

Tutorial

KHIOPS 10.1

KHIOPS & KHIOPS VISUALIZATION

KHIOPS COCLUSTERING & KHIOPS COVISUALIZATION

MULTI-TABLE FUNCTIONALITIES



Khiops

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- **Khiops**
 - Optimal data preparation based on discretization and value grouping
 - Scoring models for classification and regression
 - Correlation analysis between pairs of variables



- **Khiops Visualization**
 - Analysis of Khiops results using an interactive visualization tool

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- **Khiops Coclustering**
 - Correlation analysis of two or more variables using a hierarchical coclustering model



- **Khiops Covisualization**
 - Exploratory analysis of Khiops Coclustering results using an interactive visualization tool

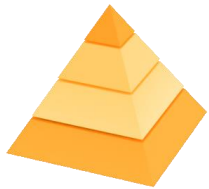
60



- **Multi-table functionalities**
 - Multi-table database
 - Automatic feature construction
 - Multi-table functionalities in Khiops and Khiops Coclustering

Khiops & Khiops Visualization

3



- **Khiops**
 - Optimal data preparation based on discretization and value grouping
 - Scoring models for classification and regression
 - Correlation analysis between pairs of variables



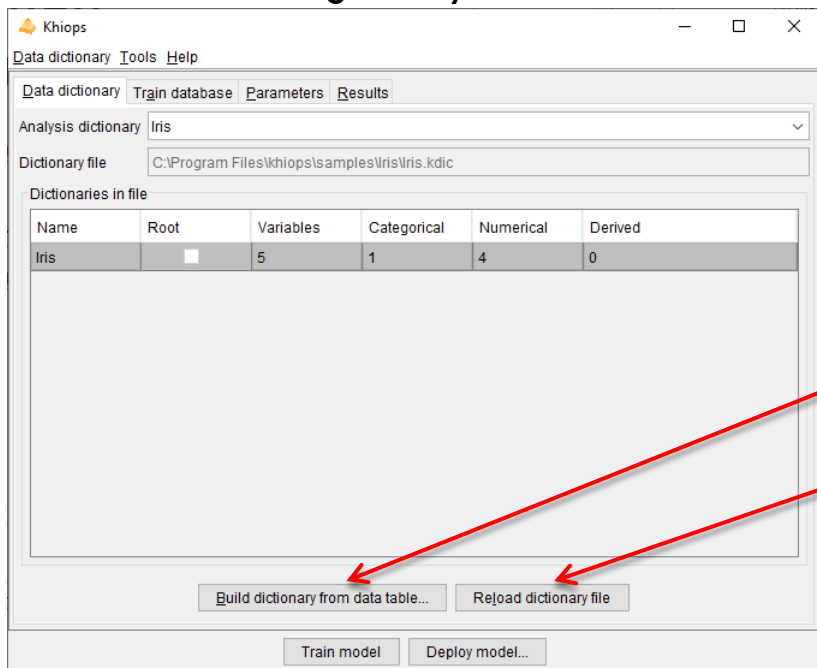
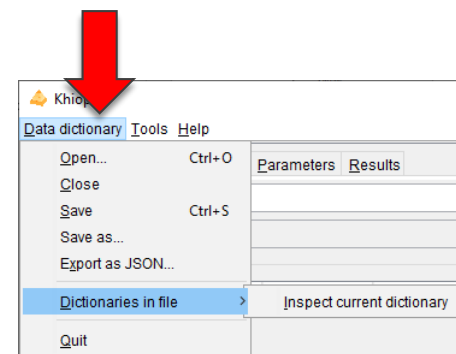
- **Khiops Visualization**
 - Analysis of Khiops results using an interactive visualization tool

Supervised classification

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- **Step 1 : Open an existing dictionary file**
(ex: sample Iris.kdic)

- Dictionary file: contains one or more dictionaries
- Dictionary: description of variables of a database to use during analysis



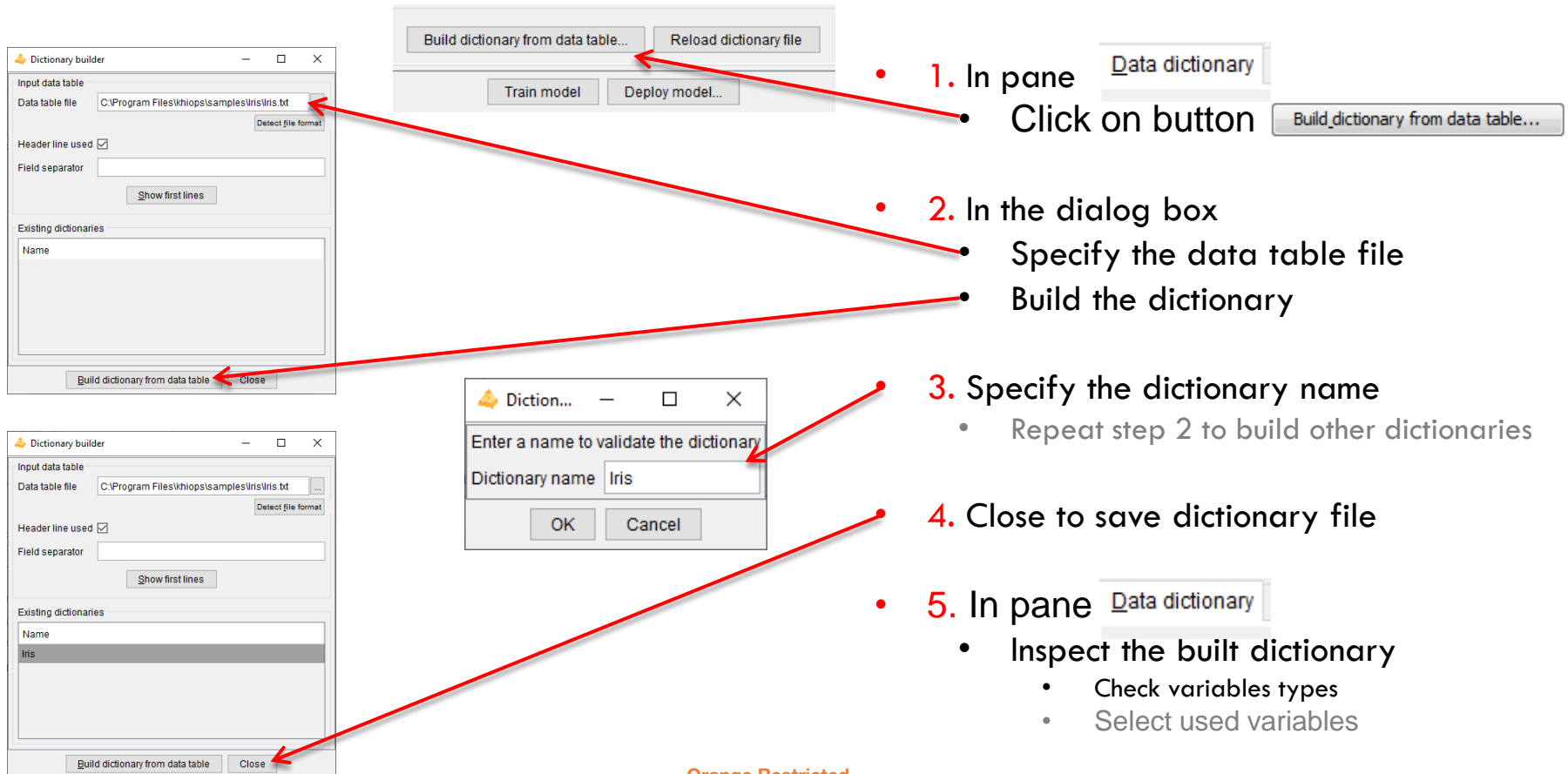
Available actions :

- Open, Save, Save as, Close
- Edition (menu « *Dictionary file/Inspect current dictionary* », or NotePad)
- Build dictionary from data table
- Reload dictionary file
 - useful if it has been modified from an external editor

Supervised classification

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- **Step 1, bis : Build a new dictionary from a data table**
(If no available dictionary)

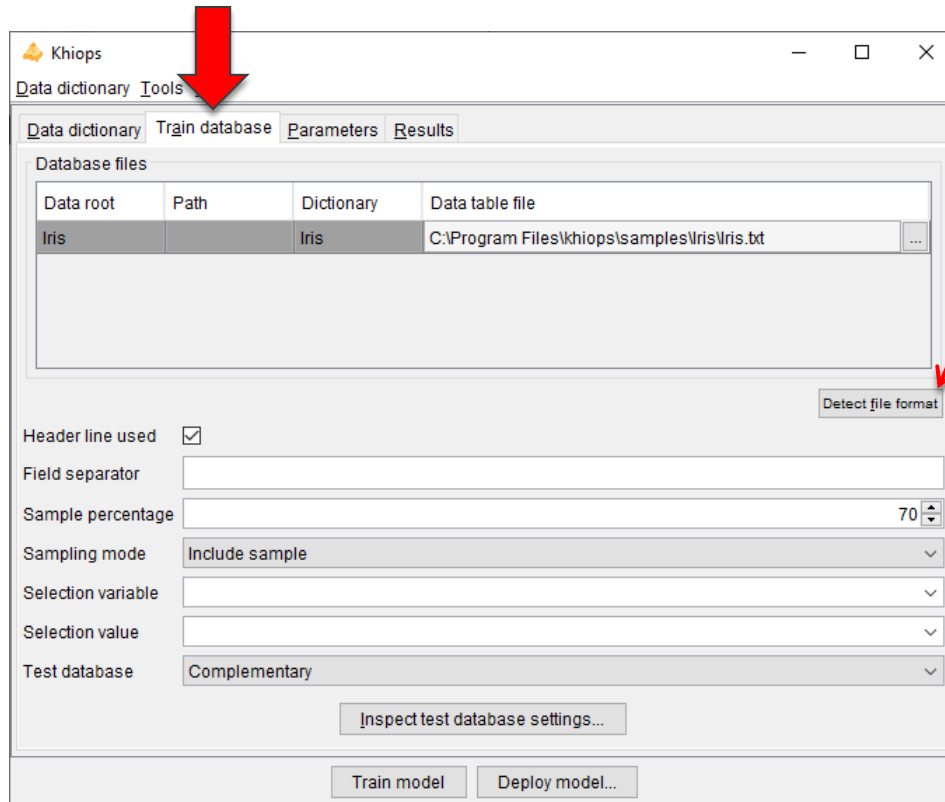


- 1. In pane **Data dictionary**
Click on button **Build dictionary from data table...**
- 2. In the dialog box
Specify the data table file
Build the dictionary
- 3. Specify the dictionary name
Repeat step 2 to build other dictionaries
- 4. Close to save dictionary file
- 5. In pane **Data dictionary**
Inspect the built dictionary
 - Check variables types
 - Select used variables

Supervised classification

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- **Step 2 : Specify train database**



| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|---|
| Iris | | Iris | C:\Program Files\khiops\samples\Iris\Iris.txt |

Header line used ☒

Field separator

Sample percentage

Sampling mode

Selection variable

Selection value

Test database

Detect file format : heuristic help that scans the first few lines to guess the file format. The header line and field separator are updated on success, with a warning or an error in the log window only if necessary.

File Format

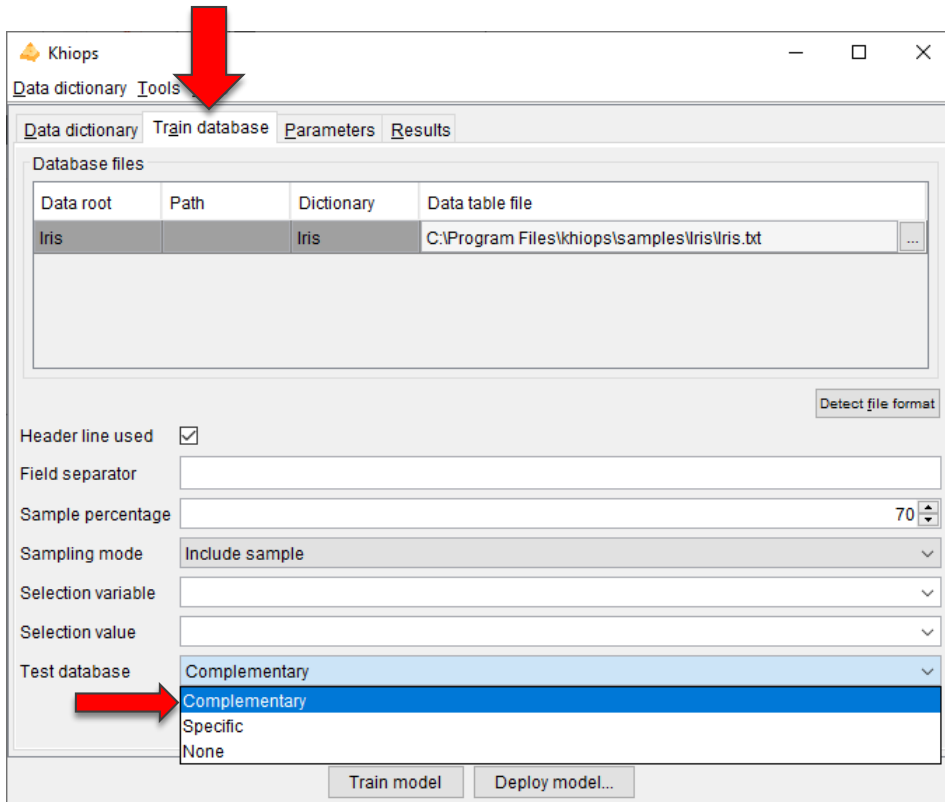
Sample percentage : default 70%

Controlled way of selecting the instances by the means of a **selection variable** and **selection value**

Supervised classification

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- **Step 2, bis : Specify test database**



The screenshot shows the 'Train database' dialog box in the Khiops software. The 'Tools' menu is highlighted with a red arrow. The 'Test database' dropdown menu is open, showing 'Complementary' as the selected option, with another red arrow pointing to it. The dialog box contains various settings for training a model, including a table for database files, a 'Header line used' checkbox, a 'Field separator' text field, a 'Sample percentage' spinner set to 70, a 'Sampling mode' dropdown set to 'Include sample', a 'Selection variable' dropdown, a 'Selection value' dropdown, and a 'Test database' dropdown. The 'Train model' and 'Deploy model...' buttons are at the bottom.

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|---|
| Iris | | Iris | C:\Program Files\khiops\samples\Iris\Iris.txt |

Header line used ☒

Field separator

Sample percentage

Sampling mode

Selection variable

Selection value

Test database

Train model Deploy model...

Three possibilities :

Complementary

Specific

None

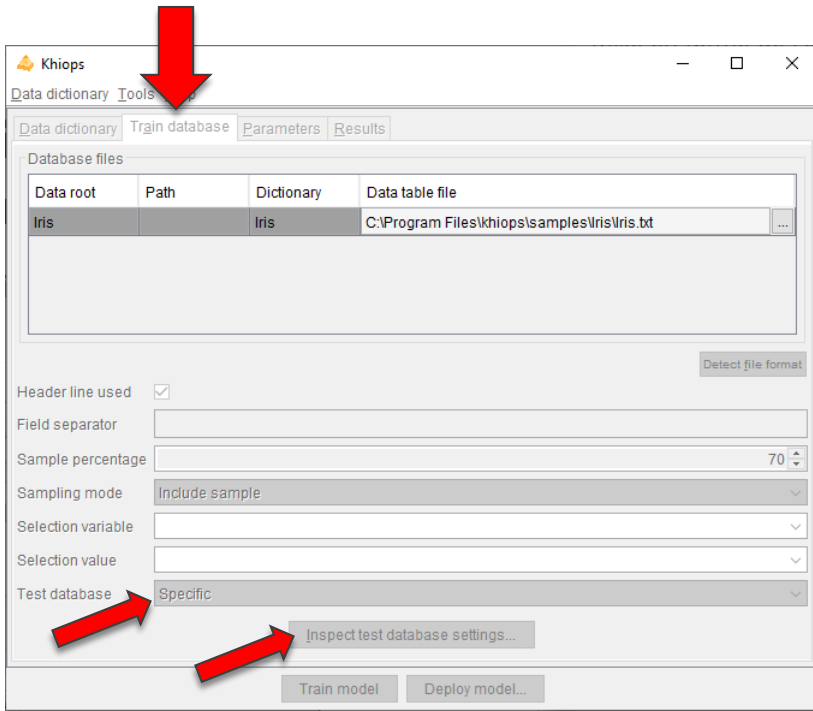
Complementary (default)

The test database is the complementary of the train database according to the chosen sample percentage

Supervised classification

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- **Step 2, ter :** Specify test database



Khops

Data dictionary Tools

Data dictionary Train database Parameters Results

Database files

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|--|
| Iris | | Iris | C:\Program Files\khops\samples\Iris\Iris.txt |

Detect file format

Header line used ☒

Field separator

Sample percentage 70

Sampling mode Include sample

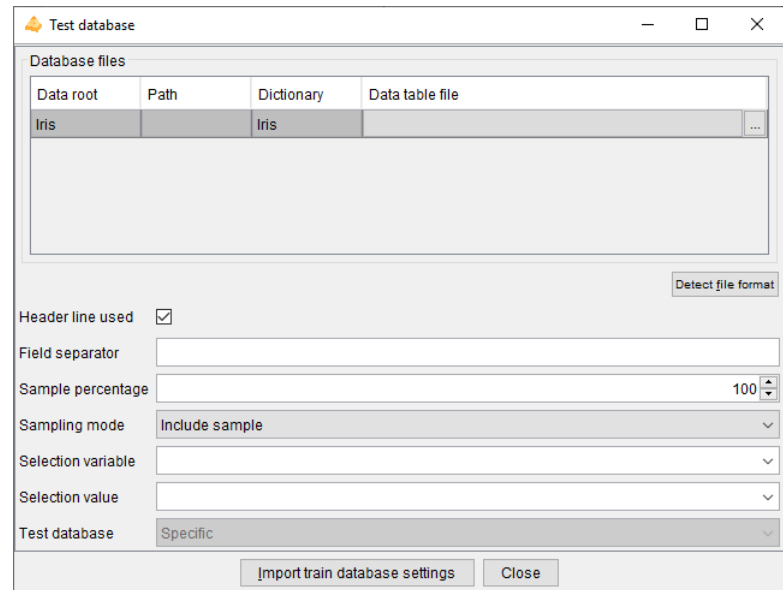
Selection variable

Selection value

Test database Specific

Inspect test database settings...

