{u,\gamma}$ components to the connected component cc_q , as follows:

$$\forall j = 1, \dots, n_{\mathcal{A}}n_{\mathcal{B}}, \Theta_j^{(q)} = \begin{cases} 0 & \text{if } j \notin cc_q \\ 1 & \text{if } j \in cc_q \end{cases}, q = 1, \dots, Q. \quad (2.11)$$

215 Let's now compute the null space of $D_{-\mathcal{S}}$, denoted $null(D_{-\mathcal{S}})$:

$$null(D_{-\mathcal{S}}) = \{\Theta \in \mathbb{R}^{n_{\mathcal{A}}n_{\mathcal{B}} \times Q} | D_{-\mathcal{S}}\Theta^{(q)} = 0_{(m-s)}, q = 1, \dots, Q\} \quad (2.12)$$

216 where $D_{-S} \in \mathbb{R}^{(m-s) \times n_{A^B}}$, $D_{-S}\Theta^{(q)} \in \mathbb{R}^{m-s}$ and $s = \text{Card}(S)$.

217 As the $D^{u,\gamma}$ matrix has a simple structure, adapting Theorem 3 of [37] in the context of 2d-
 218 Sparse Fused Lasso is equivalent to looking for the components of $\hat{\beta}^{u,\gamma}$ which have different values.
 219 This is the subject of the next corollary.

220 **Corollary 2.3.** *The degree of freedom $\hat{df}(X\hat{\beta}^{u,\gamma})$ associated to the criterion (2.8) in the context*
 221 *of 2d-Sparse Fused Lasso is equal to the number of connected components $Q^{u,\gamma}$.*

$$\begin{aligned} \text{Proof: } \hat{df}(X\hat{\beta}^{u,\gamma}) &= \dim(X^u(\text{null}(D_{-S}^{u,\gamma}))) = \dim(X^u(\Theta)) \\ &= \dim(\text{Vect}\{X^u\Theta^{(q)}, q = 1, \dots, Q^{u,\gamma}\}) = \text{rank}([X^u\Theta^{(1)}, \dots, X^u\Theta^{(Q^{u,\gamma})}]) = Q^{u,\gamma} \end{aligned}$$

222 where we omitted Θ dependencies on u and γ to lighten the notations in the corollary.

223 2.4.3. Choice of the best candidate matrix and selection of its variables

224 SPICEFP requires the construction of different candidate explanatory matrices X^u from both
 225 functional variables and partition's vector u . Constructing a GFL for a matrix of predictors
 226 associated to a fixed u requires identifying the optimal values of the penalty parameters: λ and γ in
 227 (2.8). In penalized regressions, cross-validation is often used to optimize regularization parameters,
 228 but it is time consuming. We suggest using an information criterion to achieve the same purpose
 229 [9]. To that aim, we computed an adapted information criterion for each model indexed by u , λ
 230 and γ . The best model is obtained by minimizing the information criterion chosen, which yields
 231 the best partition \hat{u} and allows to select the best variables from $X^{\hat{u}}$. The variable selection is done
 232 through the selection of $\hat{\gamma}$ and $\hat{\lambda}$ and the associated non-zero $\hat{\beta}$ components are deduced.

233 There exist various information criteria including Akaike Information Criterion (AIC) [2] and
 234 Bayesian Information Criterion (BIC) [31]. These criteria penalize log-likelihood by the number of
 235 model parameters. The BIC also penalizes log-likelihood by the sample size. A well defined penal-
 236 ization is essential to compare regression models involving different explanatory matrices. These
 237 information criteria require computing the degree of freedom $Q^{u,\gamma}$ of the GFL model, obtained in
 238 Corollary 2.3.

239 For each u and γ defined on respective grids (given by the users) and λ taken from the set
 240 $(\lambda_e)_{e=1, \dots, N_\lambda}$ delivered by the path algorithm, we considered the following information criteria:

- 241 • $AIC_e^{u,\gamma} = -2 \log(L_e^{u,\gamma}) + 2Q_e^{u,\gamma}$
- 242 • $BIC_e^{u,\gamma} = -2 \log(L_e^{u,\gamma}) + \log(n)Q_e^{u,\gamma}$

with $L_e^{u,\gamma}$ the likelihood function of the following model: $y = X^u\beta_e^{u,\gamma} + \varepsilon$ with $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$,
 associated with criterion (2.8). We have:

$$-2 \log(L_e^{u,\gamma}) = 2n \log(\sigma) + n \log(2\pi) + \frac{1}{\sigma^2} \|y - X^u\beta_e^{u,\gamma}\|_2^2$$

243 where the variance of the residuals σ^2 is unknown. As mentioned by [14], the same variance
 244 estimator must be used in the calculation of the criteria for all the constructed models, and at
 245 each iteration (see bellow). We thus decided to estimate σ^2 by the variance of the response variable:
 246 $\hat{\sigma}^2 = \frac{1}{n-1} \|y - \bar{y}\|_2^2$. It's a biased estimator of σ^2 , but this bias remains fixed for all models compared
 247 [14]. Such an estimator leads to an overestimation of the variance, which penalizes the introduction
 248 of new coefficients in the model. This bias can be partly offset by an iterative approach. That's
 249 why we have implemented an iterative algorithm where residuals are used as new response variable
 250 and so on, until shutdown conditions are verified.

251 *2.5. SPICEFP: an iterative approach*

252 To capture all potential non-zero coefficients, one should take a fine partition with values of
 253 n_A and n_B large enough. This could imply a very low or even zero number of points in the joint
 254 class intervals (making the method ineffective) and prohibitively long computation times [20]. As
 255 a trade off between thinness and work-ability we chose to develop an iterative approach to explore
 256 a large space of solutions (that allows addition of different thinness of partition).

257 Data required for the use of SPICEFP are the functional explanatory variables \mathcal{A}_i and \mathcal{B}_i dis-
 258 cretized on a grid T and a response variable y_i with $i = 1, \dots, n$. Other elements are also required
 259 at the input of the algorithm: Γ , a set of positive reals representing γ ratios of regularization pa-
 260 rameters, \mathcal{U}_A and \mathcal{U}_B the sets of numbers of class intervals n_A and n_B , n_λ the selected number of
 261 pairs (among N_λ) $(\lambda, \hat{\beta}^{u,\gamma}(\lambda))$, the information criterion to be used, and K the maximum number
 262 of iterations to explore. The n_λ values of λ are chosen equally spaced on the log scale (see Genlasso
 263 package [3]).

