Some Examples of `sivipm` Use

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Contents

1 Brief description of the sivipm package

The **sivipm** R package computes total and individual sensitivity indices, significant components, and confidence intervals for the total sensitivity indices.

- The total and individual sensitivity indices are calculated using a method based on the VIP of the PLS regression, proposed by J.P. Gauchi ([Gauchi et all (2010)], [Gauchi (2012)], [Gauchi (2015)]).
- The `Q2` are calculated either by the S. Wold's rule, — the rule used in the SIMCA software ([SIMCA Software]) — or by the Miller's formulae ([Lazraq et all (2003)]) more adapted to big datasets.
- The significant components are calculated from the `Q2` of each response variable and from the cumulated Q2 (SIMCA rule), and and by the Lazraq & Cléroux test ([Lazraq and Cléroux (2001)]).
- The confidence intervals for the total sensitivity indices are determined by the bootstrap method.

The syntax of the package functions is given in the on-line help pages. Some examples of use are given here.

2 Data

The observed inputs and outputs must be stored in data-frames.

Input dataset may be,

- either, `raw` dataset. The number of columns is then the number of X-inputs,
- or `transformed` dataset. The number of columns is then the number of monomials in the polynomial. Each column is the value of a monomial calculated on non provided X-inputs.

Output dataset, or response variable, must be stored in a data-frame with one or several columns. The response can be uni or multivariate.

Missing values are accepted. However, if there are missing values and the response is multivariate, then it is not possible to compute the significant components.

Categorical variables must be transformed into indicator variables before processing analysis:

- if the variable has more than 2 categories, it must be split into as many 0/1 indicator variables as distinct categories;
- if it has two categories, set -1 on the lines corresponding to the first category, $+1$ on the lines corresponding to the second one (or vice versa);
- if it has one category only, the dataset is then not accepted.

The function `factorsplit` can be used to do this transformation: it creates a data-frame where the *factors* are split or changed into numeric variables.

2.1 Example of a raw dataset: cornell0

`cornell0` is an example of raw dataset. The data-frame contains seven input variables, followed by one response variable ([Kettaneh-Wold (1992)]).

```
Distillation  Reformat  NaphthaT  NaphthaC Polymer Alkylat Gasoline Y
0.00          0.23      0.00      0.00     0.00    0.74    0.03     98.7
0.00          0.10      0.00      0.00     0.12    0.74    0.04     97.8
0.00          0.00      0.00      0.10     0.12    0.74    0.04     96.6
0.00          0.49      0.00      0.00     0.12    0.37    0.02     92.0
0.00          0.00      0.00      0.62     0.12    0.18    0.08     86.6
0.00          0.62      0.00      0.00     0.00    0.37    0.01     91.2
0.17          0.27      0.10      0.38     0.00    0.00    0.08     81.9
0.17          0.19      0.10      0.38     0.02    0.06    0.08     83.1
0.17          0.21      0.10      0.38     0.00    0.06    0.08     82.4
0.17          0.15      0.10      0.38     0.02    0.10    0.08     83.2
0.21          0.36      0.12      0.25     0.00    0.00    0.06     81.4
0.00          0.00      0.00      0.55     0.00    0.37    0.08     88.1
```

Creation of the input data-frame, `XCornell0`, and the output data-frame, `YCornell0`:

```
> library(sivipm, lib.loc="/home/maiage/abouvier/sivipcheck")
> XCornell0 <- cornell0[,1:7] # inputs
> YCornell0 <- as.data.frame( cornell0[,8]) # output
> dimnames(YCornell0)[[2]] <- "Y"
```

2.2 Example of a transformed dataset: XY180

`XY180` is an example of transformed dataset[1]. The data-frame contains 160 columns. The first ones are the values of 158 monomials calculated on 18 inputs and the two last are the response variables.

```
> X180 <- XY180[,1:158]
> Y180 <- XY180[, 159:160]
> dimnames(Y180)[[2]]=c("Y1", "Y2")
```

3 Polynomial

The polynomial can be described,

- either, by a character vector,
- or be chosen among a list of standard types.

Note. The first monomials must always be the X-input variables.

