globber package

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Introduction

The package globber provides two tools to estimate the function f in the following nonparametric regression model:

$$Y_i = f(x_i) + \varepsilon_i, \quad 1 \leq i \leq n, \tag{1}$$

where the ε_i are i.i.d centered random variables of variance σ^2, the x_i are observation points which belong to a compact set S of $\mathbb{R}^d$, $d = 1$ or 2 and n is the total number of observations. This estimation is performed using the GLOBER approach described in [1]. This method consists in estimating f by approximating it with a linear combination of B-splines, where their knots are selected adaptively using the Generalized Lasso proposed by [2], since they can be seen as changes in the derivatives of the function to estimate. We refer the reader to [1] for further details.

Estimation of f in the one-dimensional case ($d = 1$)

In the following, we apply our method to a function of one input variable f_1. This function is defined as a linear combination of quadratic B-splines with the set of knots $\mathbf{t} = (0.1, 0.27, 0.745)$ and $\sigma = 0.1$ in (1).

Description of the dataset

We load the dataset of observations with $n = 70$ provided within the package $(x_1, \ldots, x_{70})$:

```
## --- Loading the values of the input variable --- ##
data('x_1D')
```

and $(Y_1, \ldots, Y_{70})$:

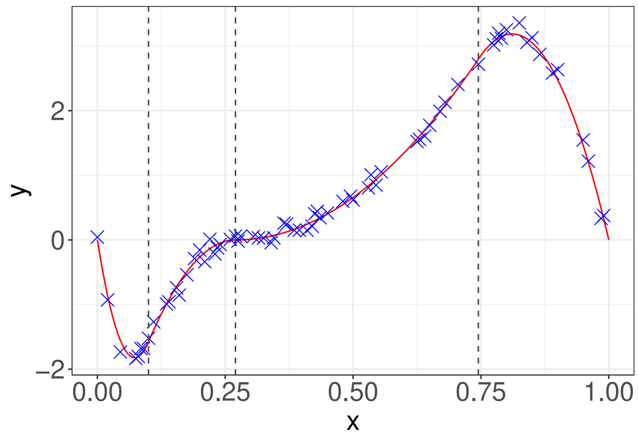
```
## --- Loading the corresponding noisy values of the response variable --- ##
data('y_1D')
```

We load the dataset containing the values of the input variable $\{x_1, \ldots, x_N\}$ for which an estimation of f_1 is sought. They correspond to the observation points as well as additional points where f_1 has not been observed. Here, $N = 201$. In order to have a better idea of the underlying function f_1, we load the corresponding evaluations of f_1 at these input values.

```
## --- Loading the values of the input variable for which an estimation
## of f_1 is required --- ##
data('xpred_1D')
## --- Loading the corresponding evaluations to plot the function --- ##
data('f_1D')
```

We can visualize it for 201 input values by using the ggplot2 package:

```
## -- Building dataframes to plot -- ##
data_1D = data.frame(x = xpred_1D, f = f_1D)
obs_1D = data.frame(x = x_1D, y = y_1D)
real.knots = c(0.1, 0.27,0.745)
```



The vertical dashed lines represent the real knots **t** implied in the definition of f_1, the red curve describes the true underlying function f_1 to estimate and the blue crosses are the observation points.

Application of `glober.1d` to estimate f_1

The `glober.1d` function of the `glober` package is applied by using the following arguments: the input values $(x_i)_{1\leq i\leq n}$ (`x`), the corresponding $(Y_i)_{1\leq i\leq n}$ (`y`), N input values $\{x_1,\dots,x_N\}$ for which f_1 has to be estimated (`xpred`) and the order of the B-spline basis used to estimate f_1 (`ord`).

```
res = glober.1d(x = x_1D, y = y_1D, xpred = xpred_1D, ord = 3, parallel = FALSE)
```

Additional arguments can also be used in this function:

- `parallel`: Logical, if set to TRUE then a parallelized version of the code is used. The default value is FALSE.
- `nb.Cores`: Numerical, it represents the number of cores used for parallelization, if parallel is set to TRUE.