264 SPICEFP constructs for each couple (u, γ) , a matrix of explanatory variables X^u and a penalty
 265 matrix $D^{u,\gamma}$. This first step (line 1 to 13, algorithm 1) is performed only once and the set of
 266 candidate explanatory matrices remains unchanged. The second step (line 14 to 34, algorithm 1)
 267 of the approach is iterative. For each candidate matrix a solution path $(\lambda, \hat{\beta}^{u,\gamma}(\lambda))$ is obtained.
 268 Once the criterion associated with each model is computed, the optimal triplet $(\hat{u}, \hat{\gamma}, \hat{e})$ is the
 269 argument that minimizes $Crit_e^{u,\gamma}$, where e is the index of the solution path-coefficients $(\lambda_e, \hat{\beta}_e^{u,\gamma})$.
 270 $X^{\hat{u}}$, $D^{\hat{u},\hat{\gamma}}$ and $\hat{\beta}_e^{\hat{u},\hat{\gamma}}$ respectively represent the optimal matrices of the explanatory, penalty and
 271 coefficient variables. At each iteration k , we denote $u^k = \hat{u}$ and $\beta^k = \hat{\beta}_e^{\hat{u},\hat{\gamma}}$. SPICEFP then checks
 272 if the selected coefficients according to the criterion $Crit_e^{u,\gamma}$ correspond to a zero vector or if the
 273 maximum number of iterations K is reached. The algorithm is stopped when at least one of these
 274 conditions is verified. When none of these conditions are verified, the residuals of the optimal
 275 model are computed and used as a response variable at the next iteration of the algorithm.

276 The third step (line 35, algorithm 1) gives the final prediction as the sum of all the predictions
 277 obtained at each iteration: $\sum_{k=1}^{k_*} X^{u^k} \beta^k$. The function corresponding to the final prediction can be
 278 written as follows :

$$F_* = \sum_{k=1}^{k_*} F_{u^k, \beta^k} = \sum_{k=1}^{k_*} \mathcal{I}^{u^k} \cdot \beta^k \quad (2.13)$$

279 hence the predicted value is given by: $E(y_i) = \sum_{t \in T} F_*(\mathcal{A}_i(t), \mathcal{B}_i(t))$. We remark that each vector
 280 β^k at each iteration may have different length $\dim(u^k)$.

281 *2.6. Adaptation of SPICEFP to the partitioning of functional variables according to a non-linear*
 282 *scale*

283 A linear partitioning of type (2.1) of the functional variables is not always suitable. Other
 284 types of partitioning may have to be chosen. Assuming for example that functional variable \mathcal{B}
 285 requires a partitioning according to a logarithmic scale, the following breaks can be used instead
 286 of Equation (2.1):

$$L_B(w) = \underline{\mathcal{B}} + \frac{1}{\alpha_B} \left((1 + \alpha_B(\bar{\mathcal{B}} - \underline{\mathcal{B}}))^{\frac{w-1}{n_B}} - 1 \right), w = 1, \dots, n_B + 1, \quad (2.14)$$

287 where parameters $\alpha_B > 0$ and n_B have to be set to determine $L_B(w)$. For a fixed n_B , high α_B value
 288 is related to high proportion of breaks close to $\underline{\mathcal{B}}$ and vice versa. So, two partitioning parameters

```

Input :  $K; \mathcal{U}_A; \mathcal{U}_B; \Gamma; n_\lambda; Crit \in \{AIC, BIC\}$ 
Output:  $k_*, (u^k)_{k \leq k_*}; (\beta^k)_{k \leq k_*}$ 
Data :  $\{y_i, i = 1, \dots, n\}; \{\mathcal{A}_i(t); \mathcal{B}_i(t), i = 1, \dots, n, t \in T\}$ 
1 foreach  $u \in \mathcal{U}_A. \mathcal{U}_B$  do
2   for  $i \leftarrow 1$  to  $n$  do
3     for  $v \leftarrow 1$  to  $n_A$  do
4       for  $w \leftarrow 1$  to  $n_B$  do
5          $C_{i,(v,w)}^u = Card \{t \in T | \mathcal{A}_i(t) \in I_A^u(v), \mathcal{B}_i(t) \in I_B^u(w)\}$ 
6       end
7     end
8      $X^u[i,] = {}^tVect(C_i^u)$ 
9   end
10  foreach  $\gamma \in \Gamma$  do
11    | Construct  $D^{u,\gamma}$  as shown in the equation (2.9)
12  end
13 end
14 for  $k \leftarrow 1$  to  $K$  do
15   foreach  $u \in \mathcal{U}_A. \mathcal{U}_B$  do
16     Center  $y$  and each joint modality in  $X^u$ 
17     foreach  $\gamma \in \Gamma$  do
18       Find the solution path  $\hat{\beta}^{u,\gamma}(\lambda) = \underset{\beta \in \mathbb{R}^{n_A n_B}}{\operatorname{argmin}} \frac{1}{2} \|y - X^u \beta\|_2^2 + \lambda \|D^{u,\gamma} \beta\|_1$ 
19       Select  $n_\lambda$  equally spaced couples  $(\lambda_e, \hat{\beta}_e^{u,\gamma})$  on the log scale with respect to  $\lambda$ 
       over the solution path and compute  $Crit_e^{u,\gamma}$  for  $e = 1 \dots n_\lambda$  :
20        $AIC_e^{u,\gamma} = \frac{1}{\sigma^2} \|y - X^u \hat{\beta}_e^{u,\gamma}\|_2^2 + 2Q_e^{u,\gamma}$  or
21        $BIC_e^{u,\gamma} = \frac{1}{\sigma^2} \|y - X^u \hat{\beta}_e^{u,\gamma}\|_2^2 + \log(n) Q_e^{u,\gamma}$ 
22     end
23   end
24    $(\hat{u}, \hat{\gamma}, \hat{e}) \leftarrow \underset{u \in \mathcal{U}_A \mathcal{U}_B, \gamma \in \Gamma, 1 \leq e \leq n_\lambda}{\operatorname{argmin}} Crit_e^{u,\gamma}$ 
25    $u^k = \hat{u}, \beta^k = \hat{\beta}_{\hat{e}}^{\hat{u}, \hat{\gamma}}$ 
26   if  $\beta^k \neq 0_{n_A n_B}$  then
27      $k_* = k$ 
28     if  $k < K$  then
29        $y \leftarrow y - X^{u^k} \beta^k$ 
30     end
31   else
32     | Leave the loop in  $k$ 
33   end
34 end
35 Construct the result:  $\sum_{k=1}^{k_*} X^{u^k} \beta^k$ 