From the input data-frame and its polynomial description, an object of class `polyX`[2] has to be created before processing the calculations. The following sections illustrate the way of creating a `polyX` object.

3.1 When the provided data are "raw" data

3.1.1 Polynomial described by a character vector

The polynomial can be described by a character vector, whose each element codes a monomial. The variables are identified either by their names or by their numbers. The character "*" (asterisk) denotes interaction between variables.

For example, we create the following polynomial of maximal degree equal to 3:

```
x1 + x2 + x3 + x4 + x5 + x6 + x7 + x1*x3 + x2*x2 +
x2*x4 + x3*x4 + x5*x5 + x6*x6 + x7*x7*x7
```

where `xi` is the X-input number `i`.
It is described by the following character vector, where the variables are identified by their numbers:

[1] This dataset is provided by S. Lefebvre (ONERA, Palaiseau, France) and described in [Gauchi (2015)].

[2] `polyX`: class which contains the polynomial description in a list structure and in an indicator matrix, and the transformed data, calculated on the raw data, if necessary.

```
> monomials <- c("1","2","3", "4","5", "6", "7",
+              "1*3", "2*2", "2*4", "3*4", "5*5",
+              "6*6", "7*7*7")
```

We could have identified the variables by their names as well:

```
> monomialsbis <- c("Distillation","Reformat","NaphthaT", "NaphthaC",
+                   "Polymer", "Alkylat", "Gasoline",
+                   "Distillation*NaphthaT", "Reformat*Reformat",
+                   "Reformat*NaphthaC",     "NaphthaT*NaphthaC",
+                   "Polymer*Polymer",       "Alkylat*Alkylat",
+                   "Gasoline*Gasoline*Gasoline")
```

The function **vect2polyX** creates the `polyX` object:

```
> PCornell0 <- vect2polyX (XCornell0, monomials)
```

3.1.2 Polynomial of standard type

The function **crpolyX** can be used to generated three types of standard polynomials:

- `full`: complete polynomial with all the terms of degree less or equal to the maximal degree. Example with 2 variables and degree 3:
  $x_1 + x_2 + {x_1}^2 + x_2 * x_1 + {x_2}^2 + {x_1}^3 + x_2 * {x_1}^2 + {x_2}^2 * x_1 + {x_2}^3$
- `power`: only power terms of degree less or equal to the maximal degree. Example with 2 variables and degree 3: $x_1 + x_2 + {x_1}^2 + {x_2}^2 + {x_1}^3 + {x_2}^3$
- `interact`: only interactions of degree less or equal to the maximal degree. Example with 2 variables and degree 3: $x_1 + x_2 + x_2 * x_1 + x_2 * {x_1}^2 + {x_2}^2 * x_1$

Note. The first monomials are always the X-input variables.

For example, we create a polynomial composed with the power terms of degree less or equal to 2 on the 3 first variables of `XCornell0`:

```
> PCornell0bis <- crpolyX(XCornell0[,1:3], 2, type="power")
> options(width=60) # set display width to avoid line truncation
> print(PCornell0bis, all=TRUE)
```

```
Distillation + Reformat + NaphthaT + Distillation*Distillation +
Reformat*Reformat + NaphthaT*NaphthaT
Polynomial description using variable numbers:
1 + 2 + 3 + 1*1 + 2*2 + 3*3
Polynomial degree:  2
Number of monomials:  6
Number of variables:  3
Number of observations: 12
```

3.2 When the provided data are transformed data

The functions which create a `polyX` object from transformed data and, respectively from a character vector, and from a standard type of polynomial, are `vect2PolyXT`, and `crpolyXT`.

3.2.1 Polynomial described by a character vector

The transformed data-frame X180 (see Section 2.2) is the result of the calculation of 158 monomials on 18 X-inputs.

