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This paper introduces local distance-based generalized linear models. These models extend (weighted) distance-based linear models firstly with the generalized linear model concept, then by localizing. Distances between individuals are the only predictor information needed to fit these models. Therefore they are applicable to mixed (qualitative and quantitative) explanatory variables or when the regressor is of functional type. Models can be fitted and analysed with the R package dbstats, which implements several distance-based prediction methods.

Keywords: Distance-based prediction, Generalized Linear Model, Local Likelihood, Iteratively Weighted Least Squares, R

1. Introduction

Boj, Delicado, and Fortiana (2010) introduced local Distance-Based Linear Model (DB-LM), a nonparametric prediction technique extending (weighted) DB-LM. In the present paper we introduce further extensions. In general, any statistical technique based on

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Weighted Least Squares (WLS) can be adapted to data presented as an inter-individual distances matrix by just replacing each WLS step by the corresponding weighted DB-LM. This procedure is easily extended to Iterative Weighted Least Squares (IWLS), as applied in many statistical methods, ranging from Generalized Linear Models (GLM) McCullagh and Nelder (1989) to Robust Regression (see, for instance, Green (1984), Street, Carroll, and Ruppert (1988)). Here we develop in detail Distance-Based Generalized Linear Models (DB-GLM), then we construct its local version.

The dbstats R package (Boj, Caballé, Delicado, and Fortiana 2012) contains classes and functions implementing distance-based prediction methods such as DB-LM, local DB-LM, DB-GLM, local DB-GLM and Distance-Based Partial Least Squares Regression (DB-PLSR) Boj, Claramunt, Grané, and Fortiana (2007).

The paper is structured as follows: In Section 2.1 we review the main features of DB-LM; in Section 2.2 we develop DB-GLM as an extension of DB-LM; in Section 2.3 we introduce local DB-GLM. In Section 3 we describe the dbstats package for R. Finally, in Section 4, we illustrate the use of dbstats to fit DB-GLM and local DB-GLM with several examples.

2. Distance-Based Prediction

In this section, after recalling the main characteristics of DB-LM, we present DB-GLM and then we show how to construct its local version.

2.1. Distance-Based Linear Model: Definition and results

DB-LM was introduced by Cuadras (1989) and has been developed in Cuadras and Arenas (1990), Cuadras, Arenas, and Fortiana (1996), Boj, Claramunt, and Fortiana (2007), Esteve, Boj, and Fortiana (2009) and Boj, Delicado, and Fortiana (2010). Here we recall its main concepts, as given in these articles, where the reader is referred to for more details and proofs.

A sketchy description of DB-LM is as follows: Let y_i be a real-valued observation for each *i*-th individual Ω_i in a given set $\Omega = {\Omega_1, \ldots, \Omega_n}$, randomly drawn from a population, and let $w_i \in (0, 1)$ be the constant positive weight of Ω_i . The $n \times 1$ weight vector $\boldsymbol{w} = (w_1, \ldots, w_n)'$ is standardized to unit sum, i.e., $\mathbf{1}' \cdot \boldsymbol{w} = 1$, where **1** is the $n \times 1$ vector of ones. We assume that the $n \times 1$ response vector $\boldsymbol{y} = (y_i)$ is \boldsymbol{w} -centered, i.e., $\boldsymbol{w}' \cdot \boldsymbol{y} = 0$.

Individuals in Ω are described by a set \mathbf{Z} of variables, henceforth observed predictors, possibly including both quantitative and qualitative measurements or, possibly, other nonstandard quantities, such as character strings or functions. A distance (metric or semi-metric) $\delta(\cdot, \cdot)$ is defined in Ω , as a function of the \mathbf{Z} variables. We denote by $\boldsymbol{\Delta}$ the $n \times n$ matrix, whose entries are the squared distances $\delta^2(\Omega_i, \Omega_j)$.

We define the $n \times n$ inner-products matrix as:

$$G_{w} = -\frac{1}{2} J_{w} \cdot \Delta \cdot J_{w}',$$

where J_w is the *w*-centering matrix, defined as $J_w = I - 1 \cdot w'$. We denote by g_w a $1 \times n$ row vector containing the (necessarily nonnegative) diagonal entries of G_w .

Any $n \times k$ matrix X_w such that $G_w = X_w \cdot X'_w$ is called a *Euclidean configuration of* Δ . $k \ge r \equiv rank G_w$ and $w' \cdot X_w = 0$.

The DB-LM of response \boldsymbol{y} with weights \boldsymbol{w} and predictor matrix $\boldsymbol{\Delta}$, an $n \times n$ square distances matrix, is defined as the WLS regression of \boldsymbol{y} on a \boldsymbol{w} -centered Euclidean configuration of $\boldsymbol{\Delta}$, $\boldsymbol{X}_{\boldsymbol{w}}$, a *latent Euclidean configuration*.

Assume a new case Ω_{n+1} is available, and we are given the $1 \times n$ vector $\boldsymbol{\delta}_{n+1}$ of squared distances from Ω_{n+1} to the *n* previously known individuals. Ω_{n+1} can be represented as a *k*-vector \boldsymbol{x}_{n+1} in the row space of $\boldsymbol{X}_{\boldsymbol{w}}$. Then, the predicted *Y* for Ω_{n+1} is $\boldsymbol{x}_{n+1} \cdot \hat{\boldsymbol{\beta}}$, where $\hat{\boldsymbol{\beta}}$ is the vector of estimated regression coefficients.

DB-LM does not depend on a specific X_w , since the final quantities are obtained directly from the distances. Usually such a configuration needs not be made explicit, and neither do $\hat{\beta}$ or x_{n+1} . In DB-LM the hat matrix is:

$$\boldsymbol{H}_{\boldsymbol{w}} = \boldsymbol{G}_{\boldsymbol{w}} \cdot \left(\boldsymbol{D}_{\boldsymbol{w}}^{1/2} \cdot \boldsymbol{F}_{\boldsymbol{w}}^{+} \cdot \boldsymbol{D}_{\boldsymbol{w}}^{1/2} \right), \tag{1}$$

where $D_{w} = \text{diag}(w)$ is the diagonal matrix whose diagonal entries are the weights w,

$$oldsymbol{F}_{oldsymbol{w}}=oldsymbol{D}_{oldsymbol{w}}^{1/2}\cdotoldsymbol{G}_{oldsymbol{w}}\cdotoldsymbol{D}_{oldsymbol{w}}^{1/2},$$

and F_w^+ is the Moore-Penrose pseudo-inverse of F_w . Thus, H_w is an intrinsic quantity, meaning that it can be expressed directly as a function of the distances or, equivalently, the inner products.

The predicted Y for a new case Ω_{n+1} , given its δ_{n+1} vector is:

$$\hat{y}_{n+1} = \frac{1}{2} \left(\boldsymbol{g}_{\boldsymbol{w}} - \boldsymbol{\delta}_{n+1} \right) \cdot \left(\boldsymbol{D}_{\boldsymbol{w}}^{1/2} \cdot \boldsymbol{F}_{\boldsymbol{w}}^{+} \cdot \boldsymbol{D}_{\boldsymbol{w}}^{1/2} \right) \cdot \boldsymbol{y}.$$
(2)

In DB-LM the rank r of the hat-matrix in (1), as in an ordinary linear regression, is equal to the number of linearly independent linear predictors. Since for n cases,

depending on the chosen metric, r can be as high as n-1, giving an overparametrized model with unstable predictions, a sensible procedure is to replace the pseudo-inverse F_{w}^{+} with a lower-rank approximation. This can be easily implemented by the Singular Value Decomposition which, by the Schmidt-Eckart-Young Theorem (see, e.g., Stewart (1993)), gives the best ℓ^2 approximation of any given rank $k, 1 \leq k \leq r$. Cross-validation can then be used to select a suitable k.

DB-LM contains WLS as a particular instance: if we start from a $n \times r$ *w*-centered matrix X_w of *r* continuous predictors corresponding to *n* individuals and we define Δ as the matrix of squared Euclidean distances between rows of X_w , then X_w is trivially a Euclidean configuration of Δ , hence the DB-LM hat matrix, response and predictions coincide with the corresponding WLS quantities of ordinary Linear Model (LM).

2.2. Distance-Based Generalized Linear Model

In this section we review the basic concepts and notations of GLM, for the sake of an easy reference. As it is well-known (see, eg., McCullagh and Nelder (1989)), in a GLM we have a linear predictor $\boldsymbol{\eta} = \boldsymbol{X} \cdot \boldsymbol{\beta}$, which is related to the response variable Y by means of a link function $g(\cdot)$, $\boldsymbol{\eta} = g(\boldsymbol{\mu})$, then,

$$\boldsymbol{\mu} = g^{-1}\left(\boldsymbol{\eta}\right). \tag{3}$$

In a GLM it is assumed that each component of the response has a distribution in the exponential family, taking the form:

$$f_Y(\boldsymbol{y};\boldsymbol{\theta},\boldsymbol{\phi}) = \exp\left\{ (\boldsymbol{y}\cdot\boldsymbol{\theta} - b(\boldsymbol{\theta}))/a(\boldsymbol{\phi}) + c(\boldsymbol{y},\boldsymbol{\phi}) \right\},\tag{4}$$

for some specific functions $a(\cdot)$, $b(\cdot)$ and $c(\cdot)$. If ϕ is known, this is an exponential family model with canonical parameter θ .