```

Algorithm 1: SPICEFP algorithm

289 $(n_{\mathcal{B}}$ and $\alpha_{\mathcal{B}}$) should be optimized for partitioning \mathcal{B} . In this case, the partition vector is written
290 $u = (n_{\mathcal{A}}, n_{\mathcal{B}}, \alpha_{\mathcal{B}})$. Let $\mathcal{V}_{\mathcal{B}}$ be the set containing the possible values of $\alpha_{\mathcal{B}}$. $\mathcal{V}_{\mathcal{B}}$ is an additional
291 input to the algorithm. The only change in the core of the algorithm is to replace $u \in \mathcal{U}_{\mathcal{A}}$. $\mathcal{U}_{\mathcal{B}}$ by
292 $u \in \mathcal{U}_{\mathcal{A}}$. $\mathcal{U}_{\mathcal{B}}$. $\mathcal{V}_{\mathcal{B}}$ (lines 1 to 15).

293 Various types of breaks (chosen between Equations (2.1), (2.14) or user-defined) can be used
294 for partitioning explanatory functional variables and the SPICEFP algorithm can be easily adapted.

295 3. Use Case: Grapevine dataset

296 3.1. Data presentation

297 Data were collected during an experiment conducted in a vineyard of the Institut Agro campus
298 at Montpellier in 2014 (Syrah vines). The aim was to study the influence of the micro-climate
299 (temperature, solar irradiation) at the grape level on the anthocyanin content of the berries.
300 Experts in viticulture assume that the accumulation of chemical compounds affecting the quality
301 of the grape berry is jointly influenced by these initial explanatory variables. This assumption is
302 reinforced by results of [33], which underlined that the anthocyanin composition of Merlot grapes
303 was influenced by a complex combined effect of berry temperature and solar irradiation.

304 The experimental plot was made of three rows of vines within the vineyard, each with eight
305 vines equipped with open-top chambers to warm the basis of the plant, and eight under control
306 conditions (without open-top chambers). The chambers were made up of 2 translucent polycar-
307 bonate panels placed on the ground at about 10cm below the bunches on each side of the vines
308 and inclined to form a mini two-pitched greenhouse roof open at its ridge. The greenhouse effect
309 created during the day in the chambers generated a flow of warm air that escaped through the
310 open top, raising the temperature of the bunches by 2 to 3 °C, mimicking global warming. The mi-
311 croclimate at bunch level was recorded through the measurement of temperature and irradiance.
312 According to [38], solar radiation can be characterized by three different quantifiers, including
313 Photosynthetic Photon Flux Density (PPFD), measured in $10^{-6}mol\ m^{-2}\ s^{-1}$. It corresponds to
314 the number of incident photons useful for photosynthesis, received per unit of time on a horizontal
315 surface unit. Rows were roughly oriented south-north, and irradiance was separately measured
316 on bunches located on the east and west side of the row. This measurement system therefore
317 enabled the observation of different modalities of the couple (temperature, irradiance) affecting
318 the grape berries. Temperature and Irradiance were recorded every twelve minutes throughout the
319 maturation period when anthocyanins are known to accumulate.

320 So the experimental design contained: rows $(1, 2, 3) \times 2$ sun exposure orientations (East, West)
321 $\times 16$ vine stocks = 96 "statistical individuals". Anthocyanin contents were measured weekly via the
322 Ferari Index FI_i for each individual i . This is a non-destructive measure of anthocyanin content
323 of the bunches [1]. The objective of our study is to understand how the couple (Temperature,
324 Irradiance) acts on a weekly variation of the Ferari Index ΔFI .

325 Temperature and Irradiance are variables of different natures. Temperature is a variable whose
326 variations are regular enough to be partitioned according to Equation (2.1). The Irradiance variable
327 is partitioned according to (2.14), as explained in the following subsection.

328 3.2. Partitioning of the Irradiance variable

329 Observed on a one-day scale, PPFD increases exponentially from sunrise to a daily peak (ob-
330 servation time t_{max}), decreases until sunset, and remains almost constant until the next sunrise.
331 Irradiance primarily influences plant photosynthesis in a nonlinear way with a maximal reached at
332 high irradiance. Therefore, the Irradiance variable was not partitioned according to a linear scale

333 as proposed by Equation (2.1), but rather according to a logarithmic scale as in Equation (2.14).
 334 The use of logarithmic transformation has consistently been used in the development of models
 335 involving solar radiation [30], [23], [4]. "

336 3.3. Objective

337 The objective of our study was to identify the ranges of temperature and irradiance that jointly
 338 influence or not the accumulation of anthocyanins between sunrise and noon. This study is an
 339 appropriate application framework to test the SPICEFP method.

340 Our study is composed of two parts. First a simulation part is presented in section 4. Temper-
 341 ature and Irradiance, measured during the week of July 17 to 24, 2014, are the input variables of a
 342 model which simulates output variables to be predicted, using two different known β : one with two
 343 distinct patches of coefficients and another with a concentric gradient of coefficients (Table 2, col-
 344 umn 1). This simulation study made it possible to evaluate the functioning and performance of the
 345 SPICEFP algorithm. Second, in section 5, the algorithm was tested on a complete dataset, obtained
 346 from July 24 to August 1, 2014, to understand the effect of Temperature and Irradiance interaction
 347 on ΔFI . Dataset and script are available online at [https://forgemia.inra.fr/exploratory-penalized-](https://forgemia.inra.fr/exploratory-penalized-regression/paper-script-and-data.git)
 348 [regression/paper-script-and-data.git](https://forgemia.inra.fr/exploratory-penalized-regression/paper-script-and-data.git).