Train model Deploy model...



Test database

Database files

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|-----------------|
| Iris | | Iris | |

Detect file format

Header line used ☒

Field separator

Sample percentage 100

Sampling mode Include sample

Selection variable

Selection value

Test database Specific

Import train database settings Close

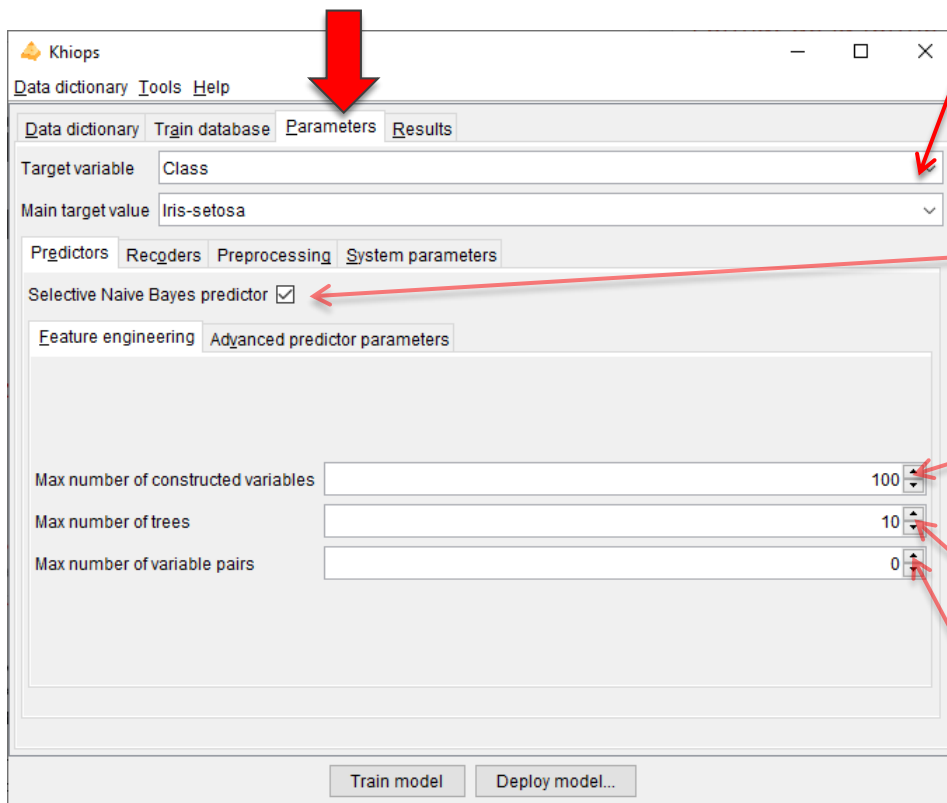
Specific

The test database has its own independent specification : specific file, sampling, selection

Supervised classification

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- **Step 3 : Parameters**



Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Target variable Class

Main target value Iris-setosa

Predictors Reducers Preprocessing System parameters

Selective Naïve Bayes predictor ☒

Feature engineering Advanced predictor parameters

Max number of constructed variables 100

Max number of trees 10

Max number of variable pairs 0

Train model Deploy model...

Type of selected target variable implies type of analysis

Categorical -> supervised classification

Numerical -> regression

Empty -> unsupervised analysis

Selective Naïve Bayes predictor

default true, to be set to false if only data preparation is wanted (without modeling)

Constructed variables are computed in multi-table schema and allow to extract numerical or categorical values resulting from computing formula applied to existing variable (default 100)

The constructed trees allow to combine variables, either native or constructed (default 10)

The pairs of variables are analyzed during data preparation using a bivariate discretization method (default 0)

Supervised classification

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- **Step 3 bis : Advanced predictor parameters (optional)**

Two other optional predictors
(only in the supervised case)

- **Baseline :** prediction of the majority class
(default false)


- **Univariate:** predictors exploiting one single variable
(default none)

Advanced parameters to inspect

Supervised classification

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- **Step 4 : Results**



Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters **Results**

Result files directory

Result files prefix **Fill a prefix**

Short description

Preparation report

2D preparation report

Modeling dictionary file

Modeling report

Train evaluation report

Test evaluation report

JSON report

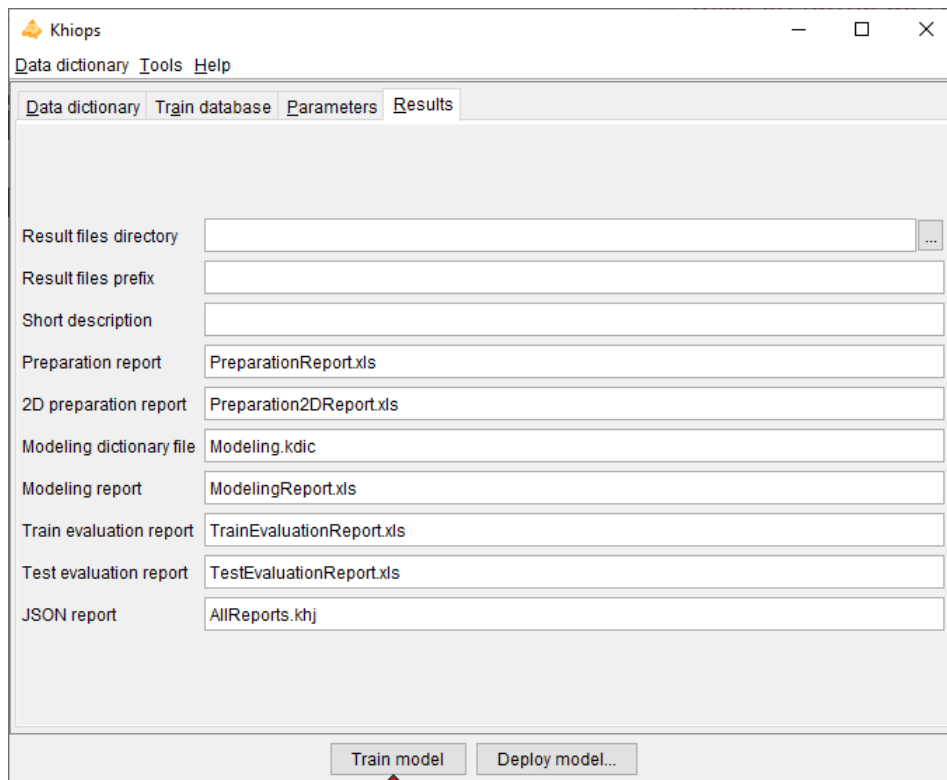
Train model Deploy model...

- Directory where all results files are written
- Prefix (ex: in case of several experiments)
- Brief description to summarize the current analysis
- Description of trained univariate preparation models
- Description of trained bivariate preparation models
- Technical description for deployment purposes
- Description of trained models with selected variables
- Evaluation on train database
- Evaluation on test database
- Json report, to get the analysis results from external tools

Supervised classification

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- Step 5 : Start the analysis**



Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Result files directory

Result files prefix

Short description

Preparation report PreparationReport.xls

2D preparation report Preparation2DReport.xls

Modeling dictionary file Modeling.kdic

Modeling report ModelingReport.xls

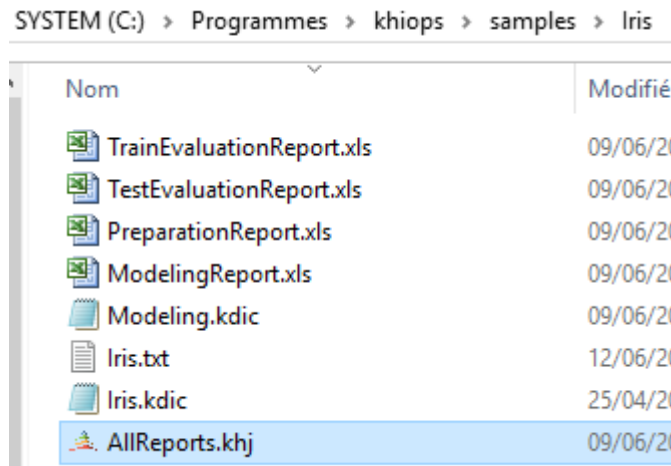
Train evaluation report TrainEvaluationReport.xls

Test evaluation report TestEvaluationReport.xls

JSON report AllReports.khj

Train model Deploy model...

1 – Train model



SYSTEM (C:) > Programmes > khiops > samples > Iris

| Nom | Modifié |
|---------------------------|----------|
| TrainEvaluationReport.xls | 09/06/21 |
| TestEvaluationReport.xls | 09/06/21 |
| PreparationReport.xls | 09/06/21 |
| ModelingReport.xls | 09/06/21 |
| Modeling.kdic | 09/06/21 |
| Iris.txt | 12/06/21 |
| Iris.kdic | 25/04/21 |
| AllReports.khj | 09/06/21 |

2 - Inspect the results using Khiops Visualization
(double-click on .khj file)



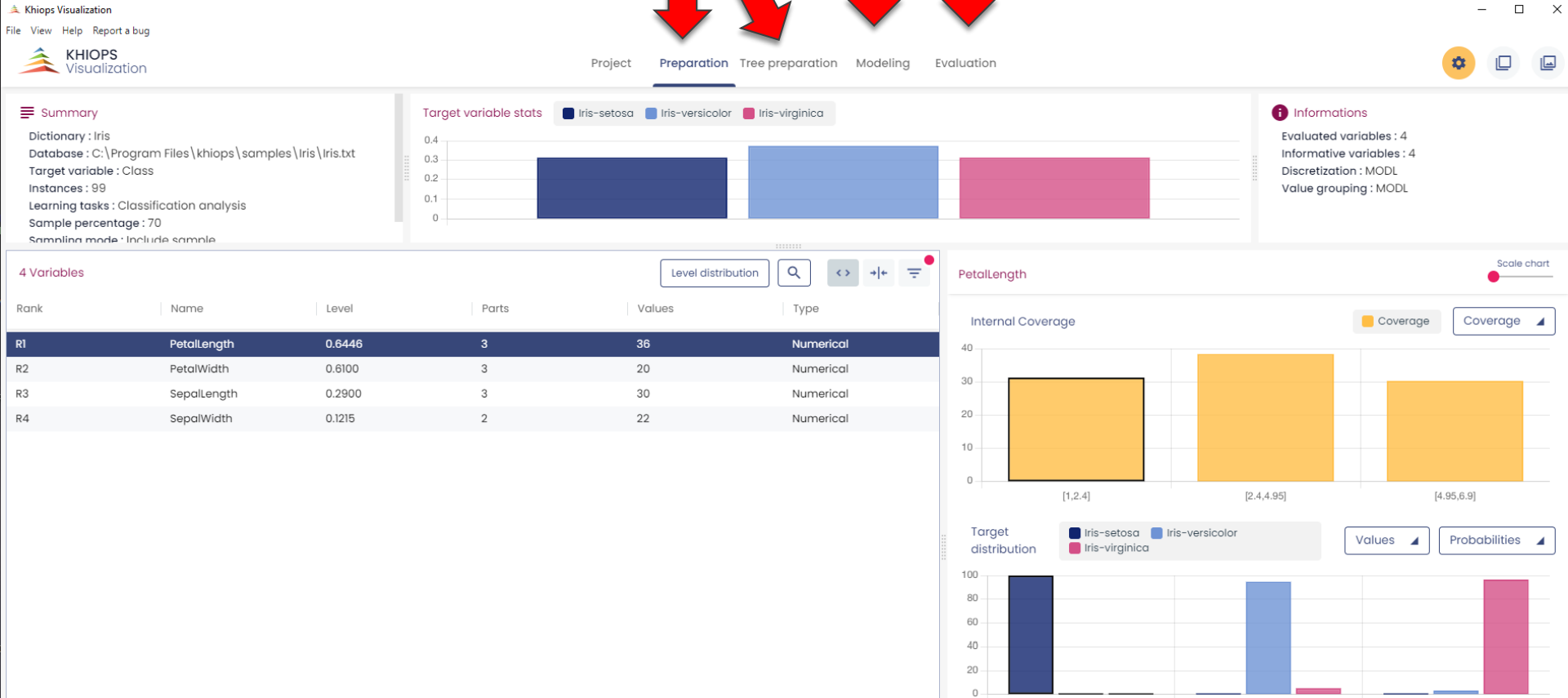
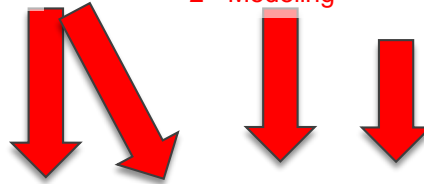
Exploratory of classification results using KHIOPS Visualization