The log-likelihood function for a GLM is $l(\boldsymbol{\theta}; \boldsymbol{y}) = (\boldsymbol{y} \cdot \boldsymbol{\theta} - b(\boldsymbol{\theta}))/a(\boldsymbol{\phi}) + c(\boldsymbol{y}, \boldsymbol{\phi})$ and the mean and the variance of Y can be derived easily from the relations $E\left(\frac{\partial l}{\partial \boldsymbol{\theta}}\right) = 0$ and $E\left(\frac{\partial^2 l}{\partial \boldsymbol{\theta}^2}\right) + E\left(\frac{\partial l}{\partial \boldsymbol{\theta}}\right)^2 = 0$. From (4) we have that $\frac{\partial l}{\partial \boldsymbol{\theta}} = \{y - b'(\boldsymbol{\theta})\}/a(\boldsymbol{\phi})$ and $\frac{\partial^2 l}{\partial \boldsymbol{\theta}^2} = -b''(\boldsymbol{\theta})/a(\boldsymbol{\phi})$ and then,

$$E(Y) = \boldsymbol{\mu} = b'(\boldsymbol{\theta}), \qquad (5)$$

and

$$var(Y) = b''(\boldsymbol{\theta}) \cdot a(\boldsymbol{\phi}).$$
(6)

The variance of Y is the product of two functions; one, $b''(\theta)$, depends on the canonical parameter only (and hence on the mean (5)) and will be called the *variance function*, while the other is independent of θ and depends only on ϕ . The variance function as a function of μ will be written $V(\mu) = b''(\theta)$. Commonly $a(\phi)$ is of the form $a(\phi) = \phi/w$ and ϕ , the *dispersion parameter*, is constant over observations. Respect w it is a known *prior weight* that varies from observations to observation. If we have n independent readings w = n. Finally, we can write (6) as

$$var(Y) = V(\boldsymbol{\mu}) \cdot \frac{\boldsymbol{\phi}}{\boldsymbol{w}}.$$
(7)

2.2.1. Construction of the Distance-Based Generalized Linear Model

In a GLM the maximum-likelihood estimates of the parameters $\boldsymbol{\beta}$ in the linear predictor $\boldsymbol{\eta}$ can be obtained by IWLS (see, e.g., McCullagh and Nelder (1989) pp. 40-43 or Wood (2006) pp. 63-66 for a more detailed description and justification of the algorithm). In the IWLS the dependent variable of the regression is not \boldsymbol{y} but \boldsymbol{z} , a linearized form of the link function applied to \boldsymbol{y} , and the weights are functions of the fitted values $\hat{\boldsymbol{\mu}}$. The process is iterative because both the adjusted dependent variable \boldsymbol{z} and the weight \boldsymbol{W} depend on the fitted values, for which only current estimates are available. The procedure underlying the iteration is as follows. Let $\hat{\boldsymbol{\eta}}_0$ be the current estimate of the linear predictor, with corresponding fitted value $\hat{\boldsymbol{\mu}}_0$ derived from the link function $\boldsymbol{\eta} = g(\boldsymbol{\mu})$. Form the adjusted dependent variate with typical value

$$\boldsymbol{z}_{0} = \hat{\boldsymbol{\eta}}_{0} + (\boldsymbol{y} - \hat{\boldsymbol{\mu}}_{0}) \cdot \left(\frac{d\boldsymbol{\eta}}{d\boldsymbol{\mu}}\right)_{0}, \qquad (8)$$

where the link derivative is evaluated at $\hat{\mu}_0$. The quadratic weight is defined by:

$$\boldsymbol{W}_{0}^{-1} = \left(\frac{d\boldsymbol{\eta}}{d\boldsymbol{\mu}}\right)_{0}^{2} \cdot \frac{\boldsymbol{V}_{0}}{\boldsymbol{w}},\tag{9}$$

where V_0 is the variance function evaluated at $\hat{\mu}_0$. Now regress z_0 on the covariates with weight W_0 to give new estimates of $\hat{\beta}_1$ of the parameters; from these form a new

estimate $\hat{\eta}_1$ of the linear predictor. Repeat until changes are sufficiently small.

Note that \boldsymbol{z} is just a linearized form of the link function applied to the data, for, to first order, $g(\boldsymbol{y}) \simeq g(\boldsymbol{\mu}) + (\boldsymbol{y} - \boldsymbol{\mu}) \cdot g'(\boldsymbol{\mu})$. The variance of \boldsymbol{z} is \boldsymbol{W}^{-1} (ignoring the dispersion parameter), assuming that $\boldsymbol{\eta}$ and $\boldsymbol{\mu}$ are fixed and known.

Both DB-GLM and DB-LM share the same elements: a set of n individuals with associated weights vector \boldsymbol{w} (standardized to unit sum), for which we have observed the \boldsymbol{w} -centered response vector \boldsymbol{y} and a set of predictors \boldsymbol{Z} . From the latter we calculate the $n \times n$ distances matrix $\boldsymbol{\Delta}$. Just as GLM with respect to LM, DB-GLM differs from DB-LM in two aspects:

- 1. We assume the responses distribution is in an exponential dispersion family (4), as in any GLM.
- 2. The relation between the linear predictor $\eta = X_w \cdot \beta$, obtained from the latent Euclidean configuration X_w , and the response y is given by a link function $g(\cdot)$ as in (3).

Then we have an underlying GLM, with link function $g: C(Supp(Y)) \to \mathbb{R}$,

$$g(\mu_i) = \eta_i, \text{ where } \mu_i = E\{Y_i\}, \quad \eta_i = \boldsymbol{x}_i \cdot \boldsymbol{\beta},$$
 (10)

where $\boldsymbol{\beta} \in \mathbb{R}^r$ is an $r \times 1$ parameter vector. Model (10) relates each response Y_i to the Euclidean coordinates of Ω_i . That is, the linear predictor η_i is a linear combination of the Euclidean coordinates \boldsymbol{x}_i of Ω_i , the *i*-th row of the $n \times r$ matrix $\boldsymbol{X}_{\boldsymbol{w}}$ of a Euclidean configuration of $\boldsymbol{\Delta}$.

The DB-GLM model definition is sound since it does not depend of the particular choice of the Euclidean configuration. Indeed, as stated, the model consists of random vectors $(Y_1, \ldots, Y_n)'$ whose expectation, $(\mu_1, \ldots, \mu_n)'$, transformed by the link function, is a vector in the column space \mathscr{G} of \mathbf{X}_{w} . Since \mathscr{G} is also the column space of $\mathbf{X}_{w} \cdot \mathbf{X}'_{w} = \mathbf{G}_{w}$, (Rao 1973, p. 27), we conclude the model depends only on $\boldsymbol{\Delta}$.

To fit DB-GLM we use the IWLS algorithm described above, where DB-LM substitutes LM in formulas (8) and (9) to regress \boldsymbol{z}_0 on the covariates with weight \boldsymbol{W}_0 , in order to obtain the new estimation $\hat{\boldsymbol{\eta}}_1$. Observe that the IWLS estimation process for DB-GLM does not depend on a specific $\boldsymbol{X}_{\boldsymbol{w}}$ since the final quantities are obtained directly from distances. In the first step we need and initial $\hat{\boldsymbol{\mu}}_0$. Then we calculate $\hat{\boldsymbol{\eta}}_0$ and $\left(\frac{d\boldsymbol{\eta}}{d\boldsymbol{\mu}}\right)_0$. These two elements only depend on the link function. Finally, we calculate \boldsymbol{V}_0 , the function (7) evaluated at $\hat{\boldsymbol{\mu}}_0$, which only depends on the fitted vales $\hat{\boldsymbol{\mu}}$ at each step.

Prediction for new observations is also independent of the choice of X_w . Given a new case Ω_{n+1} , described by the $1 \times n$ vector δ_{n+1} of squared distances from Ω_{n+1} to the *n* previously known individuals, the predicted η_{n+1} for Ω_{n+1} is $x_{n+1} \cdot \hat{\beta}$, which is calculated with formula (2) with the quantities of the last IWLS step. Then we can calculate $\mu_{n+1} = g^{-1}(\eta_{n+1})$.

DB-GLM contains GLM as a particular case: if we start from a $n \times r \, \boldsymbol{w}$ -centered matrix $\boldsymbol{X}_{\boldsymbol{w}}$ of r continuous predictors corresponding to n individuals and we define $\boldsymbol{\Delta}$ as the matrix of squared Euclidean distances between rows of $\boldsymbol{X}_{\boldsymbol{w}}$, then $\boldsymbol{X}_{\boldsymbol{w}}$ is trivially a Euclidean configuration of $\boldsymbol{\Delta}$, hence the DB-GLM hat matrix, response and predictions coincide with the corresponding IWLS quantities of ordinary GLM.