349 4. Simulation study

350 We present in this section simulations that help to better understand the SPICEFP character-
 351 istics. Remember that the approach must be able to identify an optimal partition or joint class
 352 intervals used as linear regressors.

353 4.1. Simulation design and SPICEFP setting

354 In order to carry out the simulations, a few steps were required:

- 355 • We considered the observations of temperature (\mathcal{A}) and irradiance (\mathcal{B}) in the Vine dataset
 356 obtained between sunrise and noon during the week of July 17 to 24, 2014.
- 357 • We then arbitrarily set a partition vector $u^0 = (n_{\mathcal{A}} = 17, n_{\mathcal{B}} = 20, \alpha_{\mathcal{B}} = 0.05)$.
- 358 • From \mathcal{A} , \mathcal{B} , and u^0 we constructed X^{u^0} using equations (2.2) and (2.5). X^{u^0} was computed
 359 based on observed data set in order to respect realistic frequencies for the joint class intervals.
- 360 • Based on dimensions of X^{u^0} , we drew coefficients β^{u^0} from a random distribution (values are
 361 available on git@forgemia.inra.fr) and computed the response variable of the simulation:

$$Y = X^{u^0} \beta^{u^0} + \varepsilon \text{ where } \varepsilon \sim \mathcal{N}(0, \sigma_{\varepsilon}^2 I). \quad (4.1)$$

362 After that, we used the SPICEFP approach to make the estimation.

363 In this simulation study, we chose to simulate two different coefficient vectors. They are as
 364 followed:

- 365 • Coefficients β^{u^0} for simulation 1 is made of two distinct patches (column 1, row 1 of the
 366 Table 2). Two noise levels were used and presented in table 1.
- 367 • Coefficients β^{u^0} for simulation 2 is made of a concentric gradient of coefficients (column 1,
 368 row 2 of the Table 2). Two noise levels were also used and presented in Table 1.

Table 1: Noise simulation design

	Low noise	High noise
Simulation 1	$\sigma_\varepsilon = 1.50$ ($\sigma_\varepsilon^2/\sigma_Y^2 = 0.03$)	$\sigma_\varepsilon = 2.5$ ($\sigma_\varepsilon^2/\sigma_Y^2 = 0.08$)
Simulation 2	$\sigma_\varepsilon = 0.25$ ($\sigma_\varepsilon^2/\sigma_Y^2 = 0.01$)	$\sigma_\varepsilon = 1$ ($\sigma_\varepsilon^2/\sigma_Y^2 = 0.14$)

369 We thus generated four simulation datasets (1 matrix $X^{u_0} \times 2$ simulated coefficient vectors \times
370 2 noise levels).

371 The inputs required by the algorithm were as follows:

- 372 • $\mathcal{U}_A = \{15, 16, \dots, 20\}$
- 373 • $\mathcal{U}_B = \{18, 19, \dots, 22\}$
- 374 • $\mathcal{V}_B = \{0.015, 0.05, 0.135, 0.405, 1.215\}$
- 375 • $K = 2$
- 376 • $\Gamma = \{0.0001, 0.05, 0.15, 0.45, 2, 8\}$
- 377 • $n_\lambda = 100$

378 4.2. Simulation results

379 The results of the simulations are presented in Tables 2 to 5 (Tables 4 and 5 are in the appendix).
380 Table 2 is related to the estimated coefficient vectors and Tables 4 and 5 present respectively
381 histograms of the residuals and scatter plots showing the quality of the estimates. For each of the
382 four response variables (one per row), three estimations are provided (columns 3 to 5, Table 2),
383 computed as follows:

- 384 • column 3: at the first iteration, an exploratory matrix X^{u^1} indexed by a partition vector u^1
385 is identified. The estimated coefficient at iteration 1 of SPICEFP is noted β^1 (see algorithm 1,
386 line 25). The estimated response $\hat{Y}^1 = X^{u^1}\beta^1$ and the residuals $\varepsilon^1 = Y - \hat{Y}^1$ are computed.
387 Figures in column 3 provide the visualization of β^1 . For a suitable visualization, the vector
388 of coefficients is transformed into a matrix of dimension $n_A \times n_B$, where n_A et n_B are the
389 numbers of class intervals associated to u^1 .
- 390 • column 4: at the second iteration, an exploratory matrix X^{u^2} indexed by a partition vector
391 u^2 is identified. The estimated coefficient at iteration 2 of SPICEFP is noted β^2 . The response
392 variable used at the second iteration in the model is ε^1 , the residuals obtained at iteration
393 1. The estimated response $\hat{Y}^2 = X^{u^1}\beta^1 + X^{u^2}\beta^2$ and the residuals $\varepsilon^2 = \varepsilon^1 - X^{u^2}\beta^2$ are
394 computed. Figures in column 4 give the visualization of $F(a, b) = F^1(a, b) + F^2(a, b)$ where
395 F is defined as in Equation (2.3). In the case of the visualizations in Table 4, 500 equally
396 spaced values of $a \in [\underline{A}, \bar{A}]$ and 1000 equally spaced values $b \in [\underline{B}, \bar{B}]$ were used.
- 397 • column 5: the results presented in this column are slightly out of the scope of the SPICEFP
398 approach and concerns only the outputs of iteration 1. The idea here is to consider an average
399 of the 1% best models. The best models are defined in the sense of the information criterion.
400 Best coefficients relative to the different partitions available in these 1% best models are
401 identified. Let's assume that there are n_m . They are then indexed by $u^{1,(1)}, u^{1,(2)}, \dots, u^{1,(n_m)}$.
402 The coefficients of interest can be noted $\beta^{1,(1)}, \beta^{1,(2)}, \dots, \beta^{1,(n_m)}$. The estimated response

403 is $\widehat{Y}^{1,(1:n_m)} = \frac{1}{n_m} \sum_{m=1}^{n_m} X^{u^{1,(m)}} \beta^{1,(m)}$. All the selected models have the same weight in the
404 computation of this average. The residuals can be obtained by $\varepsilon^{1,(1:n_m)} = Y - \widehat{Y}^{1,(1:n_m)}$.
405 Figures in column 5 show the visualization of $\frac{1}{n_m} \sum_{m=1}^{n_m} F^{1,(m)}(a, b)$ where $F^{1,(m)}$ is the function
406 related to model coefficients indexed by $u^{1,(m)}$.