1. The polynomial is described by a character vector. Here, the variables are identified by their numbers:

```
>   Pexp <- as.character(1:18)
> for (i in 1:13) {
+   Pexp <- c(Pexp, paste(i,"*",i, sep=""))
+ }
> for (i in 1:13) {
+   Pexp <- c(Pexp, paste(i,"*",i, "*",i, sep=""))
+ }
> for (i in 1:12) {
+   for (j in (i+1):13) {
+      Pexp <-  c(Pexp, paste(i,"*",j, sep=""))
+    }
+ }
> for (i in 1:18) {
+     if (i != 15)
+     Pexp <- c(Pexp, paste("15*",i,sep=""))
+   }
> for (i in 16:18) {
+     for (j in 9:11) {
+       Pexp <- c(Pexp, paste(i, "*", j,sep=""))
+    }
+ }
> Pexp <- c(Pexp, c("13*16"), c("13*17"), c("13*18"),
+             c("14*16"), c("14*17"), c("14*18"),
+            c("14*9"), c("14*10"), c("12*14"), c("2*14"))
```

2. We create the polyX object, by using the **vect2polyXT** function. The names of the 18 inputs must be explicitely provided, because, unlike the raw data case, they cannot be deduced from the column names of the input data-frame.

```
> varnames180 <- c("ALTI", "MACH", "POWERS", "EAI", "CAP",
+                   "YAW", "ROLL", "PITCH", "VIS", "RH",
+                   "TA", "HBASE", "HOUR", "MODEL", "CLOUDS",
+                "IHAZE1","IHAZE2", "IHAZE3")
> PX180 <- vect2polyXT(varnames180, X180, Pexp)
```

3.2.2 Polynomial of a standard type

For illustrative purpose, we suppose that the data-frame X180 is the result of the calculation of a polynomial of maximal degree 2 made up of the power terms. As this polynomial has 36 monomials only, the extra columns of X180 are ignored.

```
> PX180bis <- crpolyXT(varnames180, X180, 2, type="power")
> summary(PX180bis)
```

```
ALTI + MACH + POWERS + EAI + CAP + YAW + ROLL + PITCH + VIS +
RH + TA + HBASE + HOUR + MODEL + CLOUDS + IHAZE1 + IHAZE2 +
IHAZE3 + ALTI*ALTI + MACH*MACH + POWERS*POWERS + EAI*EAI + CAP*CAP +
YAW*YAW + ROLL*ROLL + PITCH*PITCH + VIS*VIS + RH*RH + TA*TA +
HBASE*HBASE + HOUR*HOUR + MODEL*MODEL + CLOUDS*CLOUDS + IHAZE1*IHAZE1 +
IHAZE2*IHAZE2 + IHAZE3*IHAZE3
Polynomial description using variable numbers:
1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9 + 10 + 11 + 12 + 13 + 14 +
15 + 16 + 17 + 18 + 1*1 + 2*2 + 3*3 + 4*4 + 5*5 + 6*6 + 7*7 +
8*8 + 9*9 + 10*10 + 11*11 + 12*12 + 13*13 + 14*14 + 15*15 +
16*16 + 17*17 + 18*18
Polynomial degree:  2
Number of monomials:  36
Number of variables:  18
Number of observations:  180
```

4 Polynomials handling

4.1 Binding polynomials

To put together the monomials of several polynomials calculated on the same dataset of inputs, use the `bind` method.

Example with the dataset `XCornell0`:

1. Creation of the first polynomial: a polynomial of degree 2, with the power terms only, calculated on the variables 3 and 4 of the data-frame `XCornell0`. Note that the unit monomials, those equal to the X-inputs, must always be included.

   ```
   > P1 <- crpolyX(XCornell0[, 3:4], 2, type="power")
   > print(P1, all=TRUE)

   NaphthaT + NaphthaC + NaphthaT*NaphthaT + NaphthaC*NaphthaC
   Polynomial description using variable numbers:
   1 + 2 + 1*1 + 2*2
   Polynomial degree:  2
   Number of monomials:  4
   Number of variables:  2
   Number of observations: 12
   ```

2. Creation of the second polynomial which only contains the interactions.

   ```
   > P2 <- vect2polyX(XCornell0[, 3:4], c("1", "2", "1*2"))
   > print(P2, all=TRUE)

   NaphthaT + NaphthaC + NaphthaT*NaphthaC
   Polynomial description using variable numbers:
   1 + 2 + 1*2
   Polynomial degree:  2
   Number of monomials:  3
   ```

```
Number of variables:  2
Number of observations: 12
```

3. Put together the monomials of these two polynomials:

```
> P3 <- bind(P1, P2)
> print(P3, all=TRUE)
```

```
NaphthaT + NaphthaC + NaphthaT*NaphthaT + NaphthaC*NaphthaC +
NaphthaT*NaphthaC
Polynomial description using variable numbers:
1 + 2 + 1*1 + 2*2 + 1*2
Polynomial degree:  2
Number of monomials:  5
Number of variables:  2
Number of observations: 12
```

Note. The duplicated monomials are removed.