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1 - Preparation

2 - Modeling

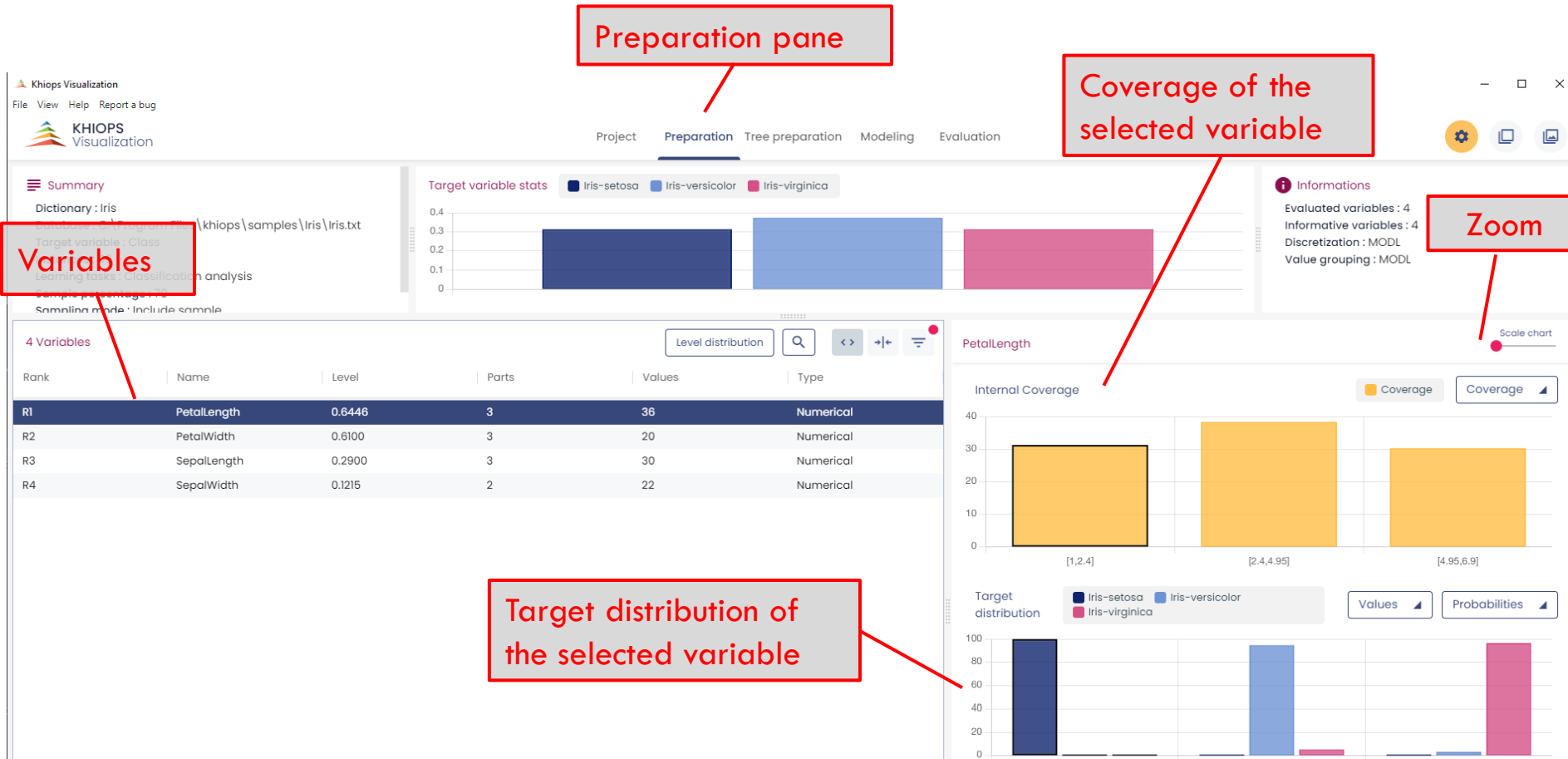
3 - Evaluation





Exploratory of classification results using KHIOPS Visualization

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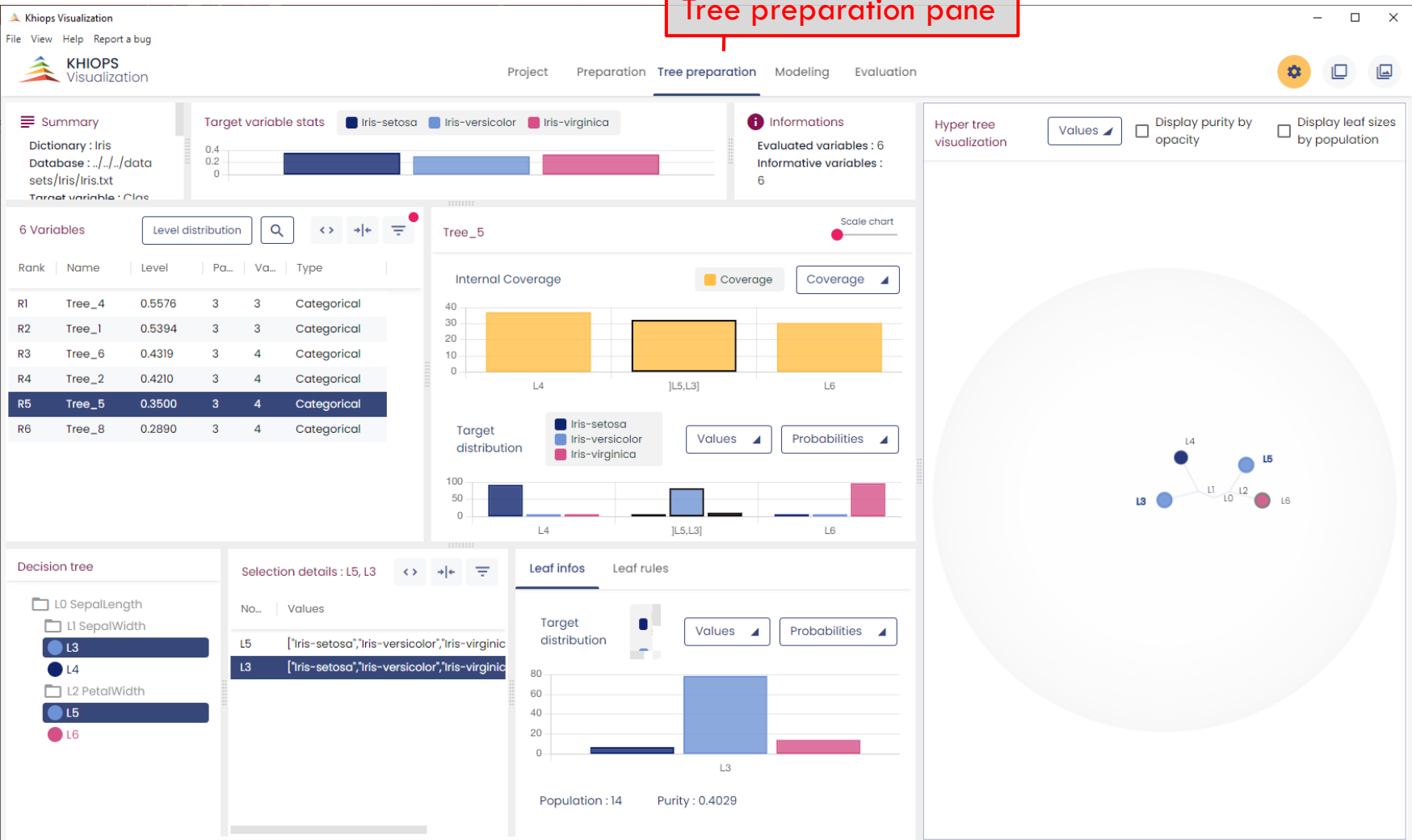




Exploratory of classification results using KHIOPS Visualization

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Tree preparation pane





Exploratory of classification results using KHIOPS Visualization

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Tree preparation pane

General information (as in Preparation pane)

Tree variables and their preparation (as in Preparation pane)

Decision tree

- ☐ L0 Sepallength
- ☐ L1 SepalWidth
- ☒ L3
- ☒ L4
- ☐ L2 PetalWidth
- ☒ L5
- ☒ L6

Hierarchy of the selected tree

Selection details : L5, L3

| No... | Values |
|-------|--|
| L5 | ["Iris-setosa","Iris-versicolor","Iris-virginica"] |
| L3 | ["Iris-setosa","Iris-versicolor","Iris-virginica"] |

Information on the selected group of leaves

Leaf infos

Leaf rules

Target distribution

Values

Probabilities

Information on the selected leaf

- infos: target distribution
- rules: sequence of tree tests

Hyper tree visualization

Values

Display purity by opacity

Display leaf sizes by population

Hypertree of the selected tree



Exploratory of classification results using KHIOPS Visualization

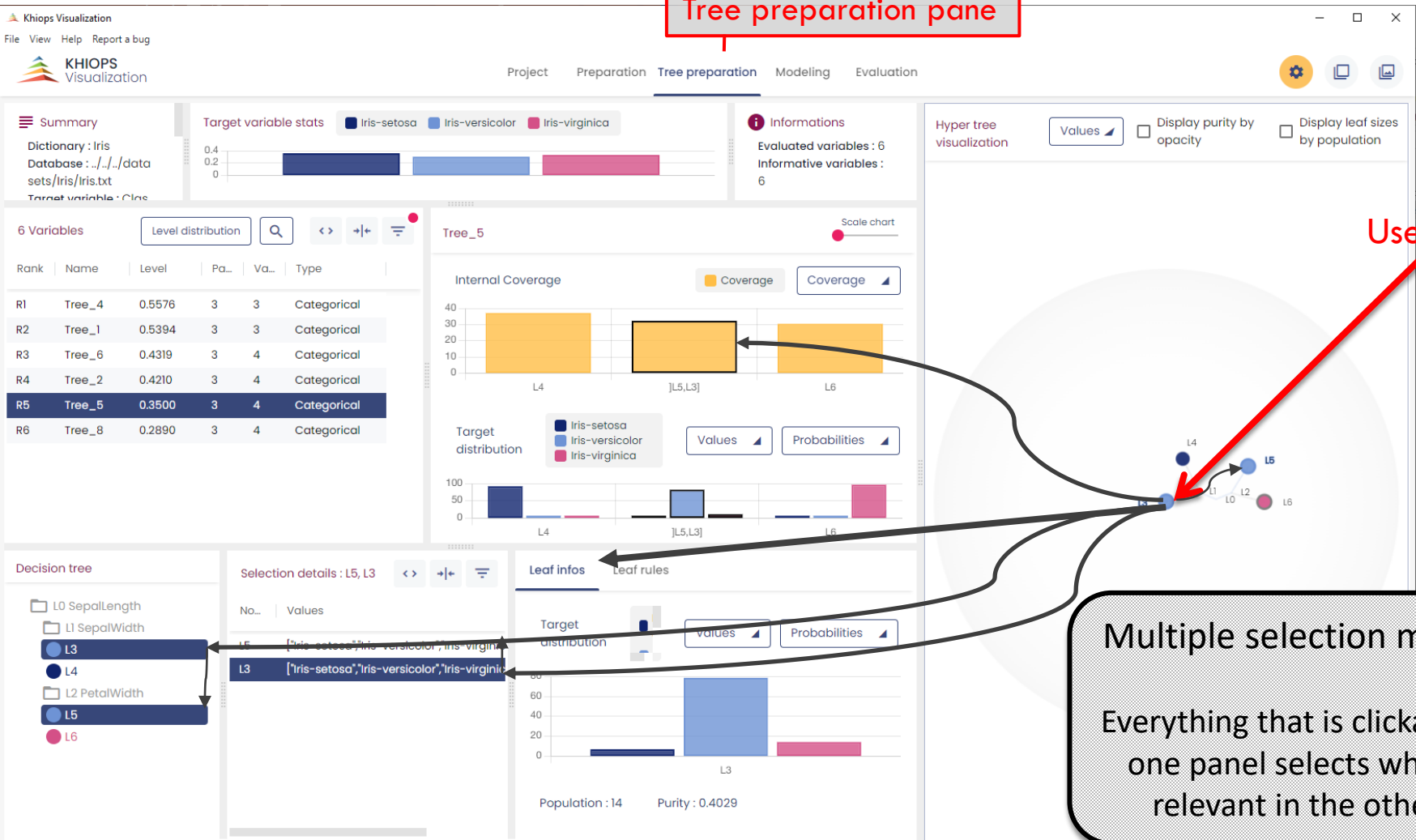
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Tree preparation pane

User click

Multiple selection modes

Everything that is clickable in one panel selects what is relevant in the others

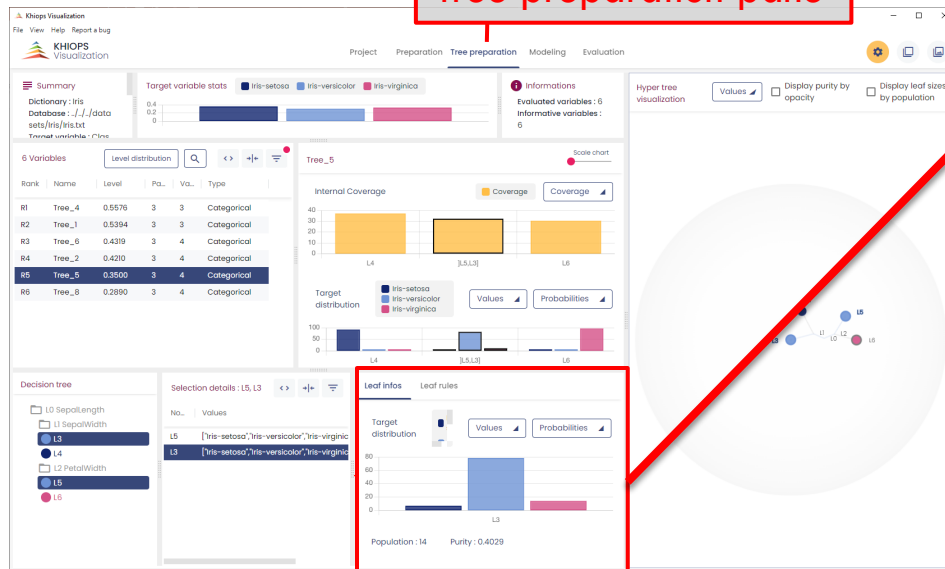




Exploratory of classification results using KHIOPS Visualization

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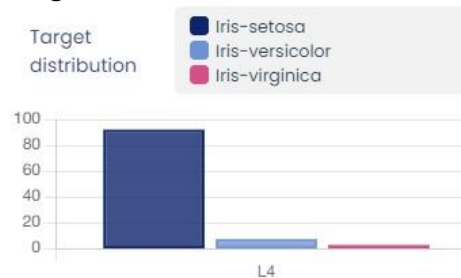
Tree preparation pane



Information on selected leaf

Leaf infos

Target distribution in leaf



Leaf rules

Sequence of trre rules leading to the leaf

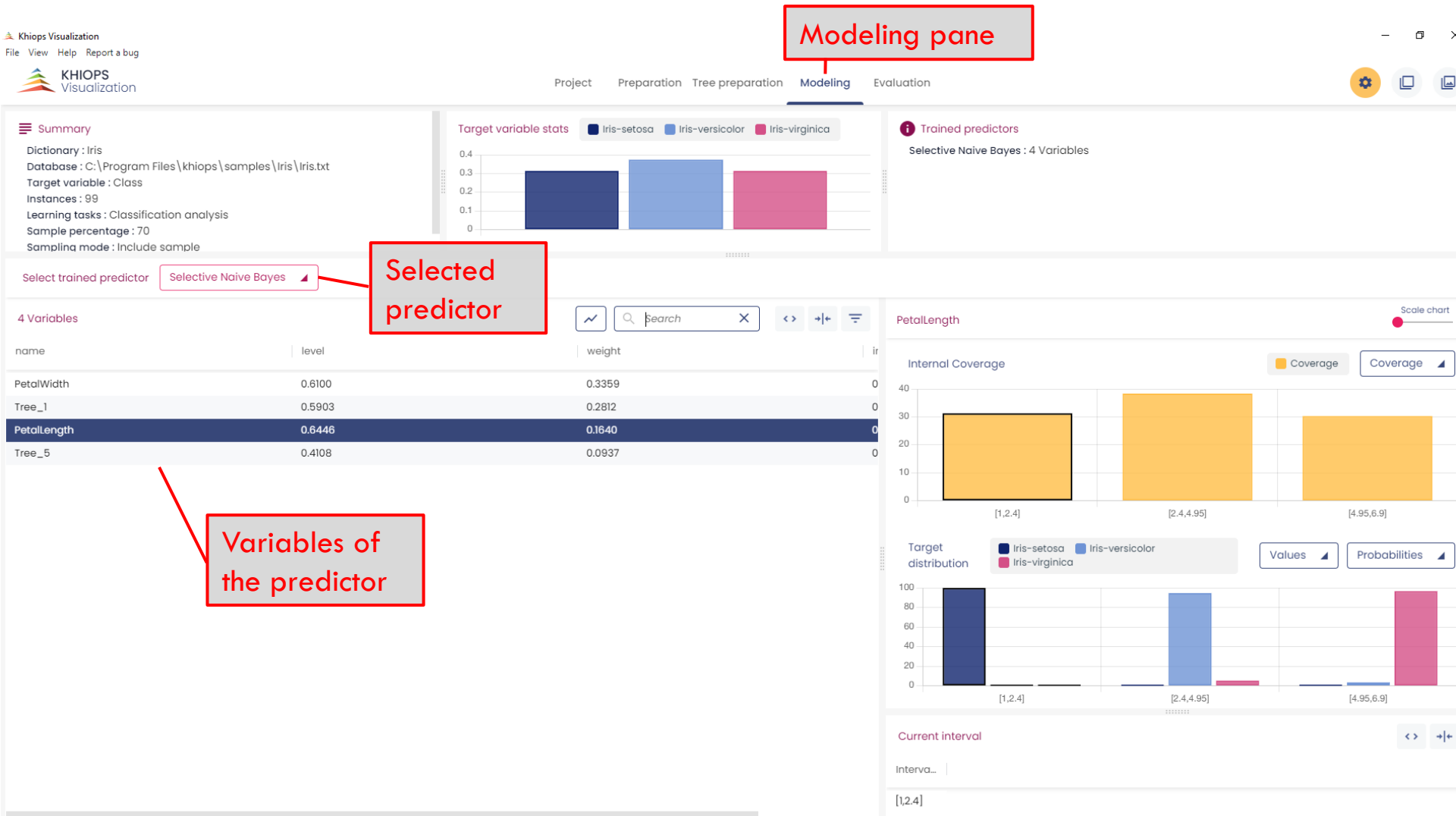
Leaf rules : L4

| Variable ↑ | Type | Partition |
|-------------|-----------|-------------|
| SepalLength | Numerical | [4.3, 5.75] |
| SepalWidth | Numerical | [2.95, 4.4] |



Exploratory of classification results using KHIOPS Visualization

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Exploratory of classification results using Khiops Visualization

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Khiops Visualization
File View Help Report a bug



Project Preparation Tree preparation Modeling **Evaluation**



Evaluation type



| Type | Dictionary | Instances |
|-------|------------|-----------|
| Train | Iris | 99 |
| Test | Iris | 51 |

Evaluation list

Predictor evaluations

Predictor evaluations



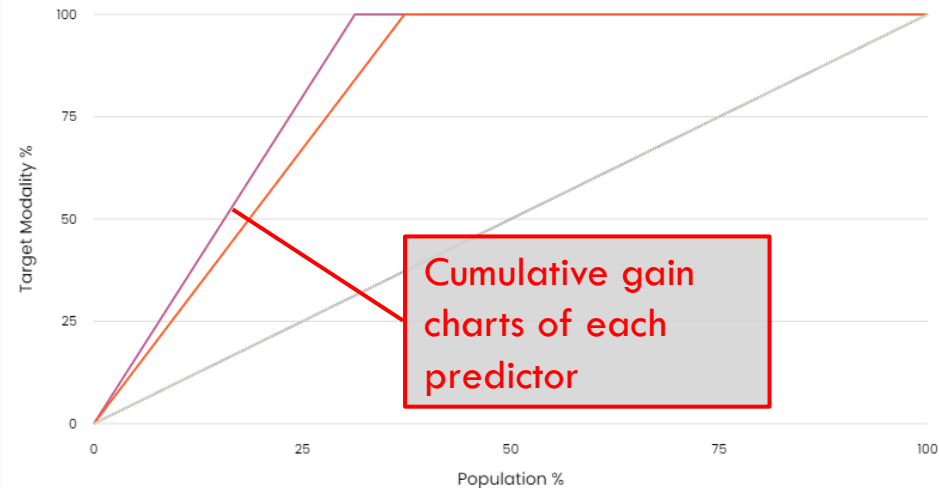
| type | name | accuracy | compression | auc | robustness | gini |
|-------|-----------------------|----------|-------------|--------|------------|--------|
| Train | Selective Naive Bayes | 0.9898 | 0.9495 | 0.9998 | | 0.9996 |
| Train | Optimal | 1 | 1 | 1 | | 1 |
| Test | Selective Naive Bayes | 0.9215 | 0.7964 | 0.9853 | 0.9854 | 0.9706 |
| Test | Optimal | 1 | 1 | 1 | 1 | 1 |

Confusion Matrix of the selected predictor

Evaluation pane

Cumulative gain chart of Iris-setosa

Filter curves



Cumulative gain charts of each predictor

Confusion matrix of Selective Naive Bayes

Frequency

| Target | Iris-setosa | Iris-versicolor | Iris-virginica |
|-------------------|-------------|-----------------|----------------|
| \$Iris-setosa | 31 | 0 | 0 |
| \$Iris-versicolor | 0 | 36 | 0 |
| \$Iris-virginica | 0 | 1 | 31 |




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Exercises A and B ...