407 Black color refers to never-observed joint modalities whereas white color refers to joint modal-
408 ities with null estimated coefficients. The histograms of residuals related to each estimation are
409 presented in Table 4. On top of these histograms, the ratio between the variance of residuals and
410 the variance of response variable are provided. Table 5 shows the goodness of fit of each estimation,
411 by presenting the slope of the regression "predicted versus simulated variables". The closer to 1
412 the slope is and the closer to 0 the ratio of variances is, the better the estimate is.

413 From the estimates provided by the algorithm (Table 2), we notice that SPICEFP effectively
414 identifies the simulated zones of influence and assigns the right color to the coefficients: the graphics
415 show two distinct areas, one with positive coefficients (red area), the other with negative coefficients
416 (blue area). The approach tends to assign the same value (same colour) to groups of estimated
417 coefficients, although with a gradient within the group. This behavior can be explained on the one
418 hand by the Generalized Fused Lasso which penalizes the difference between two related coefficients
419 and on the other hand by the variance estimate used for computing the information criterion. This
420 variance was overestimated, which penalized the introduction of new coefficients into the model.
421 With respect to the noise level contained in the response variable, we note that the more noisy Y
422 is, the more false positives are observed. Looking at the differences in the outputs of iterations 1
423 and 2, we observe that coefficients are added to those previously obtained. These new coefficients
424 lead to improved estimation when the noise is low. When the noise is high, the β estimate of the
425 second iteration has non-zero elements in some areas that are not relevant: for example for high
426 temperature and irradiance values. The average of the 1% best models underestimates, in both
427 simulations, the amplitude of the β values but, in simulation 2, it restores the β support much
428 better than the estimators obtained in iterations 1 or 2.

429 5. Modeling the evolution of a grape berry quality index

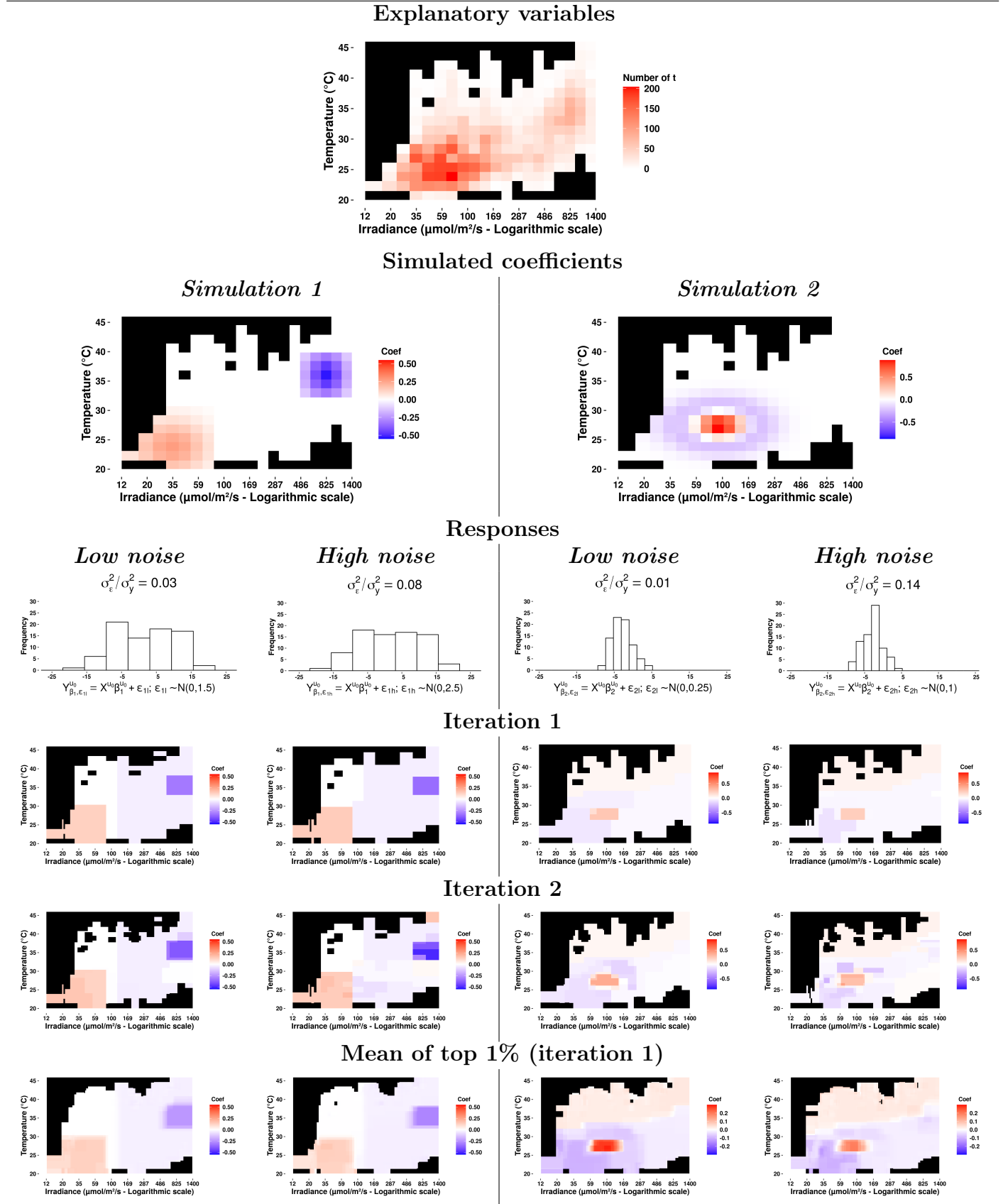
430 5.1. Methodology used for data analysis

431 We focus in this section on the modeling of the Ferari Index variation ΔFI from July 24 to
432 August 1, 2014. We selected the $n_1 = 32$ individuals which have the highest contribution to final
433 Ferari Index, with an initial index around 0.2 at the beginning of the week.