4.2 Removing monomials from a polynomial

The function **takeoff** removes monomials from a `polyX` object.

Example:

```
> X <- cornell0[,1:3]
> monos <- c("Distillation","Reformat","NaphthaT",
+            "Distillation*Reformat","Reformat*Reformat")
> P <- vect2polyX (X, monos)
> # Remove the fourth and the fifth monomials:
> P2 <- takeoff(P, c(4,5))
> print(P2, all=TRUE)
```

```
Distillation + Reformat + NaphthaT
Polynomial description using variable numbers:
1 + 2 + 3
Polynomial degree:  2
Number of monomials:  3
Number of variables:  3
Number of observations: 12
```

Same where the monomials to suppress are expressed in character strings:

```
> P2 <- takeoff(P, c("Distillation*Reformat","Reformat*Reformat"))
```

Note. Taking off the monomials equal to the X-inputs is not accepted.

5 Calculations

5.1 Individual and total sensitivity indices, significant components

The function **sivipm** is the main function of the package. It calculates the individual and total sensitivity indices and the significant components. Its arguments are the response data-frame and the `polyX` object. Its options are:

- `nc`, the number of components (2 by default);
- `options`, a vector to limit what is returned. Valid values are:
  - `"fo.isivip"`, to return first order individual sensitivity indices,
  - `"tsivip"`, to return total sensitivity indices,
  - `"simca"` and `"lazraq"`, to return the significant components calculated by the SIMCA software rule ([SIMCA Software]) and by the Lazraq and Cléroux test ([Lazraq and Cléroux (2001)]), respectively. Threshold of these tests is 0.05.

  (all is returned by default);
- `graph`, for drawing a graph of the total sensitivity indices (FALSE by default);
- `alea` to insert a random variable (FALSE by default) (see Section 5.2);
- `output` to return intermediate results (none by default) (see Section 5.3).

The returned value is an object of class `sivip` whose non-null slots depend on what has been required:

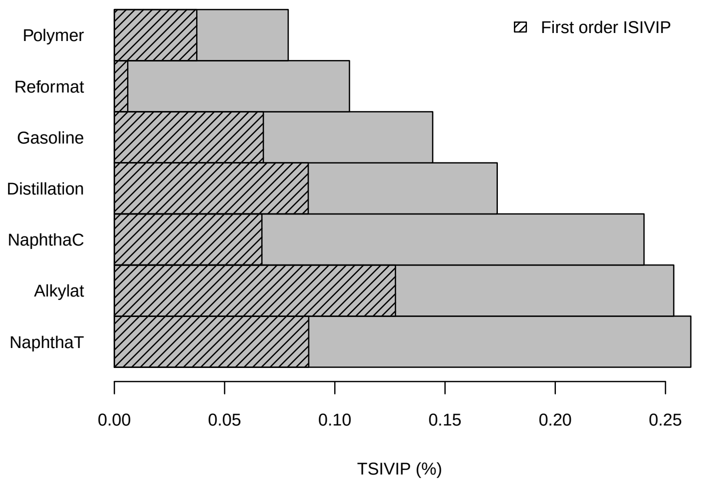
- When the vector `options` includes "fo.isivip":
  - `fo.isivip`, first order individual sensitivity indices.
- When the vector `options` includes "tsivip":
  - `tsivip`, the total sensitivity indices,
  - `percentage`, the sorted percentages of total sensitivity indices.
- When the vector `options` includes "simca" or "lazraq":
  - `simca.signifcomponents` or `lazraq.signifcomponents`, boolean vectors whose values are TRUE for the significant components.
- When the option `alea` is set (see Section 5.2):
  - `monosignif`, a boolean vector whose values are TRUE for the significant monomials,
  - `correlalea`, the correlation between the outputs and the random variable.
- When the option `output` is set:

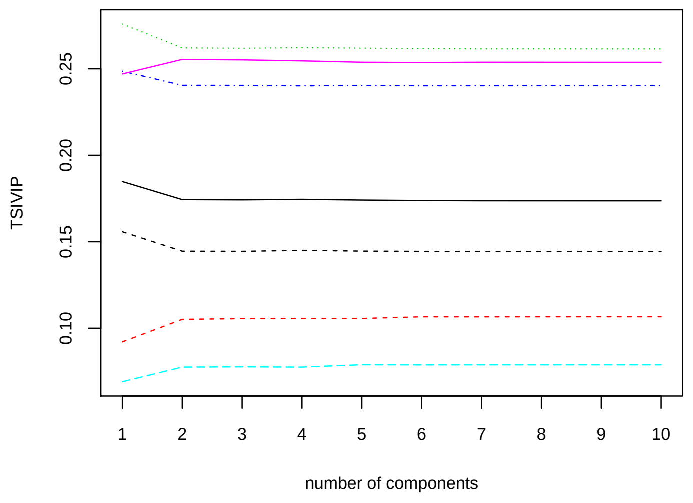
– `output`, a list of intermediate results (see Section 5.3).

The function **getNames**, applied on an object of class `sivip`, returns the names of the non-null slots.

Example with the response dataset `YCornell0` (see Section 2.1) and the `polyX` object `PCornell0` (see Section 3.1.1):

```
> sivipm(YCornell0, PCornell0, nc=10, graph= TRUE)

fo.isivip
Distillation     Reformat     NaphthaT     NaphthaC
 0.087939379  0.006049118  0.088147537  0.066914506
     Polymer      Alkylat     Gasoline
 0.037371483  0.127487898  0.067563383

tsivip
Distillation     Reformat     NaphthaT     NaphthaC
  0.17366732   0.10664095   0.26149630   0.24027001
     Polymer      Alkylat     Gasoline
  0.07884904   0.25375385   0.14440597

percentage
    NaphthaT      Alkylat     NaphthaC Distillation
   20.768783    20.153855    19.082930    13.793154
    Gasoline     Reformat      Polymer
   11.469134     8.469728     6.262416

simca.signifcomponents
        Y   Q2T
c1   TRUE  TRUE
c2   TRUE  TRUE
c3  FALSE FALSE
c4  FALSE FALSE
c5   TRUE  TRUE
c6   TRUE  TRUE
c7   TRUE  TRUE
c8   TRUE  TRUE
c9   TRUE  TRUE
c10 FALSE FALSE

lazraq.signifcomponents
   c1    c2    c3    c4    c5    c6    c7    c8    c9   c10
 TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
```



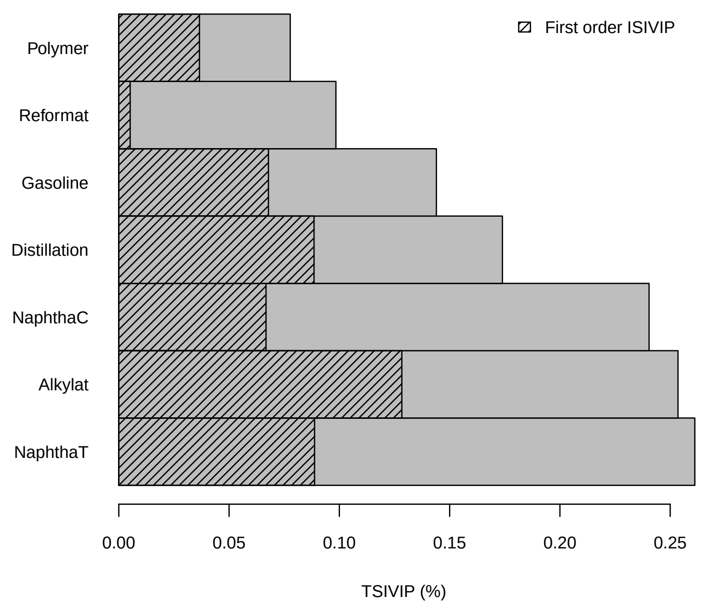


5.2 Add an alea in the computation of the total sensitivity indices

When the option **alea** is set, a uniform random variable is inserted into the computation of the total sensitivity indices. Comparison can then be made of its indices with the ones of the other variables. The non significant monomials, — those for which the individual sensitivity indices is less or equal than the one of the random variable — are excluded from the total sensitivity indices calculation. The correlation between the outputs and the random variable is returned.