A : Perform a supervised classification on sample database Iris

B : Perform a Supervised classification on sample database Adult

 Interpret the analysis results



Regression (supervised)

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- Same as classification
with a numerical target variable

Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Target variable PetalLength

Main target value

Predictors Recorders Preprocessing System parameters

Selective Naive Bayes predictor ☒

Feature engineering Advanced predictor parameters

Max number of constructed variables 100

Max number of trees 10

Max number of variable pairs 0

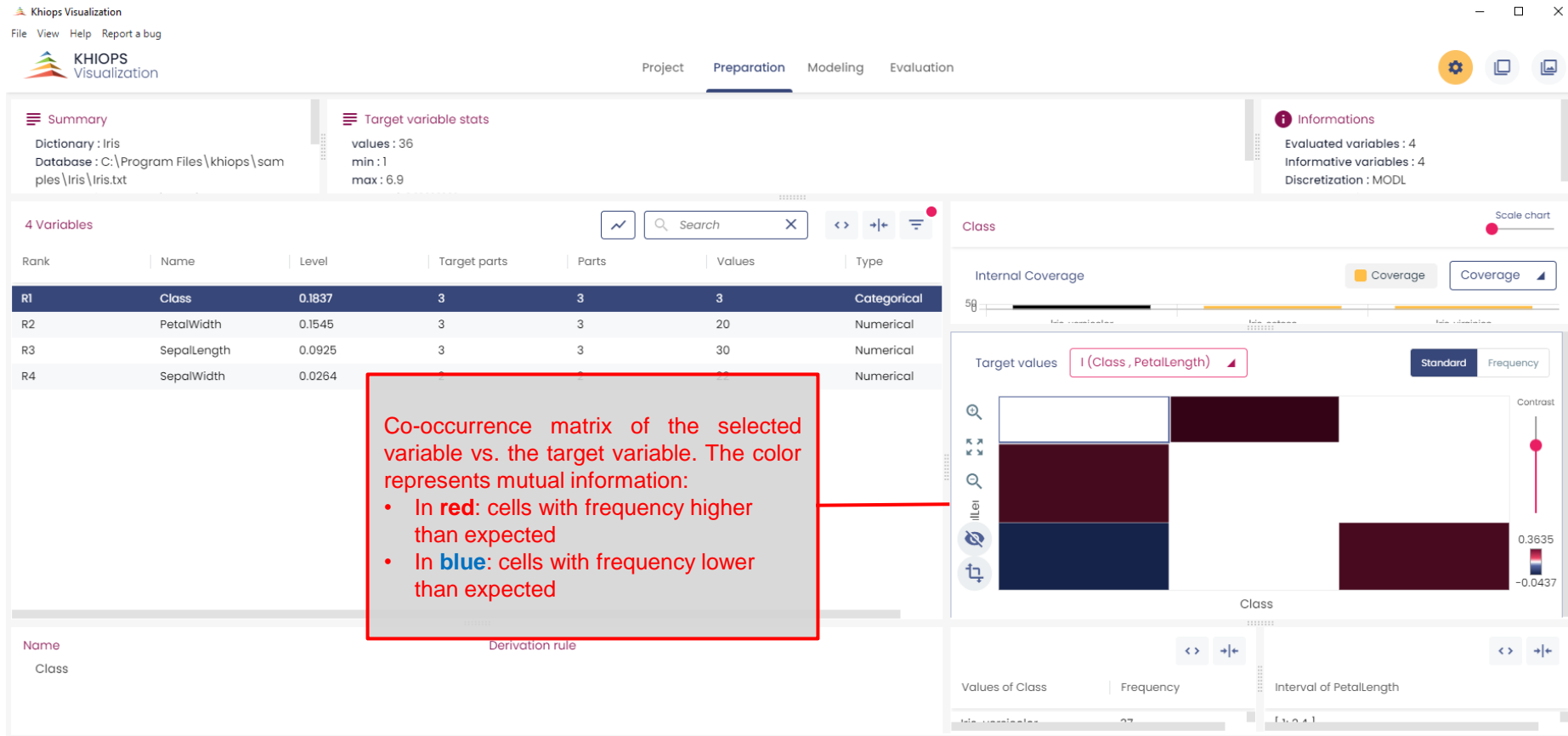
Train model Deploy model...



In this case, bivariate analysis
and tree construction are not
available!



Exploratory of regression results using Khiops Visualization





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Exercise C ...

C : Perform a regression of variable PetalLength of Iris

➡ Interpret the analysis results



Correlation analysis

(unsupervised, bivariate)

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- **Train a correlation model between two variables**
(categorical, numerical, both)

Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Target variable

Main target value

Predictors Recorders Preprocessing System parameters

Selective Naive Bayes predictor ☒

Feature engineering Advanced predictor parameters

Max number of constructed variables 100

Max number of trees 10

Max number of variable pairs 5

Train model Deploy model...

1 – Target variable must be empty

2 – Activate bivariate analysis

a – Feature engineering pane

b – Choice of a max number of pairs to analyze



Correlation analysis (unsupervised, bivariate)

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- **Train a correlation model** : advanced parameters

1 – Target variable must be empty

2 – Inspect variable pair parameters

3 – Specify the pairs

a – import/export variable pairs file

b – all potential pair

c – individual pairs or families of variable pairs involving certain variables to analyze

Variable pairs parameters

Variable pairs file

Max number of variable pairs: 5

All pairs: ☒

Specific variable pairs

| First name | Second name |
|-------------|-------------|
| SepalLength | SepalWidth |
| PetalLength | PetalWidth |

Insert pair Remove pair Clear pair list

Specific pairs number: 2

Close



Exploratory of correlation results using KHIOPS Visualization

KHIOPS Visualization

File View Help Report a bug

Project Preparation **Preparation 2D**

Summary

Dictionary : Iris
Database : C:\Program Files\khiops\samples\Iris\Iris.txt
Instances : 150
Learning task : Unsupervised analysis
Sample percentage : 100
Sampling mode : Include sample
Evaluated variables : 5

5 Pair variables

| Rank | Name 1 | Name 2 | Level | Variable 1 | Variable 2 | Cells |
|------|-------------|-------------|--------|------------|------------|-------|
| R1 | Class | PetalWidth | 0.1445 | 2 | 3 | 5 |
| R2 | Class | PetalLength | 0.1416 | 2 | 3 | 5 |
| R3 | PetalLength | PetalWidth | 0.0823 | 2 | 3 | 4 |
| R4 | Class | SepalLength | 0.0584 | 2 | 3 | 8 |
| R5 | PetalLength | SepalLength | 0.0498 | 2 | 4 | 10 |

Level distribution

Matrix Cells

Standard Frequency

Co-occurrence

I (Class, PetalWidth)

Contrast

0.3662

-0.3662

Class

Values of Class Frequency Interval of PetalWidth

Preparation 2D pane

Co-occurrence matrix of the selected variable pair

Variables pairs



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Exercises D, E, F and G...

D : Perform the correlation analysis of the two most correlated variables of Iris
(*tip: analyze all pairs to identify the most informative*)

E : Idem with variables *PetalLength* and *PetalWidth*
(*tip: inspect the Variable pairs parameters*)

F : Idem with new constructed variables *PetalArea* and *SepalArea*
(*tip: use the derivation rule Product in dictionary,*
see KhiopsGuide: sections « Derivation rules » and « Appendix »)

G : Perform the correlation analysis of all pairs of Adult involving variable *native_country*

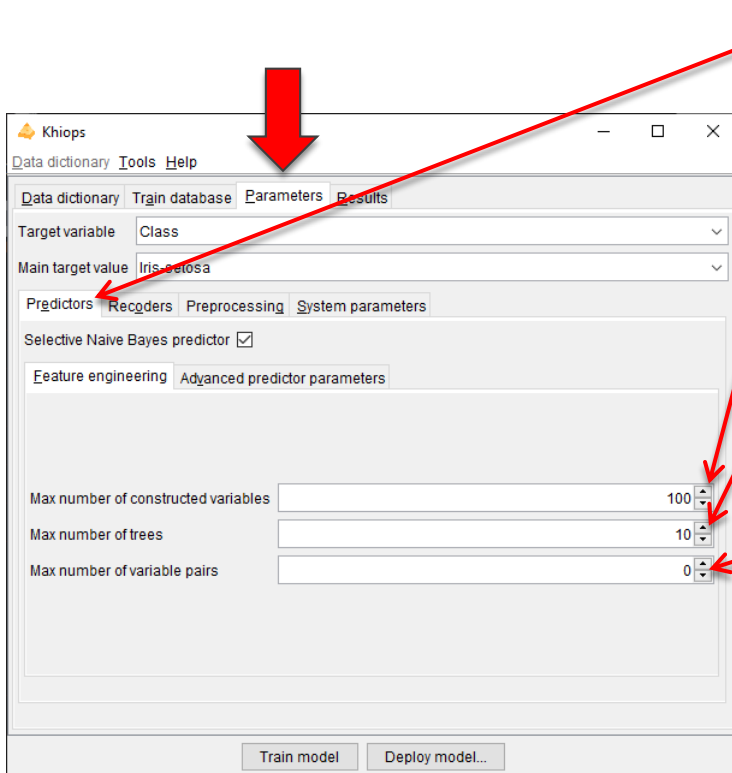
 Interpret the analysis results



Variable construction

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- Parameters



Predictors

Feature engineering

- Max number of constructed variables

- to build an analyze table from a multi-table schema (see later)
- automatic extraction of complex information to obtain accurate classifiers

- Max number of trees

- combines natives or constructed variables to extract complex information
- better accuracy, at the expense of interpretability

- Max number of pairs of variable

- to understand correlation between variables
- use rather for exploratory analysis rather than for better accuracy

Recommendation


- start with few constructed variables, and increase incrementally
- idem for trees
 - no tree for simpler, faster and more interpretable predictors
 - more and more trees for more accurate predictors



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Exercise H ...

A : Perform a supervised classification on sample database Letter
Build 0, 10, 50 trees

 Interpret the analysis results, and the trade-off between
number of trees, training time and test accuracy

Integration in information systems

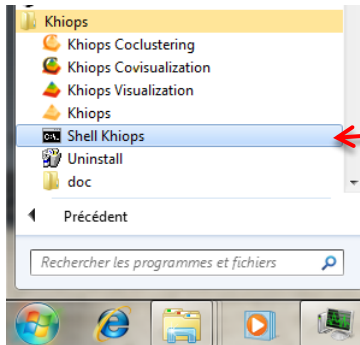
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- Batch mode
 - to record and replay Khiops scripts
 - to perform any Khiops task from any programming language
 - see next slide
- Khiops Native Interface (KNI)
 - dynamic link library (DLL) for online deployment of Khiops models
 - package to download from www.khiops.com
- Python Khiops Library (pykhiops)
 - to perform any Khiops task from python
 - to inspect any Khiops analysis results from python
 - python package available from www.khiops.com
- JSON file exports
 - Khiops dictionaries and analysis results can be exported from the Khiops tool to exploit Khiops results from any programming language

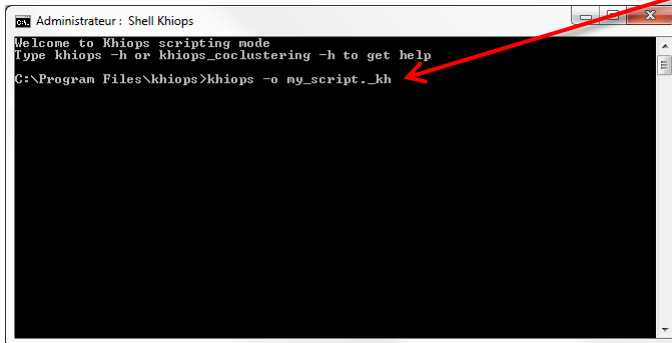


Batch mode

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Start a Shell Khiops



Record a script « automatically » using
Khiops user interface

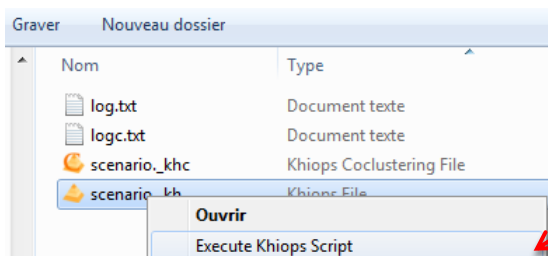
`khiops -o my_script._kh`

o = output

- Replay a script from the shell

`khiops -i my_script._kh`

i = input



Replay a script from Windows Explorer
right click on script file



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Exercise I ...

I : Record a script file, then replay it ...



Deploy a model

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Deployment dictionary: Adult

Input database

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|---|
| Adult | | Adult | C:\Program Files\khiops\samples\Adult\Adult.txt |

Detect file format

Header line used: ☒

Field separator:

Sample percentage: 100

Sampling mode: Include sample

Selection variable:

Selection value:

Output database

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|--|
| Adult | | Adult | C:\Program Files\khiops\samples\AdultT_Adult.txt |

Header line used: ☒

Field separator:

Output format: tabular

Buttons: Deploy model, Build deployed dictionary..., Close

Steps for model deployment

- 1- Start from a modeling dictionary « *Modeling.kdic* »
 - In « Data dictionary » pane
- 2- Choose the variables to deploy
 - Inspect the modeling dictionary In « Data dictionary » pane by right-click in the “Dictionaries in file” list
 - Suppress the « *Unused* » tag from identifier variables
 - Select the prediction variables to deploy
- 3- Menu : « *Tools -> Deploy model* »
- 4- Deploy model dialog box
 - Select deployment dictionary
 - Select input database
 - Select output database
 - Click on « Deploy model » button



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Exercise J ...

J: Deploy a classifier on database Iris

Khiops Coclustering & Khiops Covisualization

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- **Khiops Coclustering**
 - Correlation analysis of two or more variables using a hierarchical coclustering model



- **Khiops Covisualization**
 - Exploratory analysis of Khiops Coclustering results using an interactive visualization tool

Khiops Coclustering & Khiops Covisualization

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- **Train a coclustering model**
 - Use of **Khiops Coclustering** back-end tool
 - Co-partition of two or more categorical or numerical variables
 - At each level of the hierarchy, the merge of clusters with the minimum information loss is performed
 - Write results in a coclustering report file « .khcj »



- **Exploratory analysis of the results**
 - Use of **Khiops Covisualization** tool
 - Navigation in the hierarchy of models

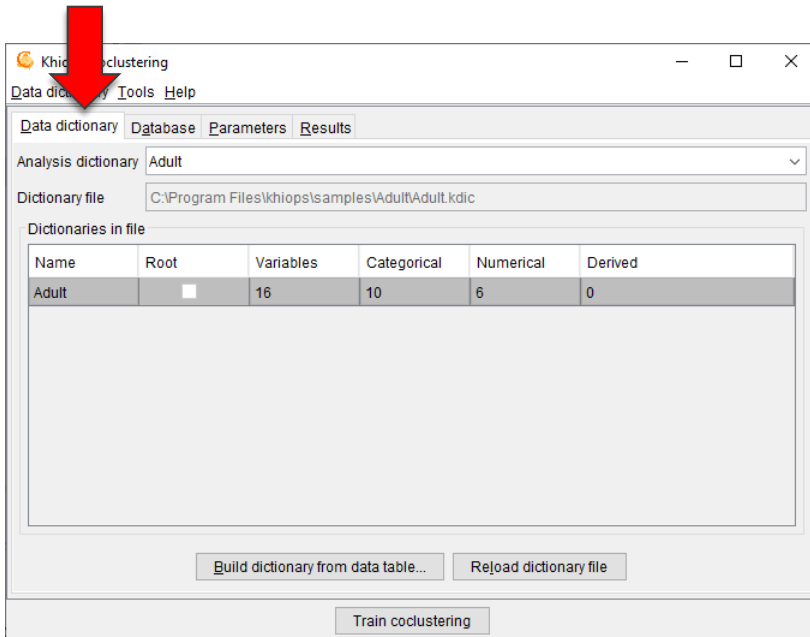




Train a coclustering model

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- **Step 1 : Open an existing dictionary**
(ex: sample Adult.kdic)
- Description of variables to use during analysis



Available actions :

- Open, Save, Save as, Close
- Edition (menu « Dictionary file/Inspect current dictionary », or NotePad)
- Reload dictionary file
- Build dictionary from data table

```

Dictionary  Adult
{
    Numerical  Label;
    Numerical  age;
    Categorical workclass;
    Numerical  fnlwtg;
    Categorical education;
    Numerical  education_num;
    Categorical marital_status;
    Categorical occupation;
    Categorical relationship;
    Categorical race;
    Categorical sex;
    Numerical  capital_gain;
    Numerical  capital_loss;
    Numerical  hours_per_week;
    Categorical native_country;
    Categorical class;
};

```



Build a coclustering model

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- **Step 2 : Specification of used database**

Khiops Coclustering

Data dictionary Database Parameters Results

Database files

| Data root | Path | Dictionary | Data table file |
|-----------|------|------------|---|
| Adult | | Adult | C:\Program Files\khiops\samples\Adult\Adult.txt |

Detect file format

Header line used ☒

Field separator

Sample percentage 100

Sampling mode Include sample

Selection variable

Selection value

Train coclustering

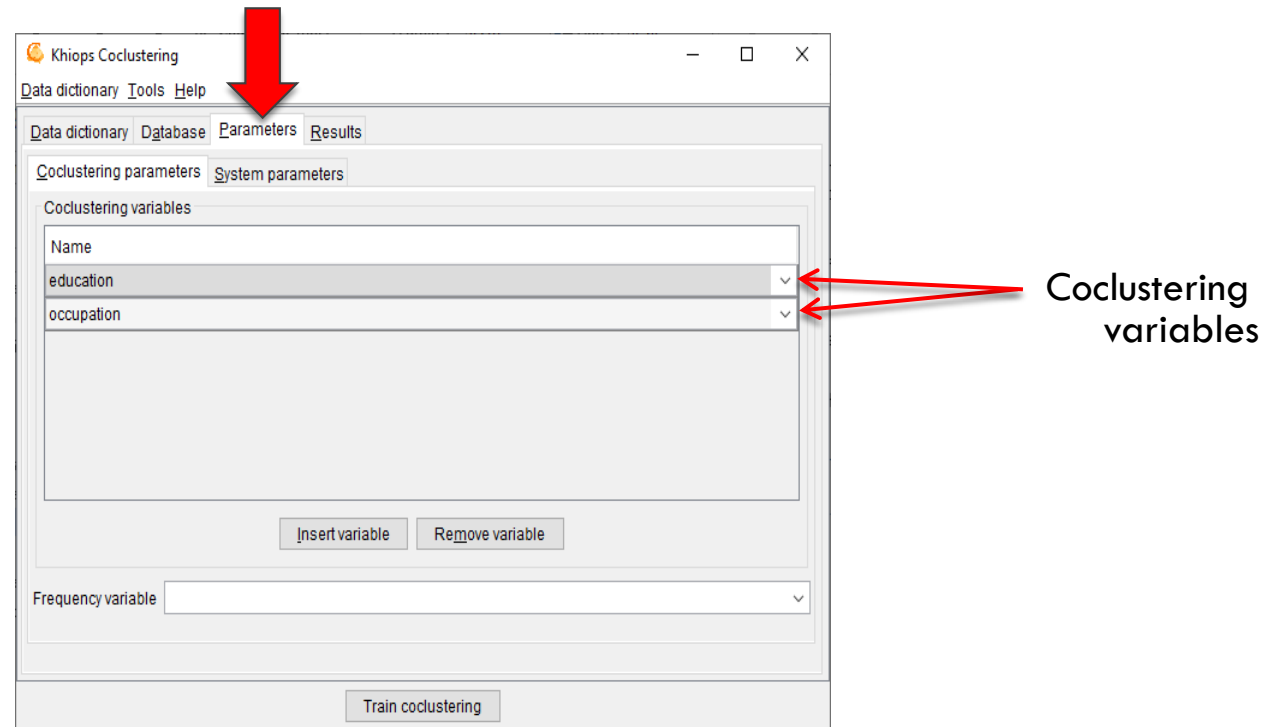
Detect file format : heuristic help that scans the first few lines to guess the file format. The header line and field separator are updated on success, with a warning or an error in the log window only if necessary.