The resulting outputs are the following:

- `festimated`: the estimated values of f_1.
- `knotSelec`: the selected knots used in the definition of the B-splines of the GLOBER estimator.
- `rss`: Residual sum-of-squares (RSS) of the model defined as: $\sum_{k=1}^{n}(Y_i - \widehat{f}_1(x_i))^2$, where $\widehat{f}_1$ is the estimator of f_1.
- `rsq`: R-squared of the model, calculated as $1 - RSS/TSS$ where TSS is the total sum-of-squares of the model defined as $\sum_{k=1}^{n}(Y_i - \bar{Y})^2$ with $\bar{Y} = (\sum_{i=1}^{n} Y_i)/n$.

Thus, we can print the estimated values corresponding to the input values $\{x_1,\dots,x_N\}$:

```
fhat = res$festimated
head(fhat)
```

```
## [1] -0.02579931 -0.26804301 -0.49284982 -0.70021972 -0.89015272 -1.06264882
```

The value of the Residual Sum-of-square:

```
res$rss
```

```
## [1] 40.91661
```

The value of the R-squared:

```
res$rsq
```

```
## [1] 0.9970843
```

We can get the set of the estimated knots $\widehat{\mathbf{t}}$:

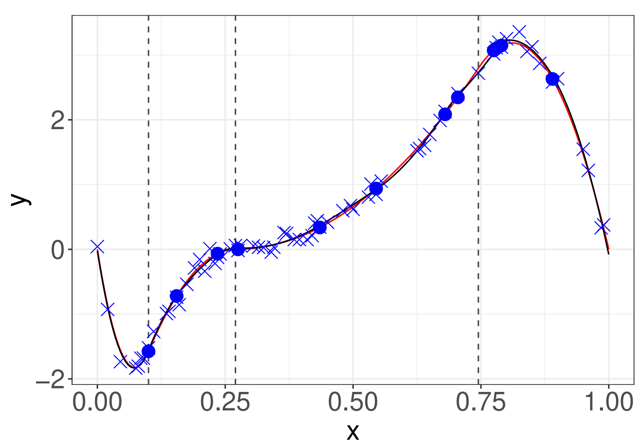
```
knots.set = res$Selected.knots
print(knots.set)
```

```
##  [1] 0.100 0.155 0.235 0.275 0.435 0.545 0.680 0.705 0.775 0.780 0.790 0.890
```

Finally, we can display the estimation of f_1 by using the ggplot2 package:

```
## Dataframe of selected knots ##
idknots = which(xpred_1D %in% knots.set)
yknots = f_1D[idknots]
data_knots = data.frame(x.knots = knots.set, y.knots = yknots)
## Dataframe of the estimation ##
data_res = data.frame(xpred = xpred_1D, fhat = fhat)

plot_1D = ggplot(data_1D, aes(xpred_1D, f_1D)) +
    geom_line(color = 'red') +
    geom_line(data = data_1D, aes(x = xpred_1D, y = fhat), color = "black") +
    geom_vline(xintercept = real.knots, linetype = 'dashed', color = 'grey27') +
    geom_point(aes(x, y), data = obs_1D, shape = 4, color = "blue", size = 4)+
    geom_point(aes(x.knots, y.knots), data = data_knots, shape = 19, color = "blue",
               size = 4)+
    xlab('x') +
    ylab('y') +
    theme_bw()+
    theme(axis.title.x = element_text(size = 20), axis.title.y = element_text(size = 20),
          axis.text.x = element_text(size = 19),
          axis.text.y = element_text(size = 19))
plot_1D
```



The vertical dashed lines represent the real knots $\mathbf{t}$ implied in the definition of f_1, the red curve describes the true underlying function f_1 to estimate, the black curve corresponds to the estimation with GLOBER, the blue crosses are the observation points and the blue bullets are the observation points chosen as estimated knots $\widehat{t}$.