2.3. Local Distance-Based Generalized Linear Model

We consider again the framework stated in Section 2.2 when DB-GLM was introduced. Our objective is now to fit a *local DB-GLM*, where *local* refers to the fact that when the DB-GLM is used to predict the value of the response variable for an object Ω_{n+1} , we use only the information provided by observed objects Ω_i , $i = 1, \ldots, n$, that are *close* to Ω_{n+1} , giving to Ω_i a weight that is a decreasing function of the distance between Ω_i and Ω_{n+1} . The idea is to translate to the DB-GLM context the principles of *local likelihood*, as stated in Loader (1999) (see also Section 3.4 in Bowman and Azzalini (1997), Section 6.5 in Hastie, Tibshirani, and Friedman (2009) or Section 5.10 in Wasserman (2006)). Our approach parallels that used in Boj, Delicado, and Fortiana (2010) when local DB-LM is defined.

Let $m(\Omega_{n+1})$ be the expected value of the response y corresponding to the object Ω_{n+1} . This is the value we want to estimate and we do that by using DB-GLM. We assume that two distance functions, δ_1 and δ_2 , are defined between the elements of Ω (the set of observable objects). We consider the weights

$$w_i(\Omega_{n+1}) = K(\delta_1(\Omega_{n+1}, \Omega_i)/h) / \sum_{j=1}^n K(\delta_1(\Omega_{n+1}, \Omega_j)/h),$$

where h is an smoothing parameter (depending on n). Let Δ_2 be the matrix of squared distances between functions defined from δ_2 . We fit a DB-GLM starting from the initial elements

$$\boldsymbol{\Delta}_{2} = (\delta_{2}(\Omega_{i}, \Omega_{j})^{2})_{i=1...n, j=1...n}, \ \boldsymbol{y} = (y_{i})_{i=1...n}, \ \text{and} \ \boldsymbol{w} = (w_{i}(\Omega_{n+1}))_{i=1...n}.$$

We consider the new individual Ω_{n+1} and we compute the squared distances from object Ω_{n+1} to other individuals Ω_i :

$$\boldsymbol{\delta}_{2,n+1} = (\delta_2(\Omega_{n+1}, \Omega_1)^2, \cdots, \delta_2(\Omega, \Omega_n)^2).$$

Then we run the IWLS algorithm for DB-GLM to obtain the local DB-GLM estimator of $m(\Omega_{n+1})$:

$$\hat{m}_{localDB-GLM}(\Omega_{n+1}) = \hat{y}_{n+1}.$$

There are two distance functions involved in the local DB-GLM: one of them, δ_1 , is used to compute the weight of observed objects Ω_i around the object Ω_{n+1} where the response function is estimated, and the other, δ_2 , defines the distances between observations for computing DB-GLM. The distances δ_1 and δ_2 can coincide or not. In the context of local DB-LM, Boj, Delicado, and Fortiana (2010) show that using two distance functions provides more flexibility than using only one (that is, $\delta_1 = \delta_2$).

3. The dbstats Package

The dbstats package for R (Boj, Caballé, Delicado, and Fortiana 2012) implements several distance-based prediction methods. Currently the response is univariate. Distances can either be directly input as an interdistances matrix, a squared interdistances matrix, an inner-products matrix or computed from observed explanatory variables. We distinguish observed explanatory variables, denoted by Z, from Euclidean coordinates X_w . Observed explanatory variables Z are possibly a mixture of continuous, qualitative or more general quantities. dbstats does not provide specific methods for computing distances, depending instead on other available functions and packages, such as:

dist in the stats package.

- daisy in the cluster package (Maechler 2012). Compared to dist above whose input must be numeric variables, the main feature of daisy is its ability to handle other variable types as well (e.g. nominal, ordinal, (a)symmetric binary) even when different types occur in the same data set.
- dist in the proxy package (Meyer and Buchta 2012). Supersedes the one in the stats package. It allows a user-provided function, entered as a parameter, for evaluating distances between observations, hence it can deal with any type of data.

Distance-related classes in dbstats are dist and dissimilarity (as in stats), D2, for squared distances matrices; and Gram, for doubly centered inner product matrices. Utility functions such as as.D2, as.Gram, D2toDist, D2toG, distoD2 and GtoD2 allow their mutual interconversions (see (Boj, Caballé, Delicado, and Fortiana 2012) for details).

The main functions of dbstats are:

Linear and local linear models with a continuous response:

- dblm for DB-LM.
- ldblm for local DB-LM.
- dbplsr for DB-PLSR.

Generalized linear and local generalized linear models with a univariate response:

- dbglm for DB-GLM.
- ldbglm for local DB-GLM.

In the next subsections we describe the usage of dblm, dbglm and ldbglm. For ldblm and plsr we refer to (Boj, Caballé, Delicado, and Fortiana 2012).

3.1. dblm

The usage of dblm depends on the input information. There are two ways to incorporate predictors information: either as a formula or as a distance-type object of any of the four classes: dist, dissimilarity, D2 or Gram.

The usage of dblm is:

For class formula

```
dblm(formula, data, ..., metric = "euclidean", method = "OCV",
full_search=FALSE, weights, rel.gvar = 0.95, eff.rank)
```

For class dist or dissimilary

```
dblm(distance, y, ..., method = "OCV", full_search = FALSE,
weights, rel.gvar = 0.95, eff.rank)
```

For class $\mathtt{D2}$

```
dblm(D2, y, ... , method = "OCV", full_search = FALSE, weights,
rel.gvar = 0.95, eff.rank)
```

For class Gram

dblm(G, y, ..., method = "OCV", full_search = FALSE, weights, rel.gvar = 0.95, eff.rank)

The arguments in dblm are:

- formula an object of class formula. A formula of the form $y^{\sim}Z$. This argument is a remnant of the lm function, kept for compatibility.
- **data** an optional data frame containing the variables in the model (both response and explanatory variables, either the observed ones, Z, or a Euclidean configuration X_w).
- **metric** metric function to be used when computing distances from observed explanatory variables. One of "euclidean" (default), "manhattan", or "gower".
- **distance** a dist or dissimilarity class object. See functions dist in the package stats and daisy in the package cluster.
- **D2** a D2 class object. Squared distances matrix between individuals Δ . See details above to learn the usage of dblm.
- **G** a Gram class object. Doubly centered inner product matrix of the squared distances matrix D2, i.e., G_w . See details above to learn the usage of dblm.Gram.
- **y** (required if no formula is given as the principal argument). Response (dependent variable) must be numeric, matrix or data.frame.
- method sets the method to be used in deciding the effective rank, which is defined as the number of linearly independent Euclidean coordinates used in prediction. There are six different methods: "AIC", "BIC", "OCV" (default), "GCV", "eff.rank" and "rel.gvar". OCV and GCV take the effective rank minimizing a cross-validatory quantity (either ordinary ocv or generalized gcv). AIC and BIC take the effective rank minimizing, respectively, the Akaike or Bayesian Information Criterion (see the R function AIC for more details). The optimizacion procedure to be used in the above four methods can be set with the full_search optional parameter.

When method is eff.rank, the effective rank is explicitly set by the user through the eff.rank optional parameter which, in this case, becomes mandatory.

When method is **rel**.gvar, the fraction of the data *geometric variability* for model fitting is explicitly set by the user through the **rel**.gvar optional parameter which, in this case, becomes mandatory.

full_search sets which optimization procedure will be used to minimize the modelling

criterion specified in method. Needs to be specified only if method is "AIC", "BIC", "OCV" or "GCV". If full_search=TRUE, *effective rank* is set to its global best value, after evaluating the criterion for all possible ranks. Potentially too computationally expensive. If full_search=FALSE, the R function optimize is called. Then computation time is shorter, but the result may be found a local minimum.

- weights an optional numeric vector of weights to be used in the fitting process. By default all individuals have the same weight.
- rel.gvar relative geometric variability (real between 0 and 1). Take the lowest effective
 rank with a relative geometric variability higher or equal to rel.gvar. Default
 value (rel.gvar=0.95) uses a 95% of the total variability. Applies only rel.gvar
 if method = "rel.gvar".
- **eff.rank** integer between 1 and the number of observations minus one. Number of Euclidean coordinates used for model fitting. Applies only if method="eff.rank".
- ... arguments passed to or from other methods to the low level.

When using method method="eff.rank" or method="rel.gvar", a compromise between possible consequences of a bad choice has to be reached. If the rank is too large, the model can be overfitted, possibly leading to an increased prediction error for new cases (even though R2, the determination coefficient, is high). On the other hand, a small rank suggests a model inadequacy (R2 is small). The other four methods are less error prone (but still they do not guarantee good predictions).

The function returns a list of class dblm containing the following components:

residuals the residuals (response minus fitted values).

fitted.values the fitted mean values.

df.residuals the residual degrees of freedom.

weights the specified weights.

y the response used to fit the model.