Build a coclustering model

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- **Step 3 : Specification of coclustering variables**





Build a coclustering model

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- **Step 4 : Results**



Khiops Coclustering

Data dictionary Tools Help

Data dictionary Database Parameters Results

Result files directory CorrelationEducationOccupation

Result files prefix

Short description

Coclustering report Coclustering.khc

Export JSON ☒

Train coclustering

- Directory where result file is written
- Prefix (ex: *in case of several experiments*)
- Synthetic coclustering report (cf. Khiops Covisualization)
- Json report, to get the analysis results from external tools

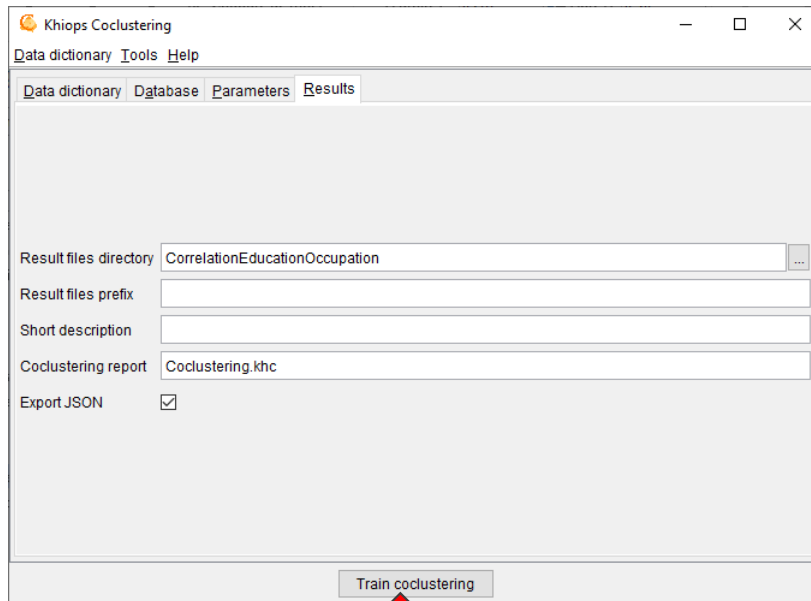




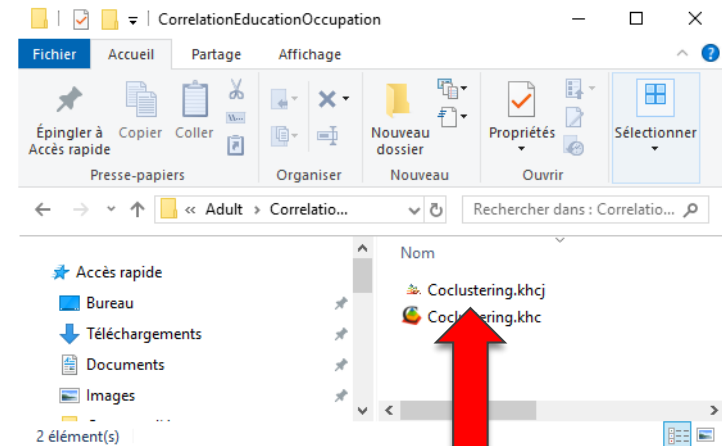
Build a coclustering model

42

- **Step 5 : Start the analysis**



1 – Train the coclustering



2 - Inspect the results using Khiops Covisualization
(double-click on .khcj file)

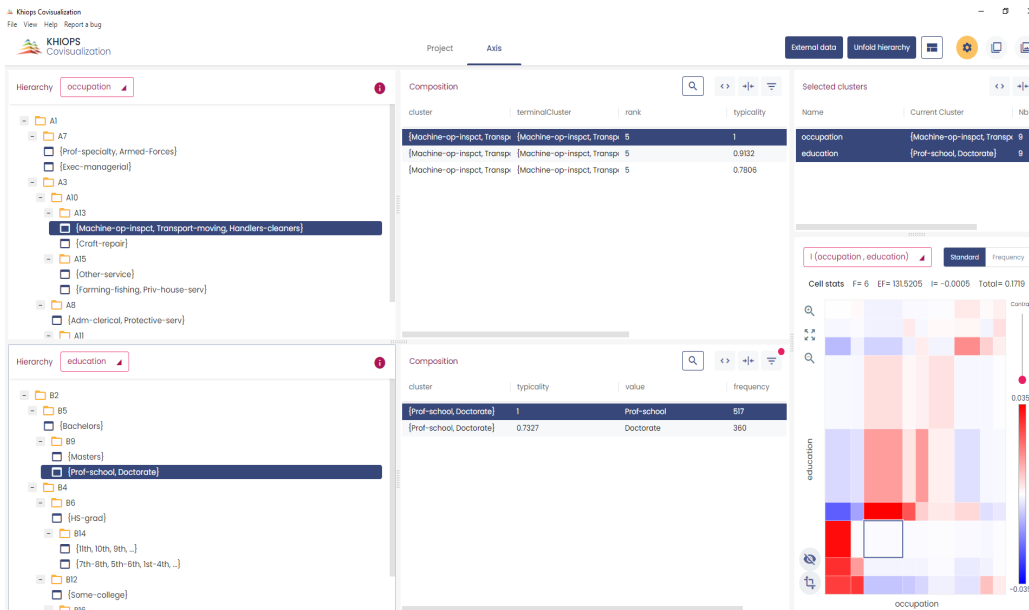
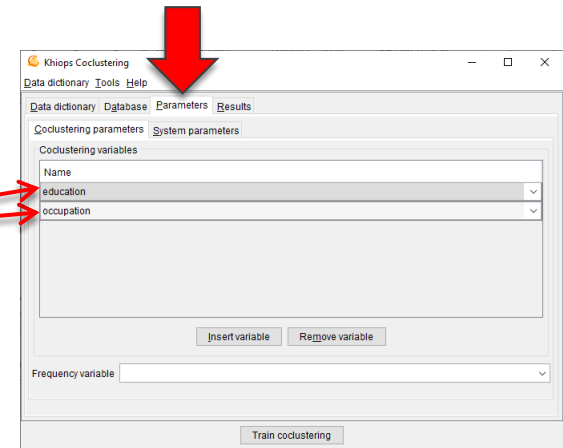


Example: base Adult education*occupation

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- With Khiops Coclustering
 - Analysis of pair of variables education*occupation



- With Khiops Covisualization
 - Exploratory analysis of the results



44

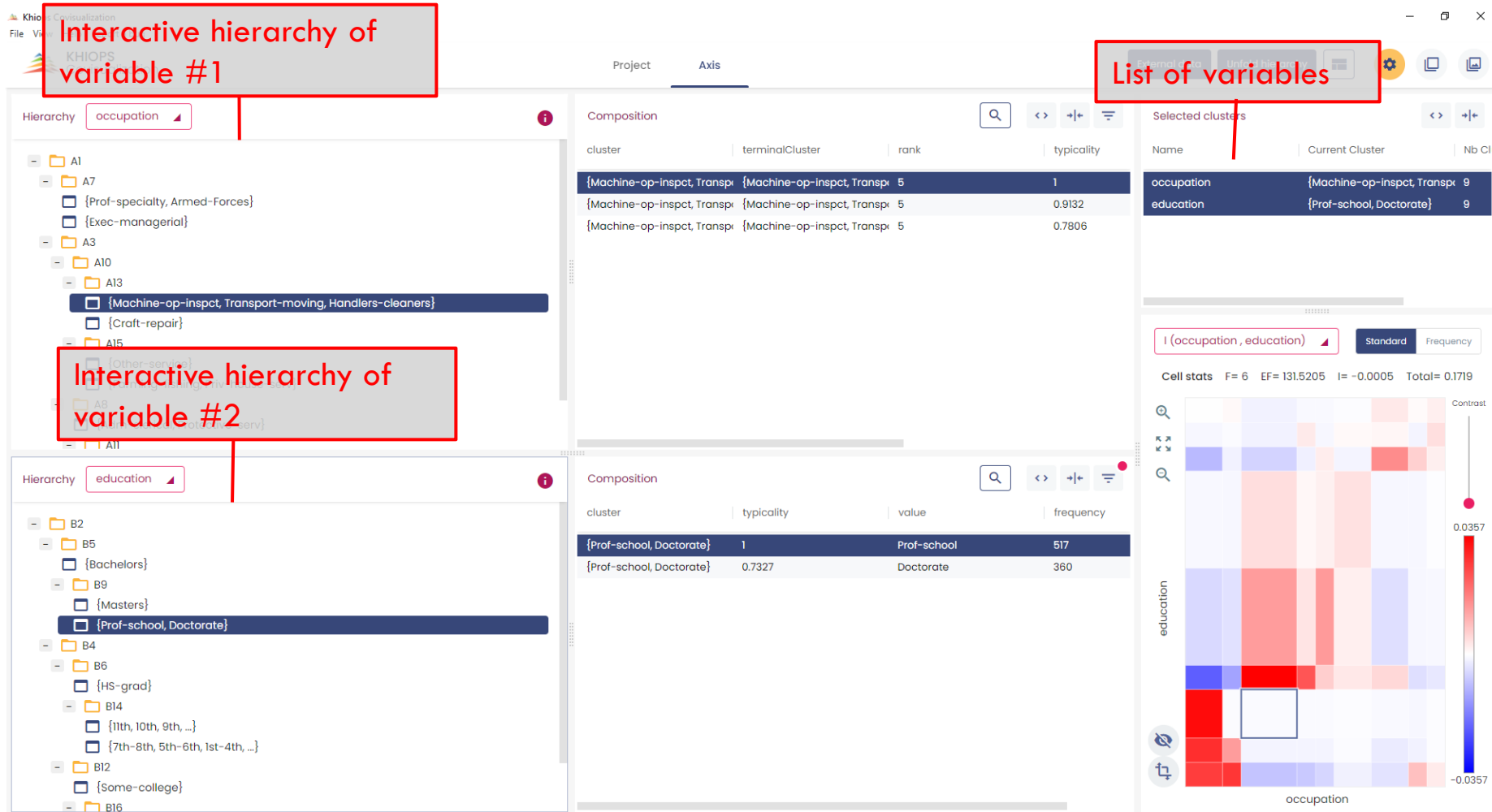
Exercise J ...

J : Train a coclustering model
on two categorical variables of sample database Adult