Estimation of f in the two-dimensional case ($d = 2$)

In the following, we apply our method to a function of two input variables f_2. This function is defined as a linear combination of tensor products of quadratic univariate B-splines with the sets of knots $\mathbf{t}_1 = (0.24, 0.545)$ and $\mathbf{t}_2 = (0.395, 0.645)$ and $\sigma = 0.01$ in (1).

Description of the dataset

We load the dataset of observations with $n = 100$, provided within the package $(x_1, \ldots, x_{100})$

```
## --- Loading the values of the input variables --- ##
data('x_2D')
head(x_2D)
```

```
##       Var1  Var2
## [1,] 0.005 0.005
## [2,] 0.005 0.385
## [3,] 0.005 0.390
## [4,] 0.005 0.395
## [5,] 0.005 0.640
## [6,] 0.005 0.645
```

and $(Y_1, \ldots, Y_{100})$:

```
## --- Loading the corresponding noisy values of the response variable --- ##
data('y_2D')
```

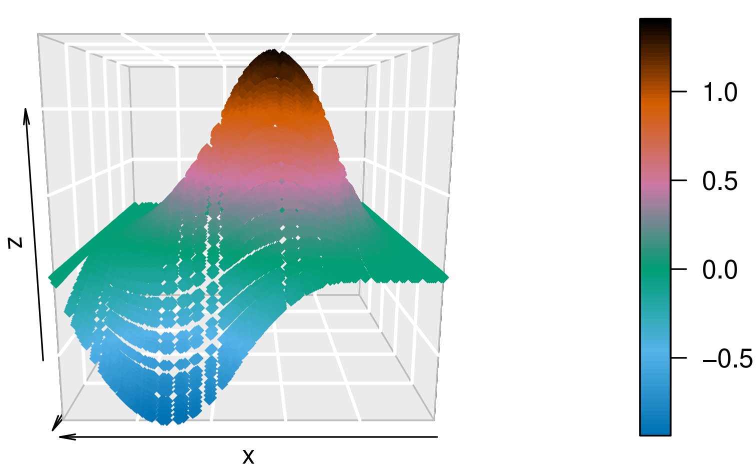
We load the dataset containing the values of the input variables $\{x_1, \ldots, x_N\}$ for which an estimation of f_2 is sought. They correspond to the observation points as well as additional points where f_2 has not been observed. Here, $N = 10000$. In order to have a better idea of the underlying function f_2, we load the corresponding evaluations of f_2 at these input values.

```
## --- Loading the values of the input variables for which an estimation
## of f_2 is required --- ##
data('xpred_2D')
head(xpred_2D)
```

```
##      Var1  Var2
## [1,]    0 0.000
## [2,]    0 0.005
## [3,]    0 0.015
## [4,]    0 0.035
## [5,]    0 0.050
## [6,]    0 0.080
```

```
## --- Loading the corresponding evaluations to plot the function --- ##
data('f_2D')
```

We can visualize it for 10000 input values by using the `plot3D` package:



Application of `glober.2d` to estimate f_2

The `glober.2d` function of the `glober` package is applied by using the following arguments: the input values $(x_i)_{1\leq i\leq n}$ (`x`), the corresponding $(Y_i)_{1\leq i\leq n}$ (`y`), N input values $\{x_1,\dots,x_N\}$ for which f_2 has to be estimated (`xpred`) and the order of the B-spline basis used to estimate f_2 (`ord`).

```
res = glober.2d(x = x_2D, y = y_2D, xpred = xpred_2D, ord = 3, parallel = FALSE)
```

Additional arguments can also be used in this function:

- `parallel`: Logical, if TRUE then a parallelized version of the code is used. Default is FALSE.
- `nb.Cores`: Numerical, it corresponds to the number of cores used for parallelization, if parallel is set to TRUE.