434 Most of the photosynthetic functioning of the grapevine happens in the morning. The time
435 period between sunrise and noon is denoted T_1 below. The following variables and parameters are
436 the input objects of SPICEFP.

- 437 • $y_i = \Delta FI_i, \mathcal{A}_i(t); \mathcal{B}_i(t); i = 1, \dots, n_1; t \in T_1;$
- 438 • $\mathcal{U}_A = \mathcal{U}_B = \{10, 11, 12, \dots, 29, 30\}$
- 439 • 10 values were chosen between 0.0025 and 1 for α based on an exponential function $\alpha \in$
440 $\{0.0025, 0.0048, 0.0094, 0.0183, 0.0357, 0.0695, 0.1353, 0.2636, 0.5134, 1.0000\}$
- 441 • $K = 3$

Table 2: Simulation results: estimation with the SPICEFP algorithm of two coefficient functions β with two types of noise (high and low). ■: Joint modalities that have never been observed.



442 • $\Gamma = \{0.001, 0.01, 0.1, 0.2, 0.4, 0.8, 1.6, 3.2, 6.4, 12.8, 25.6\}$

443 • $n_\lambda = 20$

444 5.2. Results

445 The results are presented in Table 3. The first column shows the estimated coefficients, the
446 second column the histograms of residuals and the last column the scatter plots related to the
447 goodness of fit. For this data set, SPICEFP stopped at the third iteration with a shutdown rule of
448 zero coefficients.

449 The first row of Table 3 contains the results observed at the first iteration of SPICEFP. In terms
450 of model quality, the slope is 0.558 and the residuals follow a normal distribution centered in 0. The
451 visualization of the coefficients indicates conditions (irradiance $< 100 \mu\text{mol m}^{-2} \text{s}^{-1}$, temperature
452 from 15°C to 33°C) that affect negatively the Ferari Index. The second row of Table 3 is relative
453 to the results of the second iteration. Due to the fact that the coefficients retained in iteration 3
454 are all zero, the result of the approach is therefore that of row 2. The slope of model goodness
455 of fit is 0.678 and the residuals follow a normal distribution centered in 0. The visualization of
456 the coefficients indicates, in addition to what is observed at iteration 1, a small positive influence
457 (compared to the amplitude of the negative effect) of the temperature below 30°C for an irradiance
458 higher than $100 \mu\text{mol m}^{-2} \text{s}^{-1}$.

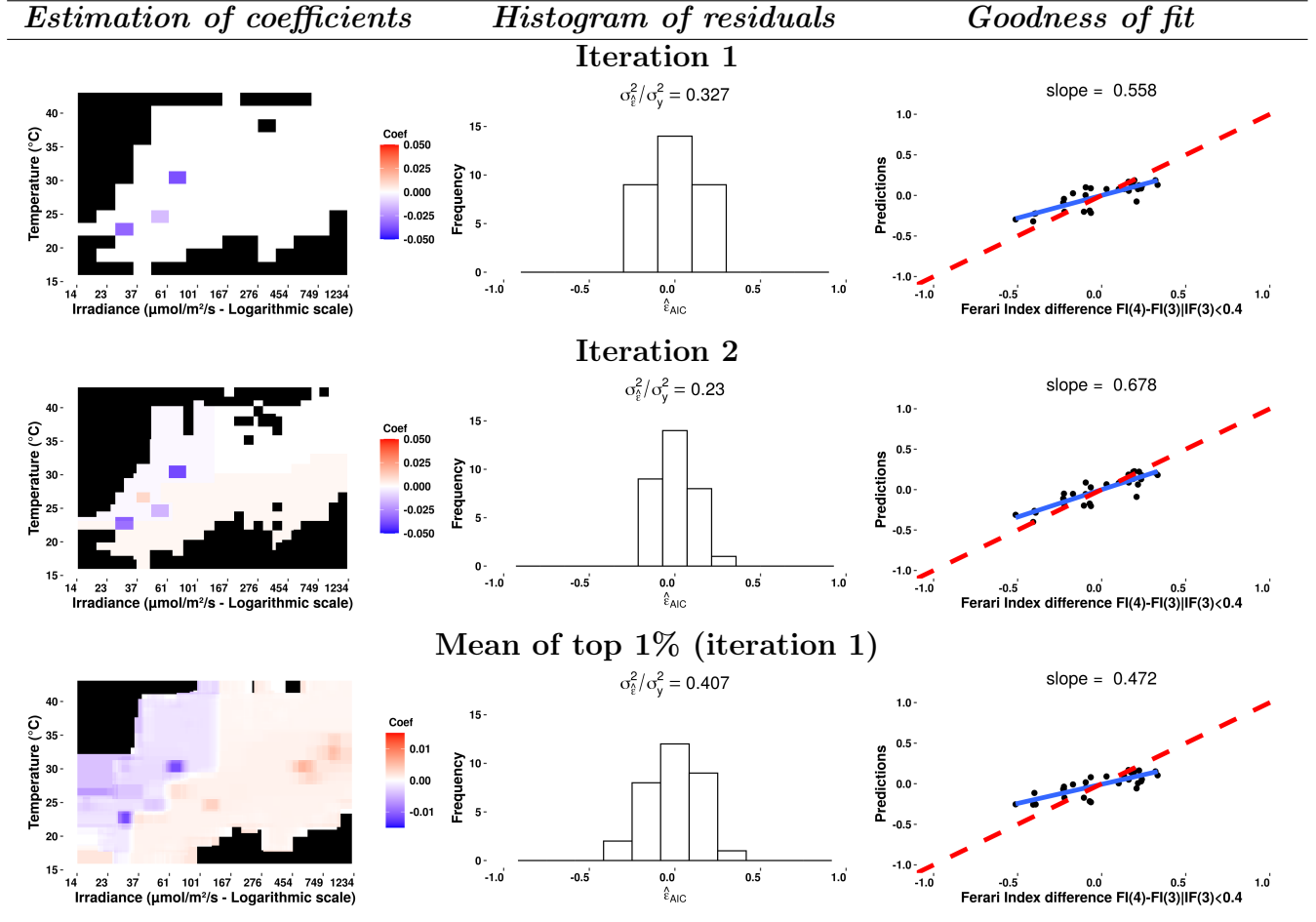
459 When focusing on the average of the 1% best models (presented in the third row), we remark
460 that the quality of this model (as indicated by the slope : 0.472) is not better than that of the
461 models chosen by SPICEFP at iteration 1 or 2. However, it should be noted that the model obtained
462 has more fused coefficients, which allows the identification of a border zone between the positive
463 and negative zones of influence.