➡ Explore the analysis results

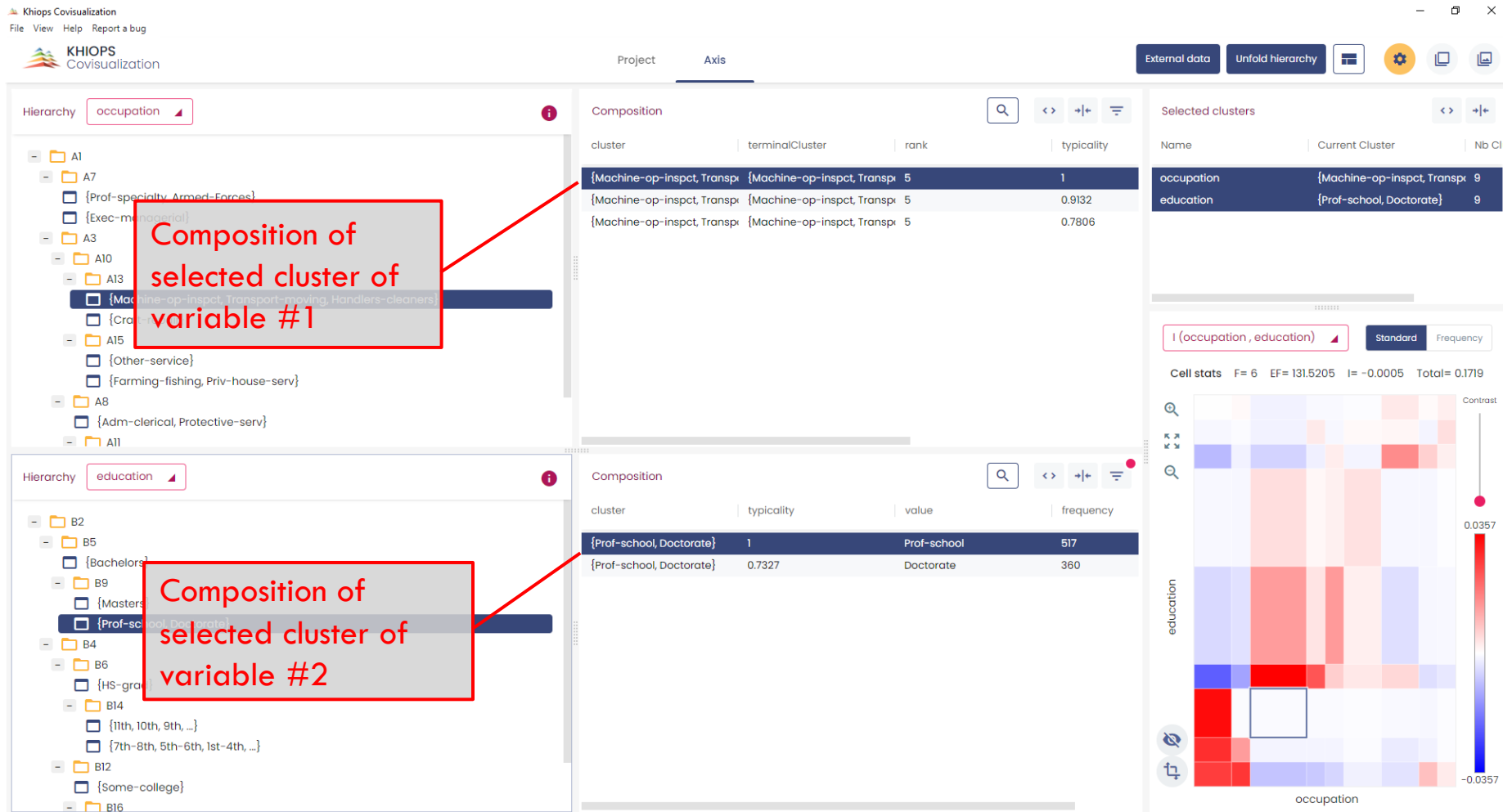
Khiops Covisualization

45



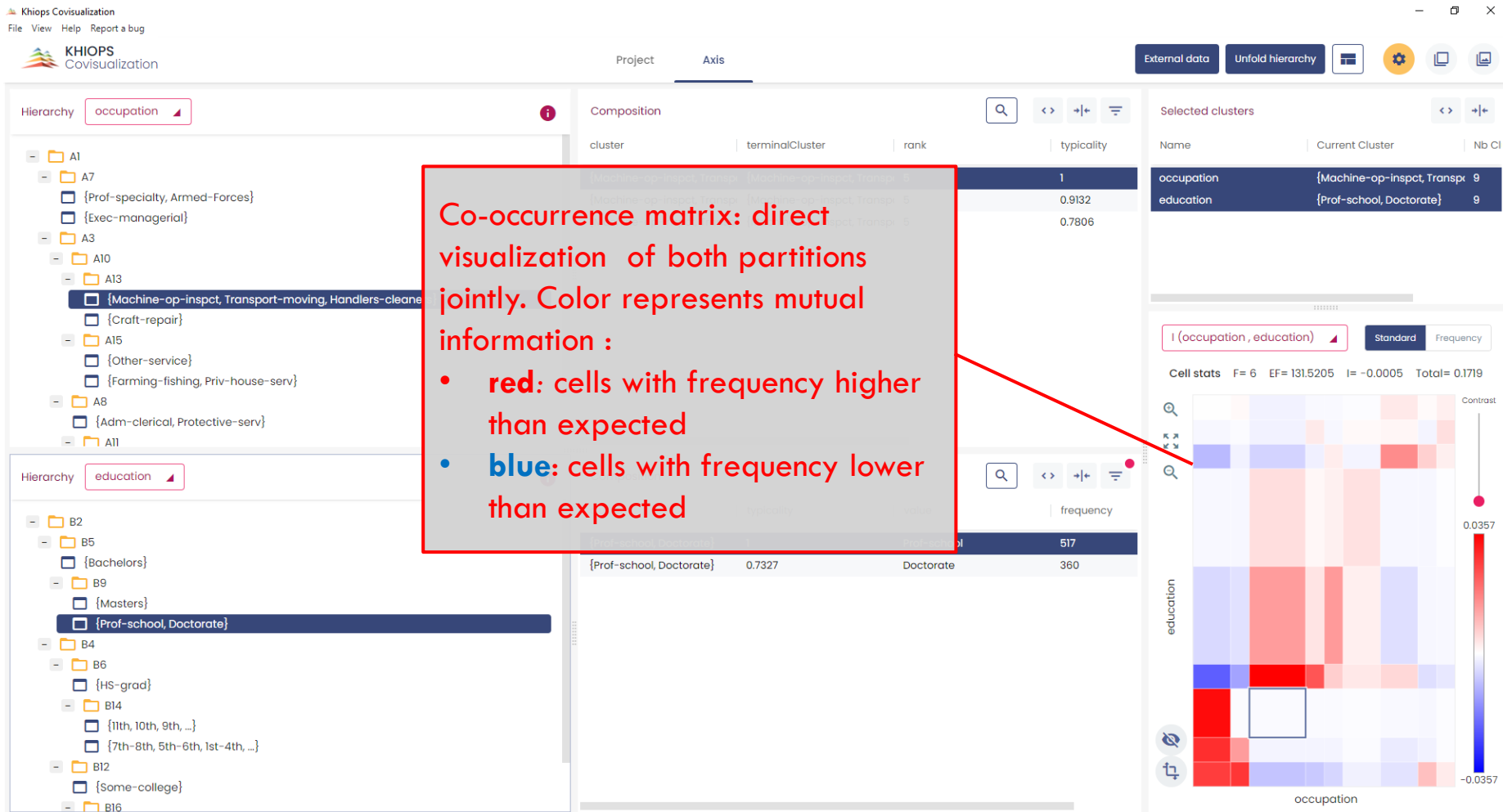
Khiops Covisualization

46



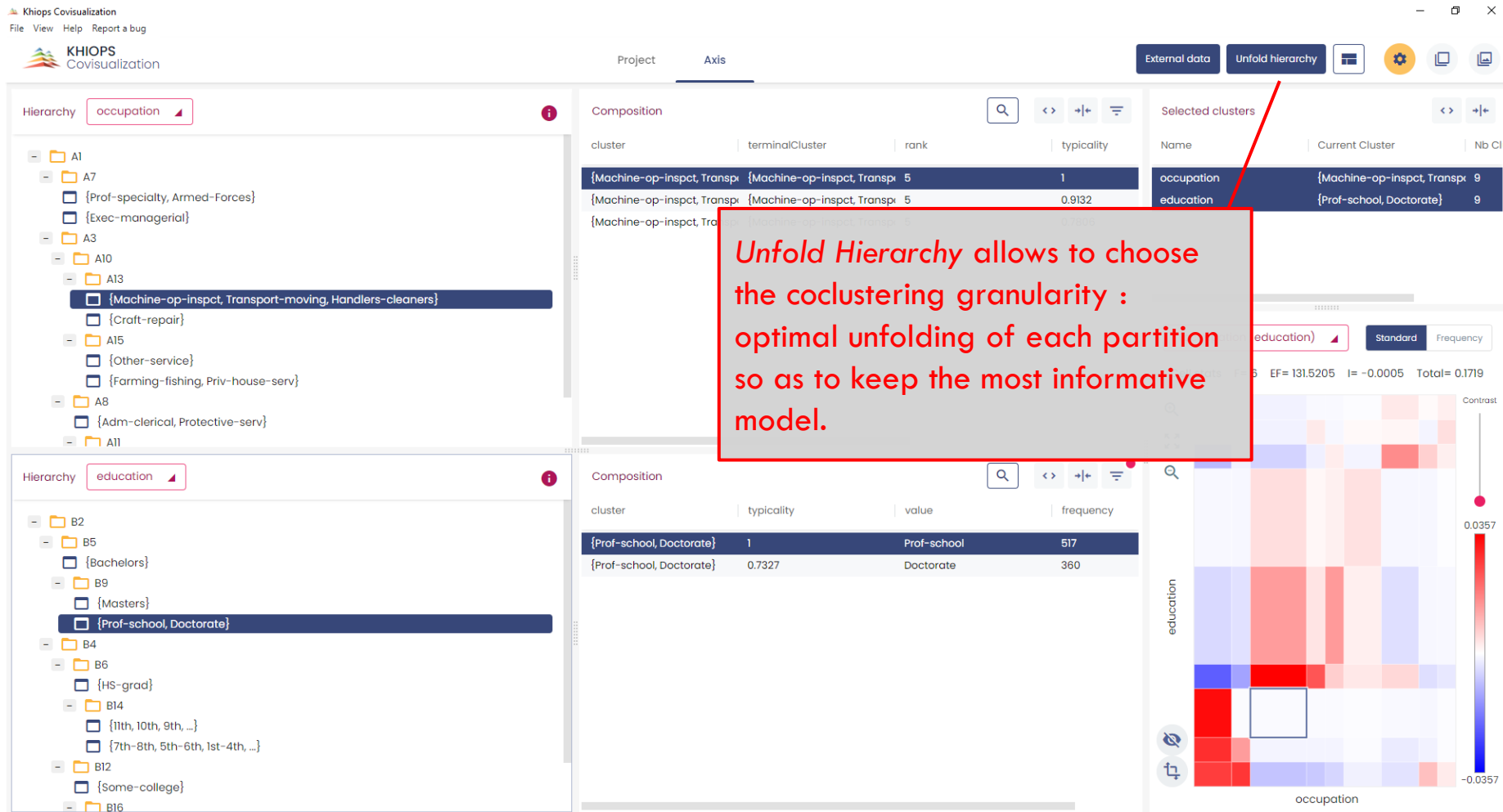
Khiops Covisualization

47



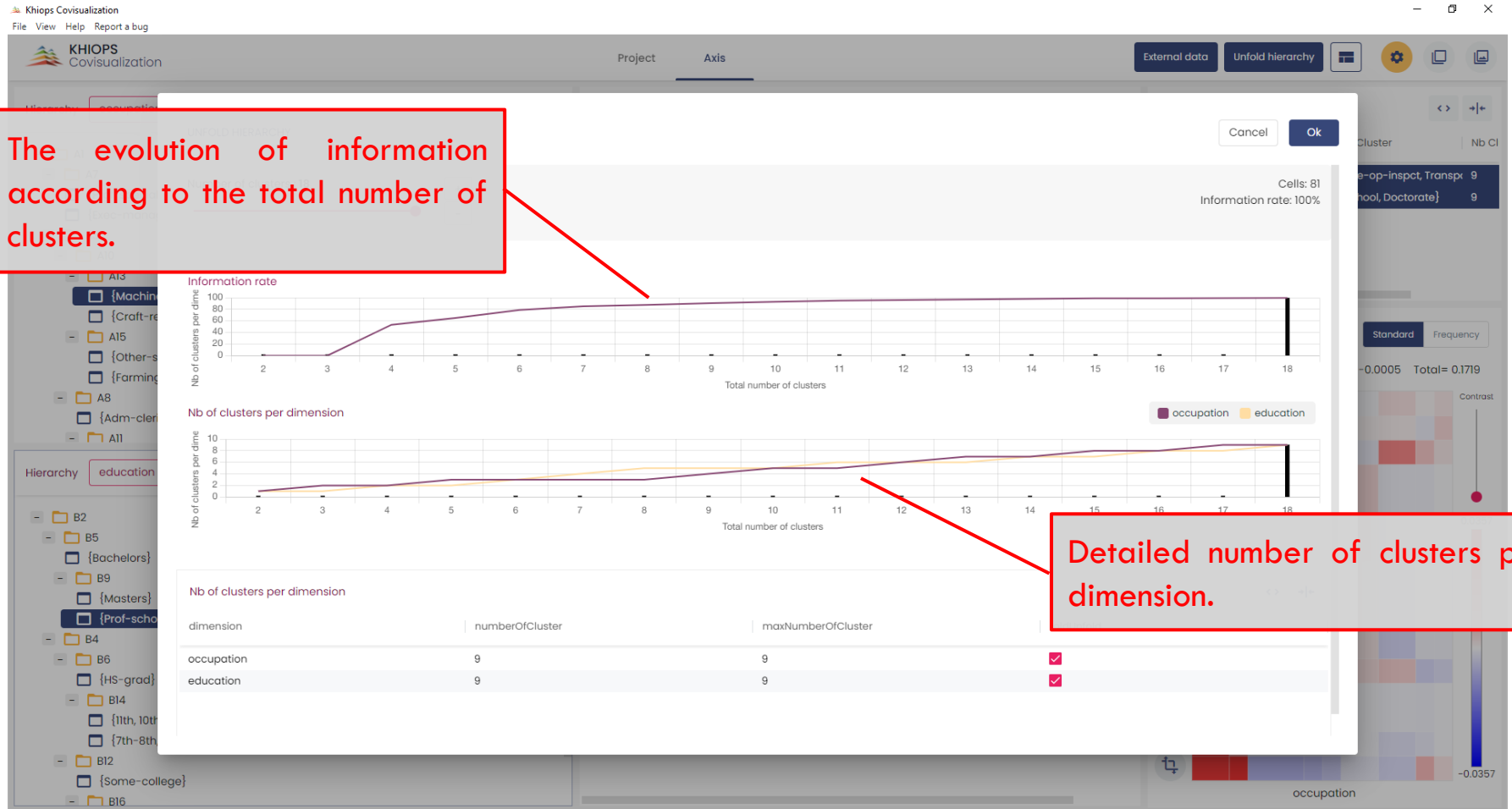
Khiops Covisualization

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Khiops Covisualization

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Training a triclustering

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- Same as coclustering (Step 3) by inserting a third variable

The screenshot shows the 'Khiops Coclustering' window with the 'Parameters' tab selected. Under the 'Coclustering parameters' sub-tab, there is a list of 'Coclustering variables'. The list contains three variables: 'education', 'occupation', and 'sex'. A red arrow points to the 'sex' variable, with the text 'The third variable' next to it. Below the list are 'Insert variable' and 'Remove variable' buttons. At the bottom of the window is a 'Train coclustering' button.