 ${\boldsymbol{\mathsf{H}}}$ the hat matrix projector.

call the matched call.

rel.gvar the relative geometric variabiliy, used to fit the model.

eff.rank the dimensions chosen to estimate the model.

ocv the ordinary cross-validation estimate of the prediction error.

gcv the generalized cross-validation estimate of the prediction error.

aic the Akaike Value Criterium of the model (only if method="AIC").

bic the Bayesian Value Criterium of the model (only if method="BIC").

3.2. dbglm

dbglm is a variety of GLM where explanatory information is coded as distances between individuals. These distances can either be computed from observed explanatory variables or directly input as a squared inter-distances matrix. Response and link function could be as in the glm function of stats for ordinary GLM.

The usage of dbglm is:

For class formula

```
dbglm(formula, data, family = gaussian, ..., metric = "euclidean",
    method = "OCV", full_search = FALSE, weights, maxiter = 100,
    eps1 = 1e-10, eps2 = 1e-10, rel.gvar = 0.95, eff.rank = NULL,
    offset, mustart = NULL)
```

For class dist or dissimilary

For class D2

```
dbglm(D2, y, ..., family = gaussian, method = "OCV", full_search =
    FALSE, weights, maxiter=100, eps1 = 1e-10, eps2 = 1e-10,
    rel.gvar = 0.95, eff.rank = NULL, offset, mustart = NULL)
```

For class Gram

rel.gvar = 0.95, eff.rank = NULL, offset, mustart = NULL)

The arguments in dbglm are:

- formula an object of class formula. A formula of the form $y \tilde{z}$. This argument is a remnant of the glm function, kept for compatibility.
- **data** an optional data frame containing the variables in the model (both response and explanatory variables, either the observed ones, Z, or a Euclidean configuration X_w).
- **metric** metric function to be used when computing distances from observed explanatory variables. One of "euclidean" (the default), "manhattan", or "gower".
- **y** (required if no formula is given as the principal argument). Response (dependent variable) must be numeric, factor, matrix or data.frame.
- **distance** a dist or dissimilarity class object. See functions dist in the package stats and daisy in the package cluster.
- **D2** a D2 class object. Squared distances matrix between individuals Δ . See details in dblm.
- **G** a Gram class object. Doubly centered inner product matrix of the squared distances matrix D2, i.e., G_w . See details in dblm.
- family a description of the error distribution and link function to be used in the model. This can be a character string naming a family function, a family function or the result of a call to a family function. (See the R function family for details of family functions.)
- method sets the method to be used in deciding the effective rank, used in prediction. There are six different methods: "AIC", "BIC", "OCV" (default), "GCV", "eff.rank" and "rel.gvar". OCV and GCV take the effective rank minimizing a cross-validatory quantity (either ordinary ocv or generalized gcv). AIC and BIC take the effective rank minimizing, respectively, the Akaike or Bayesian Information Criterion (see the R function AIC for more details). The optimizacion procedure to be used in the above four methods can be set with the full_search optional parameter.

When method is eff.rank, the effective rank is explicitly set by the user through the eff.rank optional parameter which, in this case, becomes mandatory.

When method is rel.gvar, the fraction of the data geometric variability for model

fitting is explicitly set by the user through the **rel**.gvar optional parameter which, in this case, becomes mandatory.

- full_search sets which optimization procedure will be used to minimize the modelling criterion specified in method. Needs to be specified only if method is "AIC", "BIC", "OCV" or "GCV". If full_search=TRUE, effective rank is set to its global best value, after evaluating the criterion for all possible ranks. Potentially too computation- ally expensive. If full_search=FALSE, the R function optimize is called. Then computation time is shorter, but the result may be found a local minimum.
- weights an optional numeric vector of prior weights to be used in the fitting process. By default all individuals have the same weight.
- **maxiter** maximum number of iterations in the iterated dblm algorithm. (Default = 100)
- eps1 stopping criterion 1, "DevStat": convergence tolerance eps1, a positive (small)
 number; the iterations converge when |dev dev_old|/(|dev|) < eps1. Sta tionarity of deviance has been attained.</pre>
- eps2 stopping criterion 2, "mustat": convergence tolerance eps2, a positive (small)
 number; the iterations converge when |mu mu_old|/(|mu|) < eps2. Station arity of fitted.values mu has been attained.</pre>
- rel.gvar relative geometric variability (a real number between 0 and 1). At each dblm iteration, take the lowest effective rank, with a relative geometric variability higher or equal to rel.gvar. Default value (rel.gvar=0.95) uses the 95% of the total variability.
- eff.rank integer between 1 and the number of observations minus one. Number of Euclidean coordinates used for model fitting in each dblm iteration. If specified its value overrides rel.gvar. When eff.rank=NULL (default), calls to dblm are made with method=rel.gvar.
- **offset** this can be used to specify an a priori known component to be included in the linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of cases.
- mustart starting values for the vector of means.
- ... arguments passed to or from other methods to the low level.

For Gamma-distributed responses, the domain of the canonical link function is not the same as the permitted range of the mean. In particular, the linear predictor might be

negative, obtaining an impossible negative mean. Should that event occur, dbglm stops with an error message. Proposed alternative is to use a non-canonical link function.

The function returns a list of class dbglm containing the following components:

residuals the working residuals, that is the dblm residuals in the last iteration of dblm fit.

fitted.values the fitted mean values, results of final dblm iteration.

family the family object used.

- **deviance** measure of discrepancy or badness of fit. Proportional to twice the difference between the maximum achievable log-likelihood and that achieved by the current model.
- **aic.model** A version of Akaike's Information Criterion. Equal to minus twice the maximized log-likelihood plus twice the number of parameters. Computed by the aic component of the family. For binomial and Poison families the dispersion is fixed at one and the number of parameters is the number of coefficients. For Gaussian, Gamma and Inverse Gaussian families the dispersion is estimated from the residual deviance, and the number of parameters is the number of coefficients plus one. For a Gaussian family the MLE of the dispersion is used so this is a valid value of AIC, but for Gamma and Inverse Gaussian families it is not. For families fitted by quasi-likelihood the value is NA.
- **null.deviance** the deviance for the null model. The null model will include the offset, and an intercept if there is one in the model. Note that this will be incorrect if the link function depends on the data other than through the fitted mean: specify a zero offset to force a correct calculation.

iter number of Fisher scoring (dblm) iterations.

prior.weights the original weights.

weights the working weights, that are the weights in the last iteration of dblm fit.

df.residual the residual degrees of freedom.

df.null the residual degrees of freedom for the null model.

 \boldsymbol{y} the response vector used.

convcrit convergence criterion. One of: "DevStat" (stopping criterion 1), "muStat"
 (stopping criterion 2), "maxiter" (maximum allowed number of iterations has
 been exceeded).

H hat matrix projector of the last dblm iteration.

rel.gvar the relative geometric variabiliy in the last dblm iteration.

eff.rank the working effective rank, that is the eff.rank in the last dblm iteration.

3.3. IdbgIm

ldbglm is a localized version of a DB-GLM. As in the global model dbglm, explanatory information is coded as distances between individuals. Neighborhood definition for localizing is done by the (semi)metric dist1 whereas a second (semi)metric dist2 (which may coincide with dist1) is used for distance-based prediction. Both dist1 and dist2 can either be computed from observed explanatory variables or directly input as a squared interdistances matrix or as a Gram matrix. Response and link function as in the dbglm function for ordinary generalized linear models. The model allows for a mixture of continuous and qualitative explanatory variables or, in fact, from more general quantities such as functional data.

The usage of ldbglm is:

For class formula

```
ldbglm(formula, data, ..., family = gaussian(), kind.of.kernel = 1,
    metric1 = "euclidean", metric2 = metric1, method = "GCV",
    weights, user_h = NULL, h.range = NULL, noh = 10, k.knn = 3,
    rel.gvar = 0.95, eff.rank = NULL, maxiter = 100, eps1 = 1e-10,
    eps2 = 1e-10)
```

For class dist or dissimilary

```
ldbglm(dist1, dist2 = dist1, y, family = gaussian(), kind.of.kernel
= 1, method = "GCV", weights, user_h = quantile(dist1, .25) ^ .5,
h.range = quantile(as.matrix(dist1), c(.05,.25)) ^ .5, noh = 10,
k.knn = 3, rel.gvar = 0.95, eff.rank = NULL, maxiter = 100,
eps1 = 1e-10, eps2 = 1e-10, ...)
```

For class $\mathtt{D2}$

```
ldbglm(D2_1, D2_2 = D2_1, y, family = gaussian(), kind.of.kernel = 1,
    method = "GCV", weights, user_h = NULL, h.range = NULL, noh = 10,
    k.knn = 3, rel.gvar = 0.95, eff.rank = NULL, maxiter = 100,
    eps1 = 1e-10, eps2 = 1e-10, ...)
```