464 As an interpretation, we can note that, in the morning (sunrise to noon), for low irradiance
465 values ($< 100 \mu\text{mol m}^{-2} \text{s}^{-1}$), there is a range of temperature values that are not suitable
466 for an increase of the Ferari index. On the contrary, a combination of irradiance values above
467 $150 \mu\text{mol m}^{-2} \text{s}^{-1}$ and temperature below 30°C is suitable for increasing the Ferari index. The
468 average of the coefficients shows, within each of the non-zero zones of influence, a relative variability
469 of the coefficients, suggesting the importance of some temperature and irradiance amplitudes.
470 The slope coefficients of the goodness of fit of the models are away from 1. It should be reminded
471 that the response variable is studied with respect to the variations of temperature and irradiance
472 only between sunrise and twelve. There is also a lot of information hidden in the residuals.

473 6. Discussion

474 The SPICEFP approach is a scalar-on-function approach. The response variable is real and pre-
475 dictors are functional variables. The approach is based on a transformation of functional variables,
476 which yields a contingency table. To construct this table, it is assumed that no data are missing
477 and that the times of observation are identical for both functional variables. The method takes into
478 account the multicollinearity resulting from the auto-correlations existing in the processes. More-
479 over, the constructed candidate explanatory matrices are not nested but they covered the same
480 domain. That's why model and variable selection methods (Fused Lasso, information criterion
481 selection) had to be adapted and generalized to the framework of SPICEFP. In the implementation
482 of the approach, all the candidate explanatory matrices are evaluated at each iteration. This is
483 not due to a re-sampling as is the case for bootstrap or bagging methods, but to the evaluation of
484 different partitions.

Table 3: Visualization of the combined effects of irradiance and temperature on the Ferari index (From sunrise to twelve, ■: joint modalities that have never been observed). Rows 1 and 2 present the results of iterations 1 and 2, respectively. The third row presents the average of the 1% best models obtained at iteration 1.



485 6.1. SPICEFP: a functional approach

486 In recent years, several studies in frequentist and Bayesian statistics, parametric as well as
 487 non-parametric, have focused on functional data analysis. The solutions developed can be used to
 488 achieve a wide range of goals (dimension reduction, regression, clustering, classification, etc.). They
 489 provide models that are predictive but often difficult to interpret. This lack of interpretability is
 490 partly due to the pre-processing step required on the functional data, which must be projected into
 491 bases of functions (splines, kernels...). The transformation of functional variables is a fundamental
 492 step, no matter if the variable is a response variable or a predictor.

493 The SPICEFP approach is primarily explanatory and not necessarily predictive. The first step
 494 is a transformation of the predictors into categorical variables. The choice of this transformation
 495 was motivated by the potential to interpret the results while considering the hypothesis of a joint
 496 influence of the predictors on the response variable. Each partition is a collection of 2D intervals,
 497 see §2.1. We constructed linear regressors on the basis of indicator functions associated to these
 498 2D intervals, see Equation (2.4). This basis of indicator functions is not common compared to
 499 polynomial basis, Fourier basis, wavelet basis, etc., [39]. In a previous work [21], the authors
 500 have focused on multidimensional penalized signal regression, a single surface was estimated with
 501 smooth regression coefficient using B-spline tensor products. In our case, the indicator functions
 502 facilitate the interpretation of the results, provided that both functional predictors (T in grape

503 berry dataset) are discretized over *the same set of equidistant observation times*. This constraint
504 can be released with usual pretreatment such as:

- 505 • imputation of missing data [32, 16]
- 506 • interpolation, smoothing [25] or restriction of the functional variable to an identical set of
507 observation times. Indeed, functions have uncountable supports.

508 The use of 2D class intervals implies also the assumption that the structure of the underlying
509 process does not change over the observation variable (time in the grape berry dataset). This
510 is what we can call *hypothesis of stationarity*. For example, in our use case on grapevine, this
511 hypothesis of stationarity requires to work at the scale of a week but also to split the day (working
512 with observations obtained in the morning (sunrise to noon)). When analyzing the data in section
513 5, we assumed that the underlying process is time-invariant in the mornings of the week under
514 consideration.

515 The method is design-dependent: it will not be able to properly estimate the β coefficient in
516 an area with little or no data. It is therefore necessary to have data of $(\mathcal{A}, \mathcal{B})$ in areas where there
517 is potentially something happening. There is also a limitation due to the curse of dimensionality
518 [10]: "If the number n of observations remains fixed while the dimension p of the observations
519 increases, the observations get rapidly very isolated and local methods cannot work.". The more
520 fluctuations in many directions, the more data will be needed. Our approach will work best if the
521 shapes are simple.