| Name |
|------------|
| education |
| occupation |
| sex |

Insert variable Remove variable

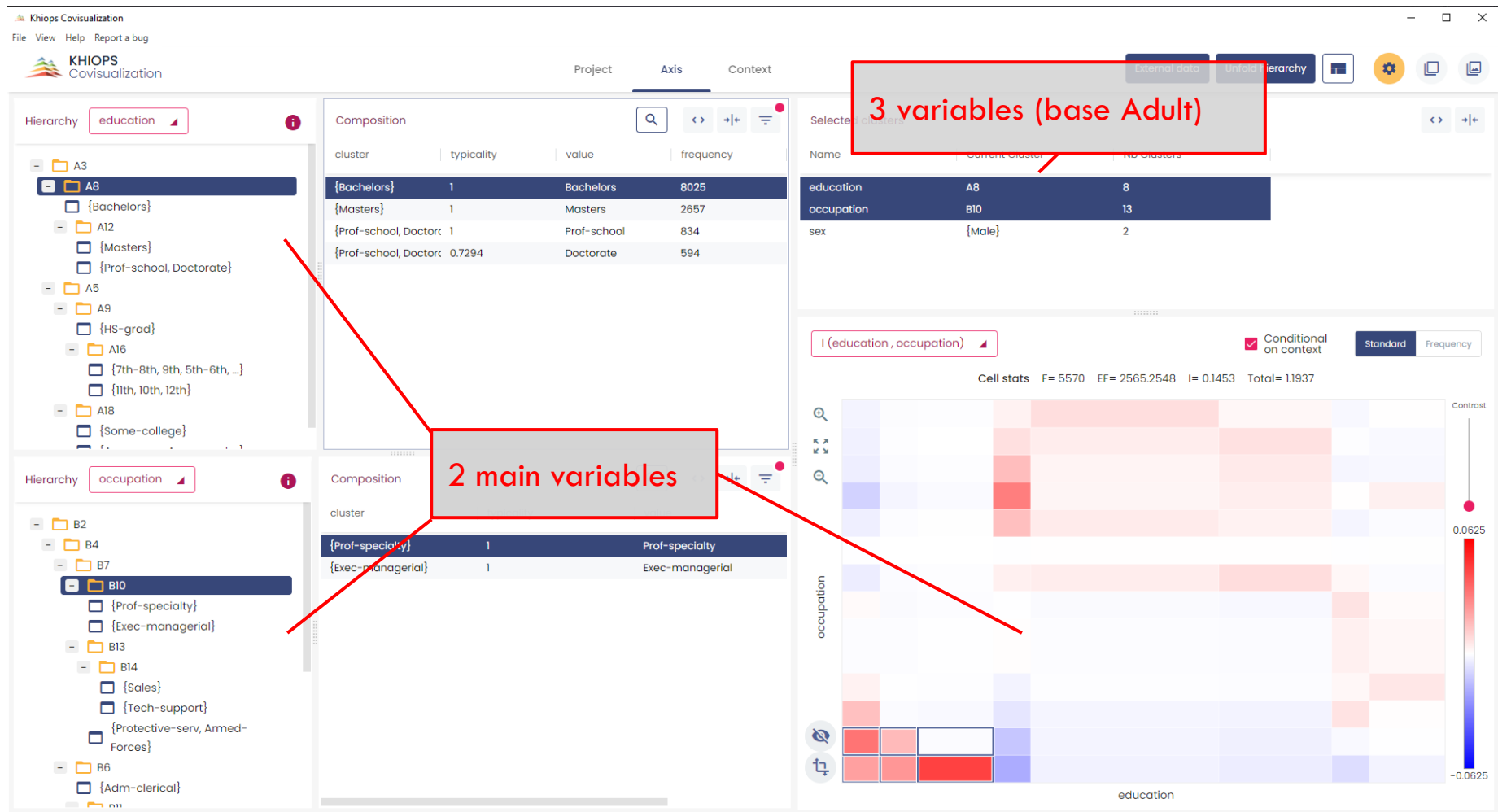
Frequency variable

Train coclustering

The third variable

Exploring a triclustering

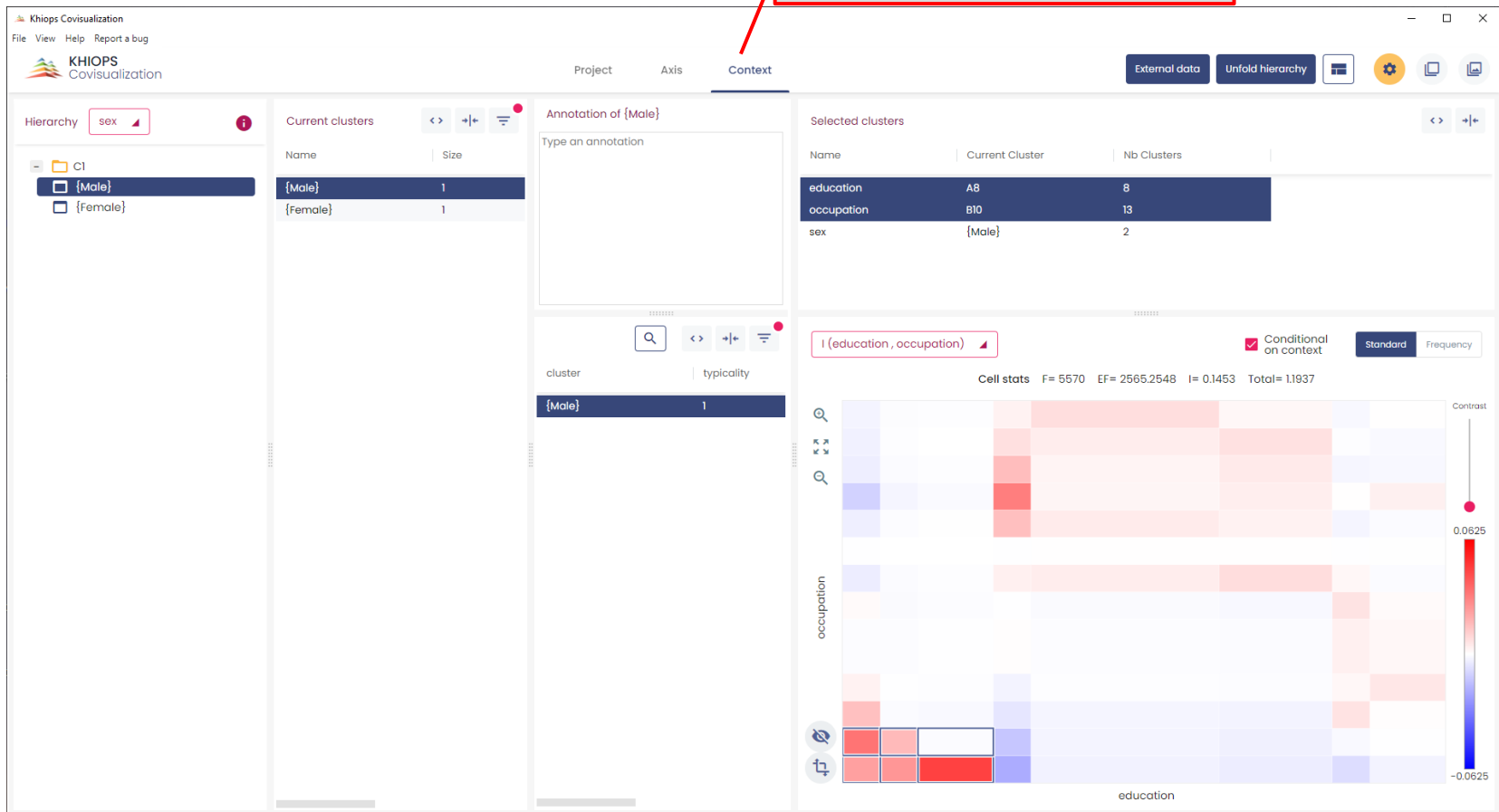
51



Exploring a triclustering

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Context pane



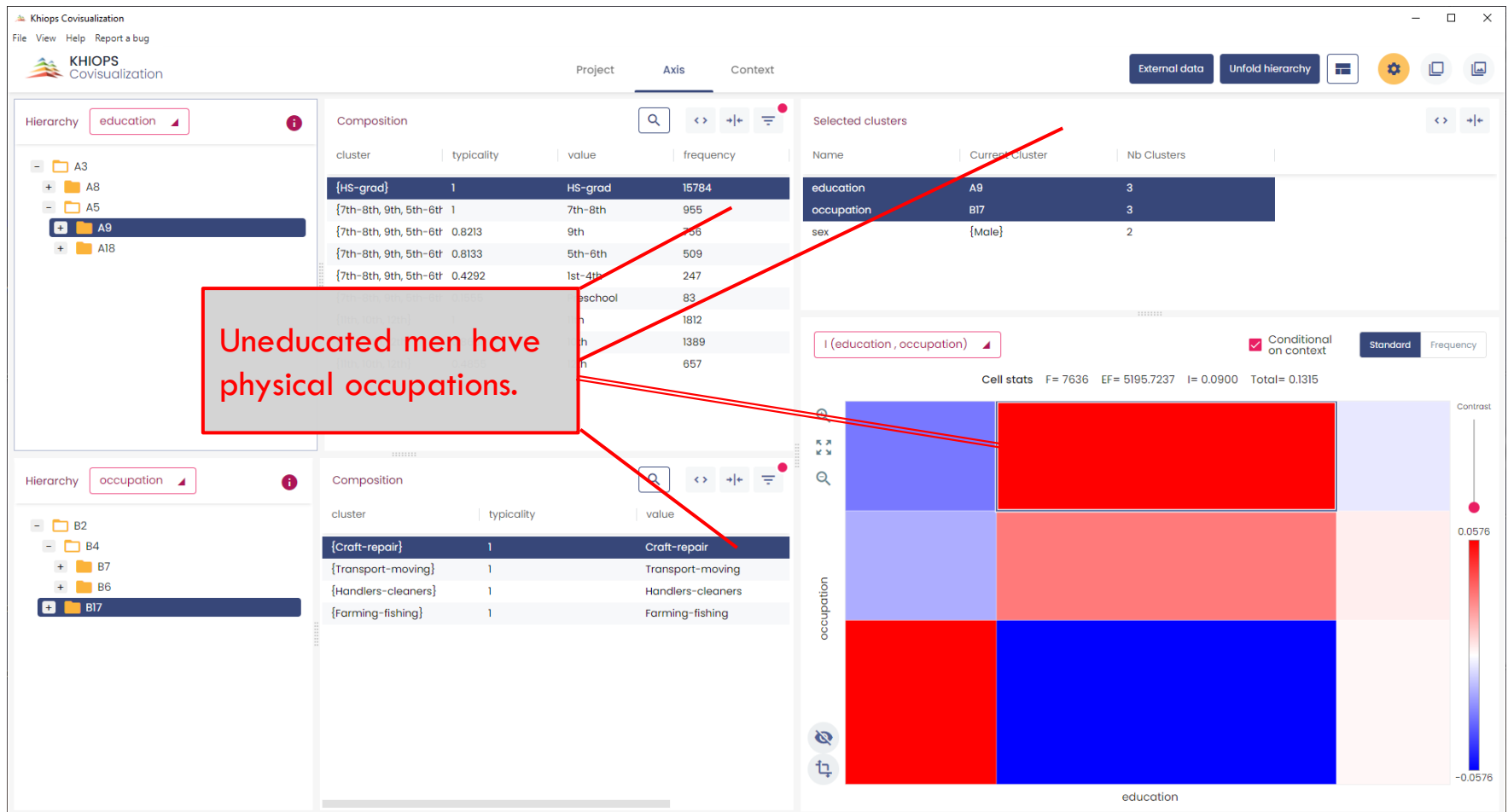
Exploring a triclustering

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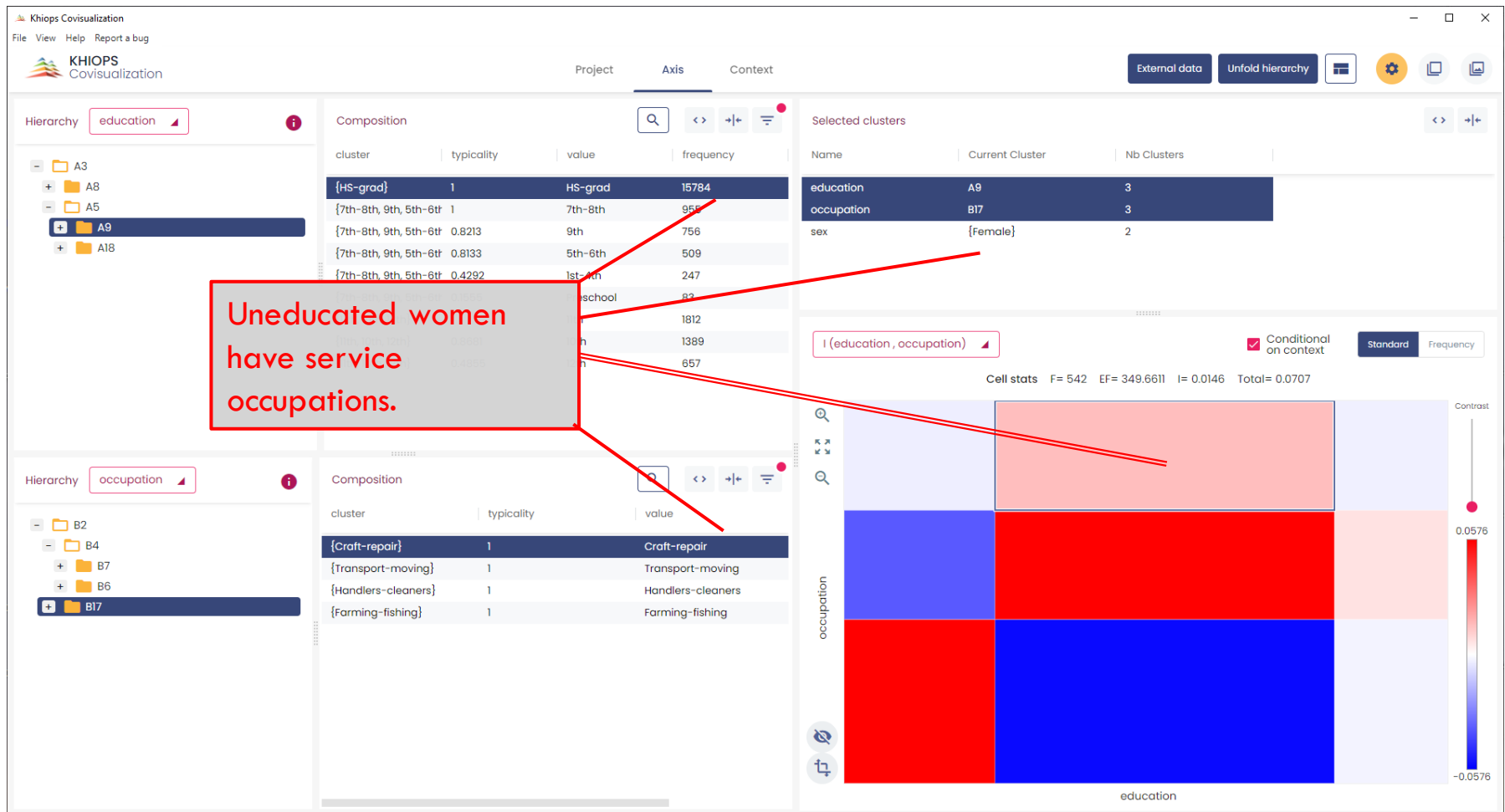
Exploring triclustering

54



Exploring a triclustering

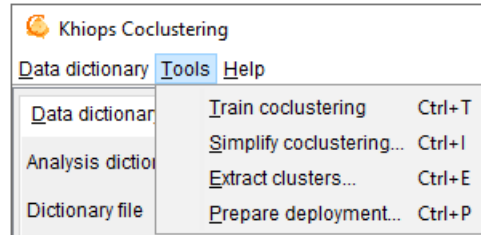
55





Exploiting a coclustering model

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- Tools menu
 - Train coclustering
 - Input: dictionary and database file
 - Train a coclustering model
 - Simplify coclustering
 - Input: coclustering model
 - Build a simplify coclustering model given user constraints
 - Extract clusters
 - Input: coclustering model
 - Extract clusters in a text file for a given coclustering variable
 - Prepare deployment
 - Input: dictionary and coclustering model
 - Enables the deployment of a coclustering model on new data by the means of a Khiops deployment dictionary
 - See multi-table section of the tutorial



Simplifying a coclustering model

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Coclustering simplification

Input coclustering report C:\Program Files\khiops\samples\Adult\CorrelationEducationO...

Simplification parameters Results

ShortDescription

Instance number 48842

Non empty cell number 81

Cell number 81

Max cell number 0

Max preserved information 0

Total part number 18

Max total part number 0

Coclustering variables

| Type | Name | Part number | Max part number |
|-------------|------------|-------------|-----------------|
| Categorical | education | 9 | 0 |
| Categorical | occupation | 9 | 0 |

Frequency variable

Select input coclustering... Simplify coclustering Close

- **Steps for coclustering model simplification**

- **1- Select input coclustering (.khc)**

- **2- Specify user simplification constraints**

- Max cell number :
 - max number of cells to keep in the simplified coclustering
 - Max preserved information
 - max percentage of information to keep in the simplified coclustering
 - Max total part number
 - max for the sum of the part number per coclustering variable
 - Per coclustering variables (in the array)
 - Max part number
 - max number of part to keep for this variable in the simplified coclustering
- (0 : no constraint)

- **3- Select result files directory**

- **4- Click on « Simplify coclustering »**

Coclustering simplification

Input coclustering report C:\Program Files\khiops\samples\Adult\CorrelationEducationO...

Simplification parameters Results

Result files directory C:\Program Files\khiops\samples\Adult\CorrelationE ...

Result files prefix

Simplified coclustering report SimplifiedCoclustering.khc

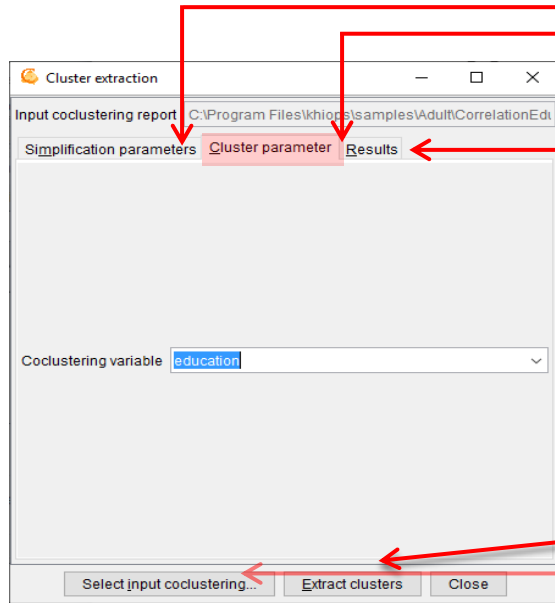
Export JSON ☒

Select input coclustering... Simplify coclustering Close



Extracting clusters in a text file

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Steps for cluster extraction

- 1- Select input coclustering (.khc)
- 2- Specify user simplification constraints
- 3- Select coclustering variable containing the clusters
- 4- Select result files directory
- 5- Click on « *Extract clusters* »

Output cluster file

- Text file with header line and separator tabulation
- Columns:
 - **Cluster:** name of the cluster (group of values)
 - **Value:** name of the value contained in the cluster
 - **Frequency:** frequency of the value
 - **Typicality:** interest measure of the value within its cluster



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Exercise K, L ...

K : Simplify previously built adult coclustering model

Keep 50% of the information in the model

➡ Explore the simplified analysis results with Khiops covisualization

L : Extract clusters from variable education of adult coclustering model

➡ Inspect the cluster file with a text editor

Multi-table functionalities

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- **Multi-table functionalities**
 - Multi-table database
 - Automatic feature construction
 - Multi-table functionalities in Khiops and Khiops Coclustering

Why extending to multi-table?

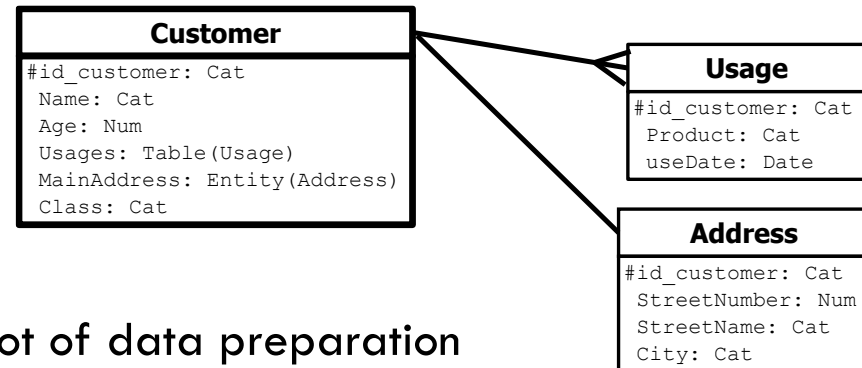
61

- Why extending to multi-table?
 - Most data mining tools work on instances*variables flat tables
 - Real data often have a structure coming from databases
 - The input representation is richer using multi-table specification
 - Data mining methods may benefit from explicit richer domain description

- Real data is usually structured

- Example

- Marketing: Customer with shopping list
 - Web analytics: cookie with web log
 - Telecommunications: Customer with call detail records
 - Bioinformatics: DNA segments with ordered list of nucleotides
 - ...



- Data mining with structured data requires a lot of data preparation
 - Constructing a representation in a flat table
 - Expert knowledge necessary to constructed new variables
 - Time expensive process to get a flat table usable for data analysis
 - This process is unreliable
 - Risk of missing informative variables
 - Risk of constructing and selecting irrelevant variables

Khops multi-table

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- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond




- Impact on Khops
 - Multi-table dictionary
 - to describe star-schema input representation
 - Multi-table database
 - to store input data on multiple files
 - Feature construction language
 - to drive automatic feature construction
 - Sort functionality on large files
 - Powerful analytic functionalities
 - Automatic feature construction
 - Recoding of multi-table databases to get a flattened representation
 - Modeling and deployment at the multi-table level



- Impact on Khops Coclustering
 - Deployment of coclustering models
 - For example, given a text*word coclustering model, assign new texts to their closest cluster


Khops multi-table

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- 
- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond
 - Impact on Khops
 - Multi-table dictionary
 - to describe star-schema input representation
 - Multi-table database
 - to store input data on multiple files
 - Feature construction language
 - to drive automatic feature construction
 - Sort functionality on large files
 - Powerful analytic functionalities
 - Automatic feature construction
 - Recoding of multi-table databases to get a flattened representation
 - Modeling and deployment at the multi-table level
 - All other Khops functionalities are available similarly
 - Classification, regression, correlation analysis
 - Deployment, recoding, evaluation
 - ...

Khops multi-table

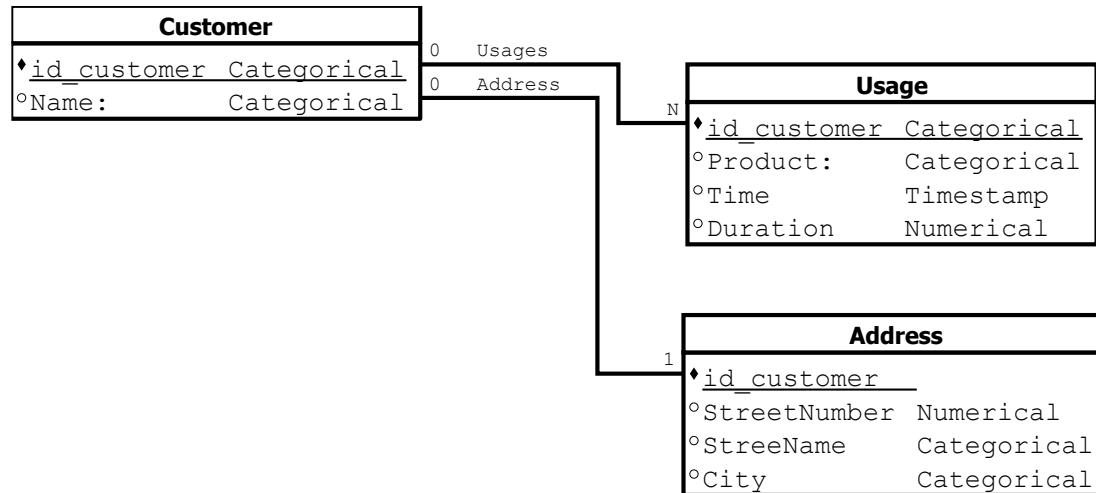
64

- 
- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond
 - Impact on Khops
 - Multi-table dictionary
 - to describe star-schema input representation
 - Multi-table database
 - to store input data on multiple files
 - Feature construction language
 - to drive automatic feature construction
 - Sort functionality on large files
 - Powerful analytic functionalities
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 - Recoding of multi-table databases to get a flattened representation
 - Modeling and deployment at the multi-table level
 - All other Khops functionalities are available similarly
 - Classification, regression, correlation analysis
 - Deployment, recoding, evaluation
 - ...