For class Gram

```
ldbglm(G1, G2 = G1, y, kind.of.kernel = 1, user_h = NULL,
family = gaussian(), method = "GCV", weights, h.range = NULL,
noh = 10, k.knn = 3, rel.gvar = 0.95, eff.rank = NULL, maxiter
= 100, eps1 = 1e-10, eps2 = 1e-10, ...)
```

The arguments in ldbglm are:

- formula an object of class formula. A formula of the form $y \tilde{z}$. This argument is a remnant of the loess function, kept for compatibility.
- **data** an optional data frame containing the variables in the model (both response and explanatory variables, either the observed ones, Z, or a Euclidean configuration X_w).
- **y** (required if no formula is given as the principal argument). Response (dependent variable) must be numeric, matrix or data.frame.
- dist1 a dist or dissimilarity class object. Distances between observations, used for neighborhood localizing definition. Weights for observations are computed as a decreasing function of their dist1 distances to the neighborhood center, e.g. a new observation whose reoponse has to be predicted. These weights are then entered to a dbglm, where distances are evaluated with dist2.
- dist2 a dist or dissimilarity class object. Distances between observations, used for fitting dbglm. Default dist2=dist1.
- **D2_1** a **D2** class object. Squared distances matrix between individuals. One of the alternative ways of entering distance information to a function. See the Details section in dblm. See above dist1 for explanation of its role in this function.
- D2_2 a D2 class object. Squared distances between observations. One of the alternative ways of entering distance information to a function. See the Details section in dblm. See above dist2 for explanation of its role in this function. Default D2_2=D2_1.
- **G1** a **Gram** class object. Doubly centered inner product matrix associated with the squared distances matrix D2_1.

- **G2** a **Gram** class object. Doubly centered inner product matrix associated with the squared distances matrix D2_2. Default G2=G1
- family a description of the error distribution and link function to be used in the model. This can be a character string naming a family function, a family function or the result of a call to a family function. (See the R function family for details of family functions.)
- kind.of.kernel integer number between 1 and 6 which determines the user's choice of smoothing kernel. (1) Epanechnikov (Default), (2) Biweight, (3) Triweight, (4) Normal, (5) Triangular, (6) Uniform.
- metric1 metric function to be used when computing dist1 from observed explanatory
 variables. One of "euclidean" (default), "manhattan", or "gower".
- metric2 metric function to be used when computing dist2 from observed explanatory
 variables. One of "euclidean" (default), "manhattan", or "gower".
- method sets the method to be used in deciding the optimal bandwidth h. There are five different methods, AIC, BIC, OCV, GCV (default) and user_h. OCV and GCV take the optimal bandwidth minimizing a cross-validatory quantity (either ocv or gcv). AIC and BIC take the optimal bandwidth minimizing, respectively, the Akaike or Bayesian Information Criterion (see the R function AIC for more details). When method is user_h, the bandwidth is explicitly set by the user through the user_h optional parameter which, in this case, becomes mandatory.
- user_h global bandwidth user_h, set by the user, controlling the size of the local neighborhood of Z. Smoothing parameter (Default: 1st quartile of all the distances d(i,j) in dist1). Applies only if method="user_h".
- **h.range** a vector of length 2 giving the range for automatic bandwidth choice. (Default: quantiles 0.05 and 0.5 of d(i,j) in dist1).
- noh number of bandwidth h values within h.range for automatic bandwidth choice (if method!="user_h").
- k.knn minimum number of observations with positive weight in neighborhood localizing. To avoid runtime errors due to a too small bandwidth originating neighborhoods with only one observation. By default k.nn=3.
- rel.gvar relative geometric variability (a real number between 0 and 1). At each dblm iteration, take the lowest effective rank, with a relative geometric variability higher or equal to rel.gvar. Default value (rel.gvar=0.95) uses the 95% of the total variability.

- eff.rank integer between 1 and the number of observations minus one. Number of Euclidean coordinates used for model fitting in each dblm iteration. If specified its value overrides rel.gvar. When eff.rank=NULL (default), calls to dblm are made with method=rel.gvar.
- **weights** an optional numeric vector of weights to be used in the fitting process. By default all individuals have the same weight.
- maxiter maximum number of iterations in the iterated dblm algorithm. (Default = 100)
- eps1 stopping criterion 1, "DevStat": convergence tolerance eps1, a positive (small)
 number; the iterations converge when |dev dev_old|/(|dev|) < eps1. Sta tionarity of deviance has been attained.</pre>
- eps2 stopping criterion 2, "mustat": convergence tolerance eps2, a positive (small)
 number; the iterations converge when |mu mu_old|/(|mu|) < eps2. Station arity of fitted.values mu has been attained.</pre>
- ... arguments passed to or from other methods to the low level.

The set of bandwidth h values checked in automatic bandwidth choice is defined by h.range and noh, together with k.knn. For each h in it a local generalized linear model is fitted and the optimal h is decided according to the statistic specified in method.

And that kind.of.kernel designates which kernel function is to be used in determining individual weights from dist1 values. See the R function density for more information.

The function returns a list of class ldbglm containing the following components:

residuals the residuals (response minus fitted values).

fitted.values the fitted mean values.

family the family object used.

y the response variable used.

S the Smoothing hat projector.

weights the specified weights.

call the matched call.

- dist2 the distance matrix (object of class "D2" or "dist") used to fit the dbglm.

4. Examples

4.1. An example of DB-GLM

We fit DB-GLM to the data set on Swedish third-party motor insurance in 1977 described in Hallin and Ingenbleek (1983). The file is included in **faraway** package with the name *motorins* (Faraway 2012). Data for factor Zone =1 can be found too in Andrews and Herzberg (1985, pp. 413-421). These data correspond to the cities of Stockholm, Gteburg and Malmo, and were obtained from a committee study of risk premiums in motor insurance. The total number of observations (for Zone=1) is n = 295 corresponding to different non-empty risk groups. For each group, Y is the number of claims suffered by the automobile insured in the exposure \boldsymbol{w} , which is the number of insured in policyyears. The factors thought to be important in modeling the occurrence of claims are three: Distance (Kilometers Travelled), Bonus (No-claims bonus) and Make (specified car makes). The number of levels of each factor are 5, 7 and 9 respectively. Distance and Bonus are continuous numerical predictors and we have coded numerically versions of them as follows:

We have represented each state of Distance by a class mark. Central classes are represented by the interval average, whereas class marks for the extreme classes are reasonably representative values. The codes are:

 $<1000\ Km\ per\ year:$ 750 Kilometers travelled per year

1000 – 15000 Km per year: 8000 Kilometers travelled per year

15000 – 20000 Km per year: 17500 Kilometers travelled per year

20000 – 25000 Km per year: 22500 Kilometers travelled per year

> 25000 Km per year: 40000 Kilometers travelled per year

Bonus is represented by the (arbitrary) numerical codes, 1 to 7. Insured starts in the class 1 and is moved up one class (to a maximum of 7) each year there is no claim.

Make will be considered as a nominal categorical variable in Gower's formula (11). It is coded numerically (as 1 to 9) just as a programming convenience. It represents 9 specified car makes.

```
R> library(dbstats)
R> require(faraway)
R> data(motorins)
R> Motor1 <- subset(motorins, Zone == 1)
R> Motor1$frequency <- Motor1$Claims / Motor1$Insured
R> y <- Motor1$frequency
R> w <- Motor1$Insured
R> Motor1$KmC <- rep(0,nrow(Motor1))
R> Motor1$KmC[Motor1$Kilometres == "1"] <-
                                              750
R> Motor1$KmC[Motor1$Kilometres == "2"] <-</pre>
                                             8000
R> Motor1$KmC[Motor1$Kilometres == "3"] <- 17500
R> Motor1$KmC[Motor1$Kilometres == "4"] <- 22500
R> Motor1$KmC[Motor1$Kilometres == "5"] <- 40000
R> Motor1$BonC <- as.numeric(Motor1$Bonus)
R> Motor1$MakeC <- as.numeric(Motor1$Make)
```

The first step in the treatment of these data by DB-GLM is the choice of a suitable metric. In principle it is possible to tailor a metric to reflect specific information on predictors and on how their proximity relates to the particular prediction under study. Here it is sufficient to utilize an omnibus metric function which satisfies the Euclidean condition. One very popular such metric for mixtures of numerical continuous, categorical and binary predictor variables is the one based on Gower's general similarity coefficient (see Gower (1971) for further details):

$$s_{ij} = \frac{\sum_{h=1}^{p_1} \left(1 - |x_{ih} - x_{jh}|/G_h\right) + a + \alpha_{ij}}{p_1 + (p_2 - d) + p_3}$$
(11)

where p_1 is the number of continuous variables, a and d are the number of positive and negative matches, respectively, for the p_2 binary variables, and α_{ij} is the number of matches for the p_3 multi-state categorical variables. G_h is the range of the h-th continuous variable. The squared distance is computed as: $\delta_{ij}^2 = 1 - s_{ij}$. Gower (1971) proves that this distance satisfies the Euclidean condition. In our example, $p_1 = 2$, $p_2 = 0$ and $p_3 = 1$ in (11).