Example with the response dataset `YCornell0` (see Section 2.1) and the `polyX` object `PCornell0` (see Section 3.1.1):

```
> set.seed(403)
> res <- sivipm(YCornell0, PCornell0, nc=2, alea=TRUE,
+                graph=TRUE, options=c("fo.isivip","tsivip"))
> res

fo.isivip
Distillation     Reformat     NaphthaT     NaphthaC
 0.088514873  0.005154289  0.088747415  0.066746055
     Polymer      Alkylat     Gasoline
 0.036573521  0.128327153  0.067852728

tsivip
Distillation     Reformat     NaphthaT     NaphthaC
  0.17393473   0.09843718   0.26116685   0.24042730
     Polymer      Alkylat     Gasoline
  0.07773183   0.25353931   0.14399843

percentage
    NaphthaT      Alkylat     NaphthaC Distillation
   20.906132    20.295555    19.245952    13.923293
    Gasoline     Reformat      Polymer
   11.526923     7.879793     6.222351

monosignif
              Distillation                  Reformat
                      TRUE                     FALSE
                  NaphthaT                  NaphthaC
                      TRUE                      TRUE
                   Polymer                   Alkylat
                      TRUE                      TRUE
                  Gasoline     Distillation*NaphthaT
                      TRUE                      TRUE
         Reformat*Reformat         Reformat*NaphthaC
                      TRUE                      TRUE
         NaphthaT*NaphthaC           Polymer*Polymer
                      TRUE                      TRUE
           Alkylat*Alkylat Gasoline*Gasoline*Gasoline
                      TRUE                      TRUE

correlalea
              Y
[1,] -0.2123951
```



5.3 Ask for more results

The expert user can require additional results by setting the option `output`. Detailed explanations of these results can be found in [Gauchi et all (2010)], [Gauchi (2012)] and [Gauchi (2015)].
`output` is a character vector whose valid values are:

- `isivip`: to return all the individual sensitivity indices
- `betaNat`: to return `betaNat` (natural β) and `betaNat0` (β coefficient)
- `VIP`: to return `VIP` and `VIPind`
- `Q2`: to return `Q2`, `Q2ckh` and `Q2cum`
- `PLS`: to return PLS results: `mweights, weights, x.scores, x.loadings, y.scores, y.loadings, cor.tx, cor.ty, expvar, X.hat, Y.hat`

Example with the response dataset `YCornell0` (see Section 2.1) and the `polyX` object `PCornell0` (see Section 3.1.1).

```
> res <- sivipm(YCornell0, PCornell0, nc=2, output= c("betaNat", "PLS"))
> getNames(res)
```

```
*** Names of the slots:
fo.isivip  tsivip  percentage  simca.signifcomponents  lazraq.signifcomponents  output
*** The slot 'output' is a list with components:
[1] "betaNat"  "betaNat0" "PLS"
```

```
*** The component 'output$PLS' is a list  with components:
 [1] "betaCR"     "mweights"   "x.scores"   "x.loadings"
 [5] "y.scores"   "y.loadings" "weights"    "cor.tx"
 [9] "cor.ty"     "expvar"     "x.hat"      "y.hat"
[13] "Q2ckh"
```

5.4 Computation Y by Y

To compute the total sensitivity indices for each response variable successively, use the R function **apply**.
Example with the two-columns data-frame `Y180`:

```
> l180 <- apply(Y180, 2, sivipm, PX180, nc=2, options="tsivip")
> names(l180)
```

```
[1] "Y1" "Y2"
```

```
> getNames(l180$Y1)
```

```
*** Names of the slots:
tsivip  percentage
```

```
> getNames(l180$Y2)
```

```
*** Names of the slots:
tsivip  percentage
```

5.5 When there are missing values

When there are missing values, it is not possible to calculate the significant components by the SIMCA software rule.
It is possible by the Lazraq and Cléroux test, if the response is univariate only.