Outputs:

- `festimated`: the estimated values of f_2.
- `knotSelec`: the selected knots used in the definition of the B-splines of the GLOBER estimator.
- `rss`: Residual sum-of-squares (RSS) of the model defined as: $\sum_{k=1}^{n}(Y_i-\widehat{f}_2(x_i))^2$, where $\widehat{f}_2$ is the estimator of f_2.
- `rsq`: R-squared of the model, calculated as $1-RSS/TSS$ where TSS is the total sum-of-squares of the model defined as $\sum_{k=1}^{n}(Y_i-\bar{Y})^2$.

Thus, we can print the estimated values corresponding to the input values $\{x_1,\dots,x_N\}$:

```
fhat_2D = res$festimated
head(fhat_2D)
```

```
## [1] -0.001507484 -0.001594391 -0.001764006 -0.002086438 -0.002313565
## [6] -0.002730025
```

The value of the Residual Sum-of-square:

```
res$rss
```

```
## [1] 1.910738
```

The value of the R-squared:

```
res$rsq
```

```
## [1] 0.9988952
```

We can get the set of estimated knots for each dimension $\widehat{\mathbf{t}}_\mathbf{1}$ and $\widehat{\mathbf{t}}_\mathbf{2}$:

```
knots.set = res$Selected.knots
print('For the first dimension:')
```

```
## [1] "For the first dimension:"
```

```
print(knots.set[[1]])
```

```
## [1] 0.255 0.540
```

```
print('For the second dimension:')
```

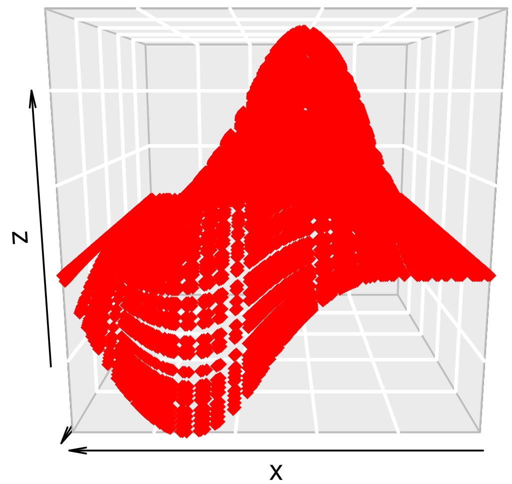
```
## [1] "For the second dimension:"
```

```
print(knots.set[[2]])
```

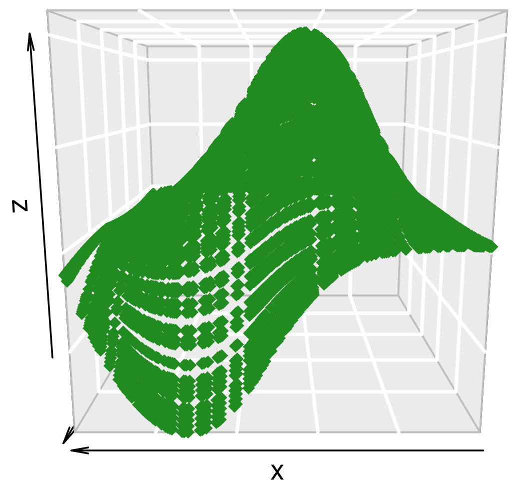
```
## [1] 0.650 0.655
```

As for f_1, we can visualize the corresponding estimation of f_2:

```r
scatter3D(xpred_2D[,1], xpred_2D[,2], f_2D, bty = "g", pch = 18, col = 'red',
          theta = 180, phi = 10)
```




```r
scatter3D(xpred_2D[,1], xpred_2D[,2], fhat_2D, bty = "g", pch = 18, col = 'forestgreen',
          theta = 180, phi = 10)
```



The red surface describes the true underlying function f_2 to estimate and the green surface corresponds to the estimation with GLOBER.

References

[1] Savino, M. E. and Lévy-Leduc, C. A novel approach for estimating functions in the multivariate setting based on an adaptive knot selection for B-splines with an application to a chemical system used in geoscience (2023), arXiv:2306.00686.

[2] Tibshirani, R. J. and J. Taylor (2011). The solution path of the generalized lasso. The Annals of Statistics 39(3), 1335 – 1371.