For GLM, we use 11 parameters: 2 for Distance and Bonus with the class marks defined above and 9 binary variables for each nominal class of Make, taking into account an intercept term. Both in GLM and DB-GLM, we assume both Poisson and Binomial distributions for claim frequency, combined with its associated canonical links. The weights of regressions are the exposures \boldsymbol{w} .

We fit three cases for the DB-GLM:

- 1. rel.gvar = 1, i.e., we take into account for the model all the dimensions of the latent Euclidean configurations;
- 2. method = "GCV", i.e., we choose the effective rank which minimizes a generalized cross-validation (leave-one-out) statistic;
- 3. rel.gvar = 0.90, i.e., we take into account for the model the 90% of explained geometric variability. In both cases (Poisson and Binomial) coincide with the choice of taking into account an effective rank of 10, which coincide with the number of parameters used in the fitted GLM (without counting the intercept term).

We obtain in both cases (the Poisson and the Binomial ones), lower residual deviances with the distance-based treatment of the GLM than those obtained with the classical GLM, see Tables 1 and 2. The detailed instructions used to elaborate these tables for the function dbglm can be found in Annex A.

To illustrate the summary command, we choose a DB-GLM, the one with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the "GCV" method. In Annex A it is the one named dbglm2. We show the results too for dbglm4 which corresponds to the case when we fit the Poisson with Logarithmic link, using the Euclidean distance and taking into account the complete geometric variability. That case is relevant because it is the particular case in which the results coincide with the classical GLM assuming Poisson and Logarithmic link (named glm1 in Annex A). Similarly, the summary of dbglm8 coincides with the summary of glm2 for Binomial response and Logit link (see Annex A)

If we compare the output of the summary command of *dbglm4* and *glm1* below, we can observe that both are similarly programmed. The main difference is that in dbglm we have not estimations of coefficients, because DB-GLM does not assign a coefficient to each explanatory variable.

R> summary(dbglm2)

Deviance Residuals: Min. 1st Qu. Median Mean 3rd Qu. Max. -6.39000 -0.71300 0.05910 0.02042 0.83250 6.72400 (Dispersion parameter for poisson family taken to be 1) Null deviance: 6977.53 on 294 degrees of freedom Residual deviance: 485.72 on 281 degrees of freedom AIC: Inf Number of Fisher Scoring iterations: 11 Convergence criterion: muStat R> summary(dbglm4) Call: dbglm.formula(formula = y ~ KmC + BonC + factor(MakeC), data = Motor1, family = poisson(link = "log"), metric = "euclidean", weights = w, rel.gvar = 1) Deviance Residuals: Min. 1st Qu. Median Mean 3rd Qu. Max. -6.51300 -0.89800 -0.06430 -0.06486 0.80760 10.09000 (Dispersion parameter for poisson family taken to be 1) Null deviance: 6977.53 on 294 degrees of freedom Residual deviance: 779.36 on 284 degrees of freedom AIC: Inf Number of Fisher Scoring iterations: 100 Convergence criterion: MaxIter R> summary(glm1) Call: glm(formula = y ~ KmC + BonC + factor(MakeC), family = poisson(link = "log"), data = Motor1, weights = w) Deviance Residuals: Median Min 1Q ЗQ Max -6.5134 -0.8980 -0.0643 0.8076 10.0902 Coefficients:

Estimate Std. Error z value Pr(|z|)(Intercept) -1.640e+00 2.637e-02 -62.181 < 2e-16 *** 22.424 < 2e-16 *** KmC 1.431e-05 6.381e-07 BonC -2.165e-01 2.762e-03 -78.387 < 2e-16 *** factor(MakeC)2 1.282e-01 4.598e-02 2.788 0.00531 ** factor(MakeC)3 -2.140e-01 5.162e-02 -4.146 3.38e-05 *** factor(MakeC)4 -5.162e-01 4.987e-02 -10.352 < 2e-16 *** factor(MakeC)5 1.270e-01 4.850e-02 2.618 0.00883 ** factor(MakeC)6 -3.976e-01 4.467e-02 -8.900 < 2e-16 *** factor(MakeC)7 -1.320e-01 5.891e-02 -2.240 0.02508 * factor(MakeC)8 1.396e-01 8.673e-02 1.609 0.10762 factor(MakeC)9 -3.079e-02 2.276e-02 -1.353 0.17618 ____ Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 (Dispersion parameter for poisson family taken to be 1) degrees of freedom Null deviance: 6977.53 on 294 degrees of freedom Residual deviance: 779.36 on 284 AIC: Inf Number of Fisher Scoring iterations: 5 We calculate the mean difference of fitted.values of glm1 and glm4:

R> mean(glm1\$fitted.values - dbglm4\$fitted.values)

[1] -2.521631e-09

obtaining that they coincide, up to a negligeable value.

Respect to the plot command, its usage is:

The arguments are:

x an object of class dblm or dbglm.

which if a subset of the plots is required, specify a subset of the numbers 1:6.

id.n number of points to be labelled in each plot, starting with the most extreme.

main an overall title for the plot. Only if one of the six plots is selected.

cook.levels levels of Cook's distance at which to draw contours.

cex.id magnification of point labels.

type_glm the type of prediction (required only for a dbglm class object). Like predict.
 dbglm, the default "link" is on the scale of the linear predictors; the alternative
 "response" is on the scale of the response variable.

The first five plots are useful for residual analysis and are the same as in plot.lm. The last plot allows us to view the "OCV", "GCV", "AIC" or "BIC" criterion according to which the rank used dblm function has been chosen. It applies only if the parameter full_search in dblm its TRUE.

It is easy to get the predicted mean values, as these are calculated by the inverse link function on the linear predictors. We refer to the R function family to view how to insert user-defined linkfun and linkinv in dbstats.

To illustrate the plot command, we exhibit for model *dbglm2* the five possible plots: Residuals vs Fitted, Normal Q-Q, Scale-location, Cook's distance and Residuals vs Leverage, which can be found in Figures 1, 2, 3, 4 and 5 respectively.

R> plot(dbglm2, type_glm = "response", which = 1:5)

Values predicted with predict may be the expected mean values of the response for the new data (type="response"), or the linear predictors evaluated at the estimated dblm of the last iteration, as is in the plot command above. Additionally, we can choose the type of the new data, which can be: "Z" if newdata contains the values of the explanatory variables, "D2" if contains the squared distances matrix or "G" if contains the inner products matrix. Its usage is:

```
predict(object, newdata, type = c("link", "response"), type_var = "Z",...)
```

With model dbglm2, for data in the original set, such as insureds with 750 kilometers travelled per year, with Bonus and Make both in class 1, we can execute:

```
R> newdata <- data.frame(KmC = 750, BonC = 1, MakeC = 1)
R> pr <- predict(dbglm2, newdata, type = "response", type_var = "Z"); pr</pre>
```

[,1] [1,] 0.1711442

Poisson / Logarithmic	Residual Deviance	Eff.rank
DB-GLM (rel.gvar = 1)	454.05	18
DB-GLM (method = "GCV")	485.72	13
DB-GLM (rel.gvar = 0.90)	539.55	10
GLM	779.36	10

Table 1: Results of the fitting for the Poisson model with the Logarithmic link

Binomial / Logit	Residual Deviance	Eff.rank
DB-GLM (rel.gvar = 1)	498.42	18
DB-GLM (method = "GCV")	538.05	13
DB-GLM (rel.gvar = 0.90)	595.74	10
GLM	889.07	10

Table 2: Results of the fitting for the Binomial model with the Logit link

Comparing this prediction with the corresponding one from fitted.values, we confirm that both values agree (with a precission of 1e-15).

R> dbglm2\$fitted.values[1] - pr

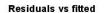
[,1] [1,] 4.746203e-15

Now, we compute the prediction for a new insured, e.g., with 900 kilometers travelled per year, with Bonus and Make both in class 1, and we obtain the prediction:

```
R> newdata <- data.frame(KmC = 900, BonC = 1, MakeC = 1)
R> pr <- predict(dbglm2, newdata, type = "response", type_var = "Z"); pr
[,1]
[1,] 0.1717889</pre>
```

4.2. An example of local DB-GLM

In this section we make an example using local DB-GLM with functional data as explanatory variable and a binary response. We say that an observed variable is functional when a whole function is registered for each individual in the sample (see Ramsay and Silverman (2005) for a general perspective on Functional Data Analysis and Ferraty and Vieu (2006a) for a nonparametric approach).