522 6.2. SPICEFP: an iterative approach

523 The SPICEFP approach can be summarized as follows: first, the functional predictors are trans-
524 formed into a set of candidate matrices X^u (and $D^{u,\gamma}$) for each (u, γ) . Then we iterate the following
525 steps: estimation of the coefficients for each of the candidate matrices, evaluation and selection
526 based on the chosen validation information criteria with respect to (u, γ) and then checking of the
527 shutdown conditions. The number of iterations performed is controlled by the shutdown condi-
528 tions. The residuals obtained at iteration k are used as response variable at iteration $k + 1$. This
529 iterative procedure has been implemented in order to:

- 530 • *extract knowledge still available in the residuals with the risk of overestimating the number*
531 *of non-zero coefficients*: This risk is linked to several factors such as:
 - 532 1. *the noise level in the response variable*: the higher the noise level in the response vari-
533 *able, the higher the risk of model misspecification in the SPICEFP approach* [13]. This
534 *situation is well illustrated by the results of the simulations at iteration 2 (row 1 vs row*
535 *2 and row 3 vs row 4, column 4, Table 2).*
 - 536 2. *the shape of the area of influence to be identified*: the number of connected components
537 *to cover the shape increases when the shape is not a combination of rectangles. For a*
538 *shape composed of rectangles of different sizes, the iterative approach allows changing*
539 *the scale of the grid to get a refined estimation.*

540 This tolerance to the overestimation of the coefficients is made in return for the identification
541 of easily interpretable areas of influence. This contributes to the explanatory character of the
542 approach. The number of non-zero coefficients is also related to the value of the γ parameter
543 presented in the Equation (2.7) which controls the ratio between parsimony and fusion of the
544 coefficients. The lower the parameter γ (conditionally to the data), the larger the estimated
545 area of influence. This increases the risk of getting unnecessary /untrue non-zero coefficients.

- *Explore the space of observations by using different partitions/pavements (fine scale, large scale)*: from the second iteration onwards, the candidate matrix selected covers the same space as the previous one, with the difference that it can cover it with different widths. Thus new areas of influence can be identified, or existing ones reinforced, etc. There is therefore no independence between the different candidate matrices because they are all constructed from the observed predictors. Even if the response of the next iteration corresponds to the residuals of the previous iteration, this approach is not orthogonal.

Eventually, the shutdown condition of SPICEFP is rather natural. The approach stops when the vector of coefficients at one iteration is null: in this case, the residuals of the model are equivalent to the response variable. This criterion is internal to the approach.

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662 **Appendix**

663 *Simulation’s residual histogram and quality of the estimate*

Table 4: Histogram of residuals

Simulations		Estimations					
Responses		iter 1	iter 2	Mean of top 1% iter 1			
<p>Irradiance ($\mu\text{mol}/\text{m}^2/\text{s}$ - Logarithmic scale)</p>	$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.03$ $Y_{\beta_1, \epsilon_1} = X^{(1)}\beta_1 + \epsilon_1; \epsilon_1 \sim \text{N}(0, 1.5)$	$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.037$	$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.02$	$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.047$			
	$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.08$ $Y_{\beta_2, \epsilon_2} = X^{(2)}\beta_2 + \epsilon_2; \epsilon_2 \sim \text{N}(0, 2.5)$	$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.06$	$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.039$	$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.073$			
	$\sigma_{\beta_3}^2 / \sigma_y^2 = 0.01$ $Y_{\beta_3, \epsilon_3} = X^{(3)}\beta_3 + \epsilon_3; \epsilon_3 \sim \text{N}(0, 0.25)$	$\sigma_{\beta_3}^2 / \sigma_y^2 = 0.155$	$\sigma_{\beta_3}^2 / \sigma_y^2 = 0.048$	$\sigma_{\beta_3}^2 / \sigma_y^2 = 0.135$			
	$\sigma_{\beta_4}^2 / \sigma_y^2 = 0.14$ $Y_{\beta_4, \epsilon_4} = X^{(4)}\beta_4 + \epsilon_4; \epsilon_4 \sim \text{N}(0, 1)$	$\sigma_{\beta_4}^2 / \sigma_y^2 = 0.212$	$\sigma_{\beta_4}^2 / \sigma_y^2 = 0.063$	$\sigma_{\beta_4}^2 / \sigma_y^2 = 0.241$			
<p>Irradiance ($\mu\text{mol}/\text{m}^2/\text{s}$ - Logarithmic scale)</p>							

■: Joint modalities that have never been observed (no t counted for these joint modalities for all individuals)

Table 5: Quality of the estimate

Simulations	Estimations				
	Responses	iter 1	iter 2	Mean of top 1% iter 1	
<p>Temperature (C)</p> <p>Irradiance ($\mu\text{mol}/\text{m}^2/\text{s}$ - Logarithmic scale)</p>	<p>Frequency</p> <p>$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.03$</p> <p>$Y_{\beta_1, \epsilon_1} = X^{(1)}\beta_1 + \epsilon_1 \epsilon_1 \sim \text{N}(0, 1.5)$</p>	<p>frequency</p> <p>slope = 0.882</p>	<p>frequency</p> <p>slope = 0.972</p>	<p>frequency</p> <p>slope = 0.848</p>	
	<p>Frequency</p> <p>$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.08$</p> <p>$Y_{\beta_2, \epsilon_2} = X^{(2)}\beta_2 + \epsilon_2 \epsilon_2 \sim \text{N}(0, 2.5)$</p>	<p>frequency</p> <p>slope = 0.891</p>	<p>frequency</p> <p>slope = 0.951</p>	<p>frequency</p> <p>slope = 0.836</p>	
	<p>Temperature (C)</p> <p>Irradiance ($\mu\text{mol}/\text{m}^2/\text{s}$ - Logarithmic scale)</p>	<p>Frequency</p> <p>$\sigma_{\beta_1}^2 / \sigma_y^2 = 0.01$</p> <p>$Y_{\beta_1, \epsilon_1} = X^{(1)}\beta_1 + \epsilon_1 \epsilon_1 \sim \text{N}(0, 0.25)$</p>	<p>frequency</p> <p>slope = 0.712</p>	<p>frequency</p> <p>slope = 0.888</p>	<p>frequency</p> <p>slope = 0.726</p>
		<p>Frequency</p> <p>$\sigma_{\beta_2}^2 / \sigma_y^2 = 0.14$</p> <p>$Y_{\beta_2, \epsilon_2} = X^{(2)}\beta_2 + \epsilon_2 \epsilon_2 \sim \text{N}(0, 1)$</p>	<p>frequency</p> <p>slope = 0.68</p>	<p>frequency</p> <p>slope = 0.875</p>	<p>frequency</p> <p>slope = 0.623</p>

■: Joint modalities that have never been observed (no t counted for these joint modalities for all individuals)