To illustrate, we created the data-frame `cornell1` from `cornell0` by introducing some missing values. `lazraq.signifcomponents` are calculated:

```
> X <- cornell1[,1:7]
> Y <-as.data.frame( cornell1[,8])
> polyXm <- vect2polyX (X, monomials)
> sivipm(Y, polyXm, nc=8, options="lazraq")
```

```
lazraq.signifcomponents
   c1    c2    c3    c4    c5    c6    c7    c8
 TRUE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
```

5.6 When there is no polynomial description

The polynomial description is only required to calculate the total sensitivity indices. It can be omitted to compute the individual sensitivity indices of each column of the input dataset, and the significant components.
For example, we calculate the first order individual sensitivity indices of all the columns of the transformed dataset `XY180`, without having to describe the polynomial:

```
> b <- new("polyX", dataX.exp=X180)
> res <- sivipm(Y180, b, nc=2, options="fo.isivip")
> slotNames(res)
```

```
[1] "fo.isivip"                 "tsivip"
[3] "percentage"                "monosignif"
[5] "correlalea"                "simca.signifcomponents"
[7] "lazraq.signifcomponents" "output"
```

5.7 When the dataset is big

When the dataset is big, it is advised to set the option `fast` of the **sivipm** function. Then, the `Q2` and relative results are calculated from the Miller's formulae ([Lazraq et all (2003)]) more adapted to big datasets.

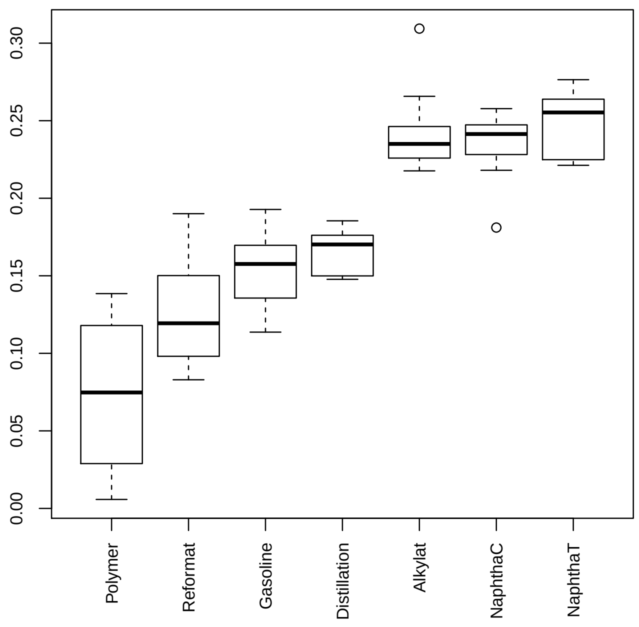
```
> resbis <- sivipm(Y180, b, nc=2, fast=TRUE, options="fo.isivip")
```

5.8 Confidence intervals for the total sensitivity indices by a bootstrap method

The function `sivipboot` calculates confidence intervals for the total sensitivity indices. Its arguments are the response data-frame, the `polyX` object, and the number of bootstrap loops. Its options are `nc`, the required number of components (2 by default), `alpha`, the test threshold (0.05 by default), and `graph` for a boxplot of the results. The option `fast` (see 5.7) is also available.
In the following example, confidence intervals are calculated in ten bootstrap loops:

```
> sivipboot(YCornell0, PCornell0, B=10 , nc=4, alpha=0.05, graph=TRUE)
```

```
                  IC.inf    IC.sup
Distillation 0.147709256 0.1854368
Reformat     0.082951362 0.1900557
NaphthaT     0.221228476 0.2764461
NaphthaC     0.181112141 0.2577898
Polymer      0.005790846 0.1385232
Alkylat      0.217641106 0.3093869
Gasoline     0.113681952 0.1927613
```



6 References

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