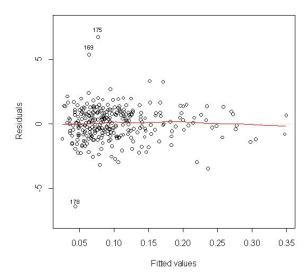


Figure 1: Residuals vs Fitted plot for DB-GLM with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the GCV method

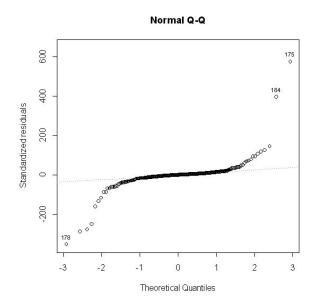


Figure 2: Normal Q-Q plot plot for DB-GLM with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the GCV method

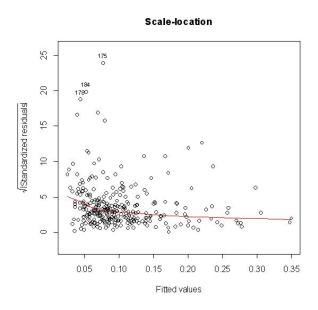


Figure 3: Scale-location plot for DB-GLM with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the GCV method

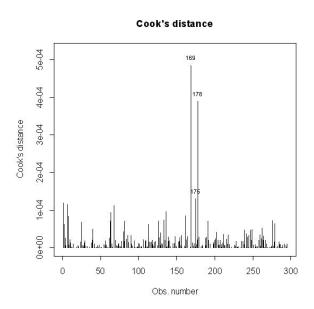


Figure 4: Cook's distance plot for DB-GLM with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the GCV method



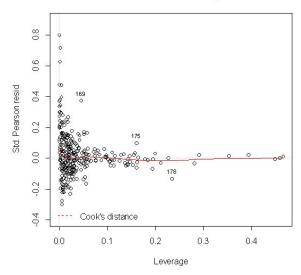


Figure 5: Residuals vs Leverage plot for DB-GLM with Poisson response and Logarithmic link, using Gower's distance and fitted taking into account the GCV method

We consider the near infrared (NIR) spectral data set contending with wheat samples that was described in Kalivas (1997). This data set contains data from 100 wheat samples. The available information for each sample consists of two scalar measures (protein and moisture contents; only protein content are used here) and a functional variable, the NIR spectra: samples were measured using diffuse reflection in units of log inverse reflectance $\log(1/R)$ at wavelengths going from 1100 to 2500 nm in 2 nm intervals (reflectance refers to the fraction of incident electromagnetic power that is reflected by the sample; see Brenchley, Hörchner, and Kalivas (1997) for more details about NIR measurements). The protein and spectrum data are available at ftp://ftp.clarkson.edu/users/h/o/hopkepk/chemdata/kalivas/, at files protein. asc and whtspec.asc, respectively.

Let us define the binary variable y indicating for each wheat sample in the data set whether its protein content is over the median value or not:

```
R> whtspec <- read.table("whtspec.asc")
R> protein <- read.table("protein.asc")
R> wave.length <- seq(1100, 2500, by = 2)
R> y <- as.numeric(protein > median(protein[, 1]))
```

Our goal is to predict the variable y using the NIR spectra function (whtspec) as predictor.

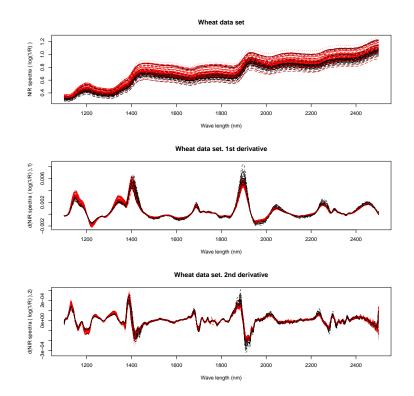


Figure 6: Wheat data set. NIR spectra functions, jointly with their first and second derivatives. Functions in red corresponds to wheat samples with protein content over the median.

We use the R package fda.usc (Febrero-Bande and Oviedo 2012) to deal with NIR spectra data as functional data:

This way the functions, as well as their first and second derivatives, are plotes as Figure 6 shows. Wheat samples have been colored according to the value of the binary variable y (red when y == 1). From the figure it is not obvious how NIR spectra functions or their derivatives could allows us to predict the value of y, the indicator of high protein content.

In order to measure the prediction ability of a given prediction rule we randomly divide the data set into a training set (with 60 wheat samples) and a validation set (with the remaining 40 samples):

R> set.seed(2)
R> trai <- sample(1:100)[1:60]</pre>

We will compare the performance of the following binary prediction tools, all of them using functional predictors:

- Generalized linear model with functional predictor using basis representation, as it is implemented in function fregre.glm, form package fda.usc.
- DB-GLM: Distance based generalized linear model, developed in Section 2.2.
- Local DB-GLM: Local distance based generalized linear model, developed in Section 2.3.

For each of these three prediction tools we have used three different functional predictors: NIR spectra functions, their first derivatives and their second derivatives. The measure of prediction quality that we are using for comparing the 9 procedures under consideration will be the number of bad classified wheat samples among the 40 in the validation set.

The following code was used to prepare the functional data to fit the functional GLM with fregre.glm:

```
R> yt <- y[trai]
R> yt.df <- as.data.frame(yt); names(yt.df) <- "protein"
R > yv < - y[-trai]
R> yv.df <- as.data.frame(yv); names(yv.df) <- "protein"</pre>
R> wst.d0 <- whtspec.fdata[trai,]</pre>
R> wsv.d0 <- whtspec.fdata[-trai, ]
R> wst.d1 <- fdata.deriv(wst.d0, nderiv = 1)
R> wsv.d1 <- fdata.deriv(wsv.d0, nderiv = 1)
R> wst.d2 <- fdata.deriv(wst.d0, nderiv = 2)
R> wsv.d2 <- fdata.deriv(wsv.d0, nderiv = 2)
R> ldata <- list("df" = yt.df, "ws.d0" = wst.d0, "ws.d1" = wst.d1,
   "ws.d2" = wst.d2)
R> newldata <- list("df" = yv.df, "ws.d0" = wsv.d0, "ws.d1" = wsv.d1,
   "ws.d2" = wsv.d2)
R> basis1 <- create.bspline.basis(rangeval = range(wave.length),
   nbasis = 18)
```

```
R> basis2 <- create.bspline.basis(rangeval = range(wave.length),
    nbasis = 18)
```

	Prediction tool		
	Functional glm	DB-GLM	local DB-GLM
Functional predictor:			
NIR spectra functions	9	14	8
First derivative	12	10	8
Second derivative	14	12	11

Table 3: Number of bad classified wheat samples among the 40 in the validation set.

```
R> basis.ws <- list("x" = basis1); basis.b <- list("x" = basis2)</pre>
```

The choice of a basis of B-splines with 18 elements (nbasis = 18) is arbitrary and it could be improved by using a choice based on leave-one-out prediction error criterium. These code lines allows us to call the function fregre.glm when the functional predictor used is observed NIR spectra function:

```
R> f0 <- protein~ws.d0
R> res.glm.0 <- fregre.glm(f0, ldata, family = binomial, basis.x =
    basis.ws, basis.b = basis.b)
R> pred.glm.0 <- predict.fregre.glm(res.glm.0, newldata)
R> glm.err.0 <- (abs(pred.glm.0 - yv) > .5)
R> print(sum(glm.err.0))
```

In order to use the first or the second derivatives the definition of formula f0 must be modified as follows:

R> f1 <- protein~ws.d1 R> f2 <- protein~ws.d2

Then the call to fregre.glm must be changed accordingly (see Annex B). The first column of Table 3 shows the number of wheat samples in the validation set that are bad classified when using the functional GLM. It can be seen that the best results are obtained when using the observed functions.

In order to fit a DB-GLM with the function dbglm the first step is to compute the inter-individual distance matrix. When dealing with functional data our choice is to use one of the semimetrics defined in Ferraty and Vieu (2006a) as they are implemented in their own R library NPFDA (Ferraty and Vieu (2006b); free access on line at http://www.lsp.ups-tlse.fr/staph/npfda/), also available at the package fda.usc (see functions metric.lp, semimetric.basis and semimetric.NPFDA in this package). In particular here we use L^2 distances between NIR spectra functions or their derivatives calculated after representing functions in a B-spline basis.

The following code was used to fit the functional DB-GLM with dbglm. NIR spectra functions are used as predictors:

```
R> ws.d0 <- whtspec.fdata
R> D2.0 <- semimetric.basis(ws.d0, ws.d0, nderiv = 0, nbasis1 = 18,
    nbasis2 = 18) ^2
R> D2.0.trai <- D2.0[trai,trai]
R> class(D2.0) <- "D2"; class(D2.0.trai) <- "D2"
R> res.dbglm.0 <- dbglm(D2.0.trai, y = yt, family = "binomial",
    maxiter = 25, rel.gvar = 0.9)
R> pred.dbglm.0 <- predict(res.dbglm.0, D2.0[-trai,trai],
    type_var = "D2", type = "response")
R> dbglm.err.0 <- (abs(pred.dbglm.0 - yv) > .5)
R> print(sum(dbglm.err.0))
```

In order to use the first or the second derivatives, the parameter nderiv at the second sentence must be set equal to 1 or 2, respectively, to obtain the corresponding distance matrices D2.1, D2.1.trai, D2.2 and D2.0.trai. The rest of the code must be changed accordingly (see Annex B). The results of DB-GLM fits, in term of the number of wheat samples in the validation set that are bad classified, are shown at the second column of Table 3. In this case the use of derivatives improves the results. The performances of functional GLM and DB-GLM are comparable.

We are fitting now local distance based generalized linear models (local DB-GLM) with the function ldbglm. We are using again L^2 distances between NIR spectra functions or their derivatives. The automatic choice of the smoothing parameter h will be done with the Generalized Cross Validation criterium (method="GCV"; results using different methods are similar).

We show the code used for fitting the local DB-GLM when NIR spectra functions are used as predictors.

```
R> res.ldbglm.0 <- ldbglm(D2.0.trai, y = yt, family = "binomial",
maxiter = 25, method = "GCV", h.range = c(2,4), rel.gvar = 0.9)
```

Observe that it has been necessary to modify the default range of candidate values for h (h.range = c(2,4)). By default the range for h was [.5,2] and the optimum value for h was the upper limit of this interval. Plotting the fitted DB-GLM model (using plot(res.ldbglm.0, which = 3)) it can be seen that the range [2,4] is addequate for h. The optimal value is attained at h = 2.3331, as it can be seen when doing the summary of the fitted model:

R > summary(res.ldbglm.0)

```
call:
        ldbglm.D2(D2_1 = D2.0.trai, y = yt, family = "binomial", method = "GCV",
    h.range = c(2, 4), rel.gvar = 0.9, maxiter = 25)
Residuals:
   Min. 1st Qu.
                 Median
                            Mean 3rd Qu.
                                             Max.
-0.7100 -0.2875 -0.0550 -0.0150 0.2150
                                          0.8400
Number of Observations: 60
R-squared : 0.3852
Trace of smoother matrix: 4.74
family: binomial
kind of kernel= (1) Epanechnikov
optimal bandwidth h : 2.333058
GCV value criterion : 3.323117e-03
Now the prediction for the validation set is done:
```

```
R> pred.ldbglm.0 <- predict(res.ldbglm.0, D2.0[-trai,trai],
    type_var = "D2", type = "response")$fit
R> ldbglm.err.0 <- (abs(pred.ldbglm.0 - yv) > .5)
R> print(sum(ldbglm.err.0))
```

The number of bad classified wheat samples is 8, as it can be seen at the third column of Table 3. In order to use the first or the second derivatives of NIR spectra functions as predictors, distance matrices D2.0 and D2.0.trai must be replaced by D2.1 and D2.1.trai, or by D2.2 and D2.0.trai. The rest of the code must be changed accordingly (see Annex B). Care must be taken when choosing a sensible range where bandwidth h must be, because the range of values for distances between the observed functions is quite different to that corresponding to their first or second derivatives. In this case the range used h when using first derivatives whas h.range=c(0.003,0.007) and it was h.range=c(0.0004,0.001) when using second derivatives. Look at the third column of Table 3 to see the number of bad classified samples in the validation set. It follows from these number that the three local DB-GLM fits performs similarly and that they do a little better job than functional GLM or global DB-GLM.

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A. Code excerpts

```
R> ###### Poisson (Logarithmic link) and Gower's distance
R> ## Case: rel.gvar = 1
R> dbglm1 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = poisson (link = "log"), metric = "gower", weights
= w, rel.gvar = 1)
R> ## Case: method = "GCV"
R> dbglm2 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,</pre>
family = poisson (link = "log"), metric = "gower", weights
= w, method= "GCV", full_search=TRUE)
R> ## Case: rel.gvar = 0.90
R> dbglm3 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = poisson(link = "log"), metric = "gower", weights
= w, rel.gvar = 0.90)
R> ###### Poisson (Logarithmic link) and Euclidean distance
R> ## With dbglm, case: rel.gvar = 1
R> dbglm4 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = poisson(link = "log"), metric = "euclidean", weights
= w, rel.gvar = 1)
R> ## With glm
R> glm1 <- glm(y ~ KmC + BonC + factor(MakeC), family =
poisson(link = "log"), data = Motor1, weights = w)
R> ###### Binomial (Logit link) and Gower's distance
R > ## rel.gvar = 1
R> dbglm5 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = binomial(link = "logit"), metric = "gower", weights
= w, rel.gvar = 1, full_search=TRUE)
R > ## method = "GCV"
R> dbglm6 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = binomial(link = "logit"), metric = "gower", weights
= w, method = "GCV")
R > \#\# rel.gvar = 0.90
R> dbglm7 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,</pre>
family = binomial(link = "logit"), metric = "gower", weights
 = w, rel.gvar = 0.90)
```

```
R> ###### Binomial (Logit link) and Euclidean distance
R> ## With dbglm, case: rel.gvar = 1
R> dbglm8 <- dbglm(y ~ KmC + BonC + factor(MakeC), Motor1,
family = binomial(link = "logit"), metric = "euclidean", weights
= w, rel.gvar = 1)
R> ## With glm
R> glm2 <- glm(y ~ KmC + BonC + factor(MakeC), family =
binomial(link = "logit"), data = Motor1, weights = w)
```

B. Code excerpts

```
## fregre.glm. Functional predictor:
## 1st derivative of NIR spectra function
R> f1 <- protein~ws.d1
R> res.glm.1 <- fregre.glm(f1, ldata, family = binomial,
basis.x = basis.ws, basis.b = basis.b)
R> pred.glm.1 <- predict.fregre.glm(res.glm.1, newldata)
R> glm.err.1 <- (abs(pred.glm.1 - yv) > .5)
R> print(sum(glm.err.1))
## fregre.glm. Functional predictor:
## 2nd derivative of NIR spectra function
R> f2 <- protein~ws.d2
R> res.glm.2 <- fregre.glm(f2, ldata, family = binomial,
basis.x = basis.ws, basis.b = basis.b)
R> pred.glm.2 <- predict.fregre.glm(res.glm.2, newldata)
R> glm.err.2 <- (abs(pred.glm.2 - yv) > .5)
R> print(sum(glm.err.2))
## dbglm. Functional predictor:
## 1st derivative of NIR spectra function
R> ws.d1 <- fdata.deriv(whtspec.fdata)
R> D2.1 <- semimetric.basis(ws.d1, ws.d1, nbasis1 = 18,
nbasis2 = 18) ^2
R> class(D2.1) <- "D2"
R> D2.1.trai <- D2.1[trai,trai]</pre>
R> class(D2.1.trai) <- "D2"</pre>
R> res.dbglm.1 <- dbglm(D2.1.trai, y = yt, family = "binomial",</pre>
maxiter = 25, rel.gvar = 0.9)
R> pred.dbglm.1 <- predict(res.dbglm.1, D2.1[-trai,trai],</pre>
 type_var = "D2", type = "response")
```

```
R> dbglm.err.1 <- (abs(pred.dbglm.1 - yv) > .5)
R> print(sum(dbglm.err.1))
## dbglm. Functional predictor:
## 2nd derivative of NIR spectra function
R> ws.d2 <- fdata.deriv(ws.d1)</pre>
R> D2.2 <- semimetric.basis(ws.d2, ws.d2, nbasis1 = 18,
nbasis2 = 18) ^2
R> class(D2.2) <- "D2"
R> D2.2.trai <- D2.2[trai,trai]
R> class(D2.2.trai) <- "D2"</pre>
R> res.dbglm.2 <- dbglm(D2.2.trai, y = yt, family = "binomial",
maxiter = 25, rel.gvar = 0.9)
R> pred.dbglm.2 <- predict(res.dbglm.2, D2.2[-trai,trai],</pre>
 type_var = "D2", type = "response")
R> dbglm.err.2 <- (abs(pred.dbglm.2 - yv) > .5)
R> print(sum(dbglm.err.2))
## ldbglm. Functional predictor:
## 1st derivative of NIR spectra function
R> res.ldbglm.1 <- ldbglm(D2.1.trai, y = yt, family = "binomial",
maxiter = 25, method = "GCV", h.range = c(0.003, 0.007),
rel.gvar = 0.9)
R> pred.ldbglm.1 <- predict(res.ldbglm.1, D2.1[-trai,trai],</pre>
type_var = "D2", type = "response")$fit
R> ldbglm.err.1 <- (abs(pred.ldbglm.1 - yv) > .5)
R> print(sum(ldbglm.err.1))
## ldbglm. Functional predictor:
## 2nd derivative of NIR spectra function
R> res.ldbglm.2 <- ldbglm(D2.2.trai, y = yt, family = "binomial",
maxiter = 25, method = "GCV", h.range = c(0.0004, 0.001),
rel.gvar = 0.9)
R> pred.ldbglm.2 <- predict(res.ldbglm.2, D2.2[-trai,trai],</pre>
type_var = "D2", type = "response")$fit
R> ldbglm.err.2 <- (abs(pred.ldbglm.2 - yv) > .5)
R> print(sum(ldbglm.err.2))
```

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