Star schema

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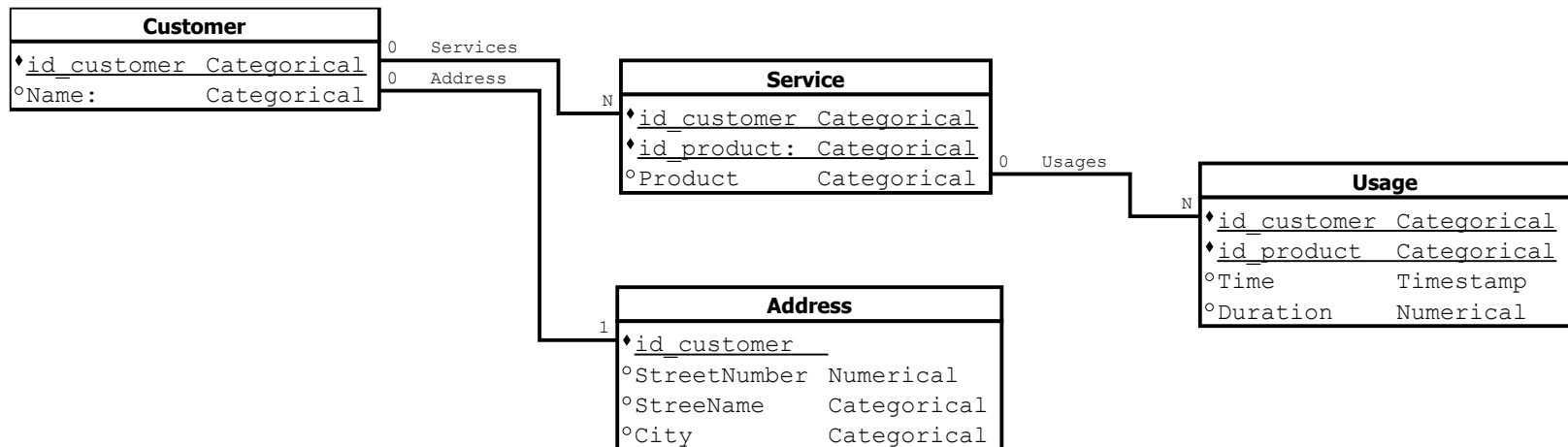
- One root entity
 - secondary tables in 0-1 relationship: Entity
 - secondary tables in 0-n relationship: Table



Snowflake schema

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- One root entity
 - secondary tables in 0-1 relationship: Entity
 - secondary tables in 0-n relationship: Table
- Each table may have secondary tables

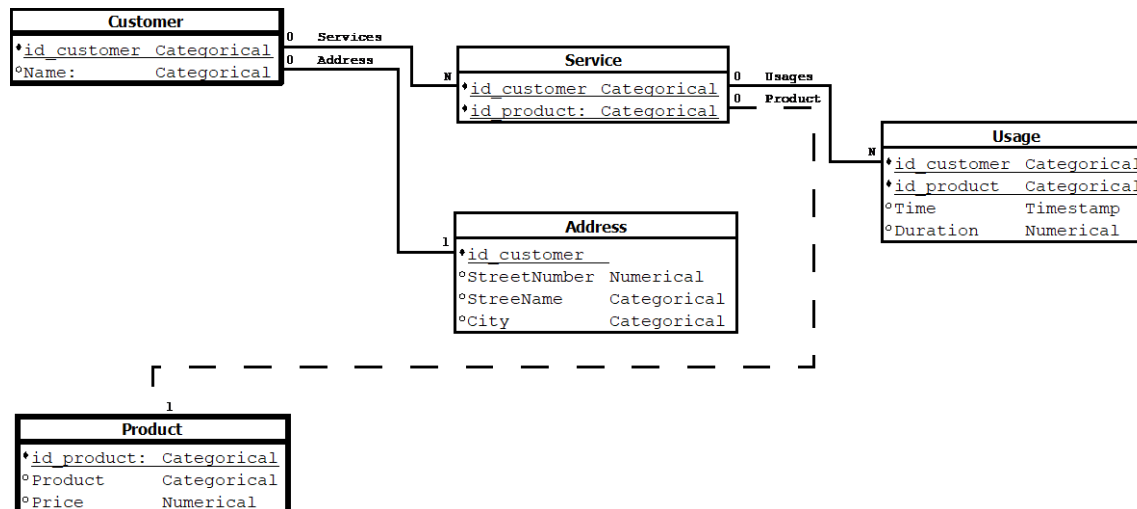


- Example in samples/Customer
 - detailed explanations in sample

External tables

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- One root entity
 - secondary tables in 0-1 relationship: Entity
 - secondary tables in 0-n relationship: Table
- Each table can have secondary tables
- **External tables**
 - to reuse common table shared by all analysis entities
 - can be referenced from any table, with specific keys

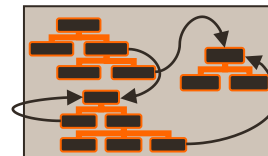
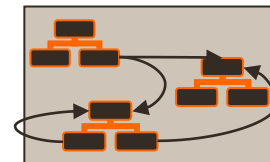
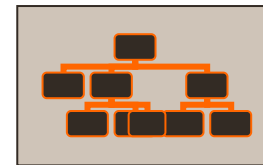
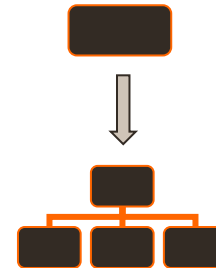


- Example in samples/CustomerExtended
 - detailed explanations in sample

Multi-table schemas: synthesis

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- Khiops 8.0:
 - from mono-table to star schema
 - Automatic variable construction
 - a technological disruption
- Khiops 9.0:
 - extended data schema
 - Snowflake schema
 - External data
 - Multiple snowflake schema



Example of a multi-table database

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French road accidents database

The `AccidentsSummary` is described using the following **star schema**:



```
Accident
|
| -- 1:n -- Vehicle
```

Each accident has associated one or more vehicles. In the Khiops dictionary Accident-Vehicle 1:n relationship is described with the `Table` keyword. The key linking both tables is `AccidentId`.

Objective: predict fatal traffic accidents (target variable: Gravity field of Accident table)

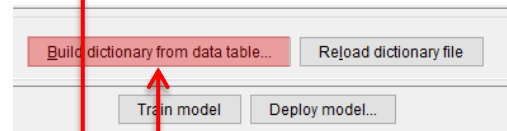
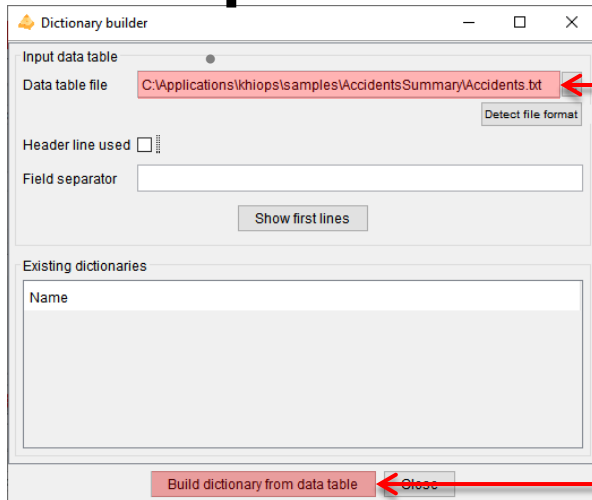


Build a multi-table dictionary

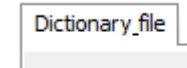
70

- Step 1: Build one dictionary per data table**

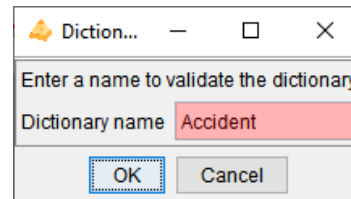
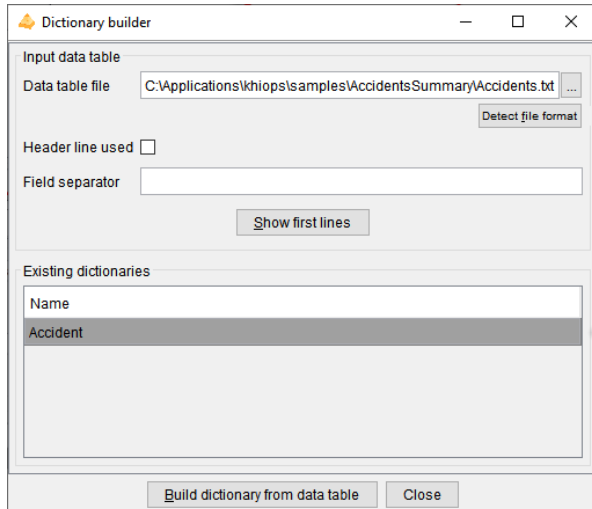
a : Build the first dictionary for the **Accidents.txt** table



1. In pane
Click on button *Build dictionary...*



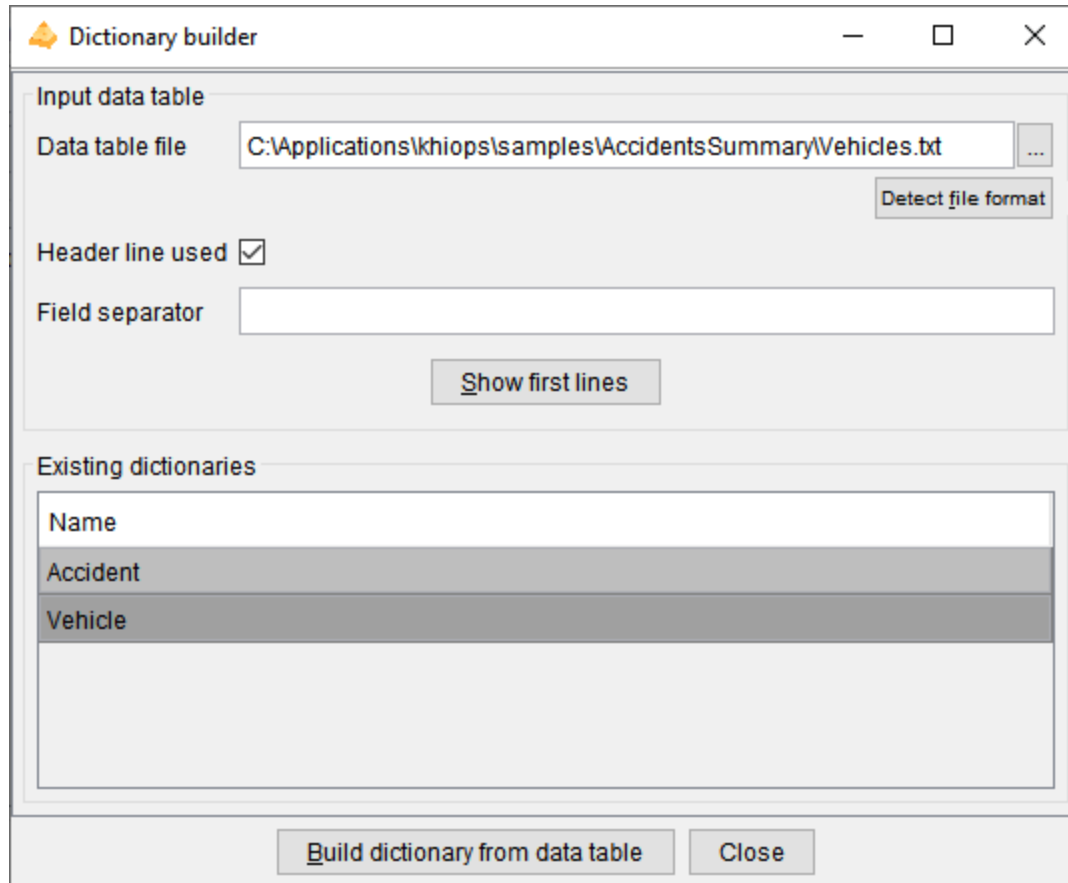
2. Build the first dictionary
Specify the data table file: **Accidents.txt**
Build the dictionary
Specify the dictionary name : **Accident**



Build a multi-table dictionary

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- **Step 1:** Build one dictionary per data table
 - b : Repeat for the `vehicles.txt` table



Dictionary builder

Input data table

Data table file ...

Detect file format

Header line used ☒

Field separator

Show first lines

Existing dictionaries

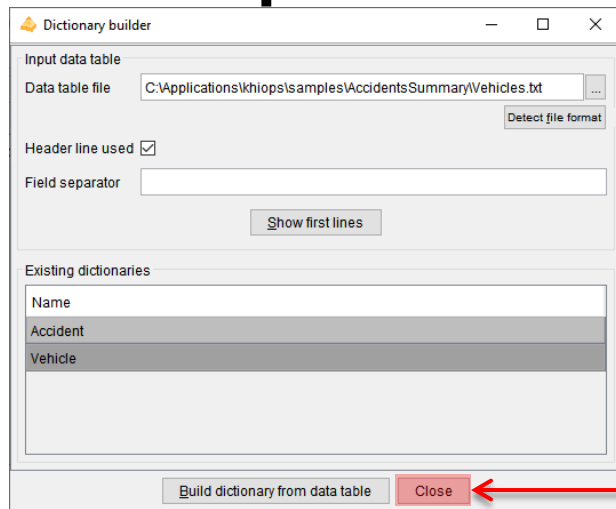
| Name |
|----------|
| Accident |
| Vehicle |

Build dictionary from data table Close

Build a multi-table dictionary

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• **Step 1:** save the constructed dictionary into a .kdic file



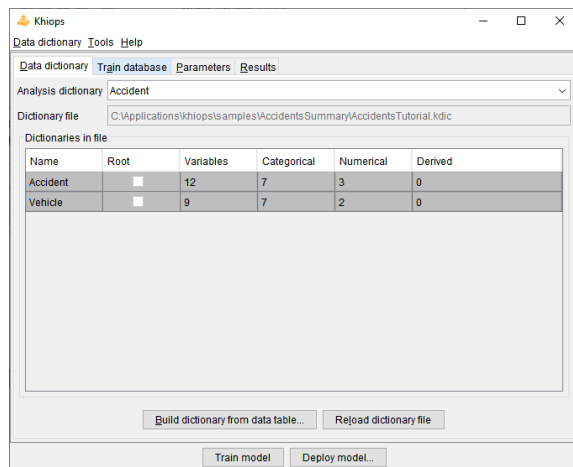
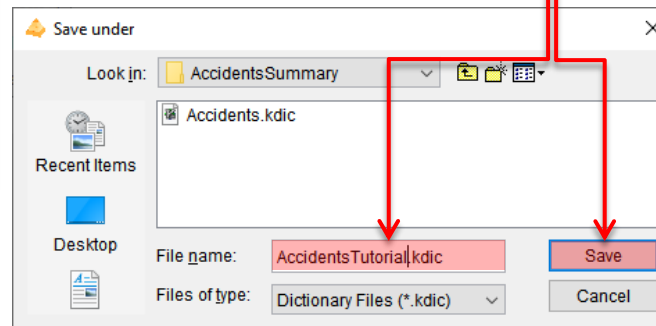
4. Save in dictionary file

• Close

• Specify the dictionary file name:

`AccidentsTutorial.kdic`

• Save



Build a multi-table dictionary

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• **Step 2:** Describe the table relationships in the .kdic file

5. Open the dictionary file with a text editor

5.1 Specify the root entity

5.2 Fix the types of the fields in green

5.3 Specify the key fields for each entity
Key fields must be Categorical and not derived

5.4 Specify the relation between the root entity and the secondary entity
Add a variable per relation to root dictionary

- *Table* for 0-n relationship
- *Entity* for 0-1 relationship

6. Save the dictionary file

```
Root Dictionary Accident(AccidentId)
{
    Categorical AccidentId;
    Categorical Gravity;
    Date Date;
    Time Hour;
    Categorical Light;
    Categorical Department;
    Categorical Commune;
    Categorical InAgglomeration;
    Categorical IntersectionType;
    Categorical Weather;
    Categorical CollisionType;
    Categorical PostalAddress;
    Table(Vehicle) Vehicles;
};

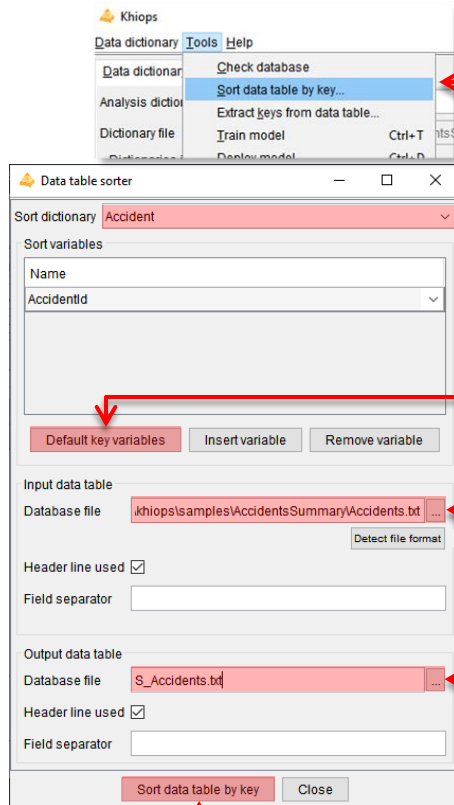
Dictionary Vehicle(AccidentId, VehicleId)
{
    Categorical AccidentId;
    Categorical VehicleId;
    Categorical Direction;
    Categorical Category;
    Numerical PassengerNumber;
    Categorical FixedObstacle;
    Categorical MobileObstacle;
    Categorical ImpactPoint;
    Categorical Maneuver;
};
```

Sort data table files (if necessary)

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For multi-table analyses data table files must be sorted by their keys

- Sorting is done only once before any Khops analysis
 - Note: Records of the root table **must** be unique by key
- It is necessary for efficiency, specially when treating large databases
 - Records of the root and secondary tables are read synchronously from their data table files



1. Open the multi-table dictionary file

This allows to obtain the definition of the tables to sort

2. Menu: *Tools* → *Sort data table by key*

In the *Data table sorter* window, for each data table to sort

2.1 Specify the sort dictionary

2.2 Specify the sort variables

Default key variables to use the keys defined in dictionary

2.3 Specify the input and output data table files

2.4 Sort

- The output file is sorted by key
- All native variables are kept (used or not in the dictionary)
- Derived variables are ignored

Supervised classification

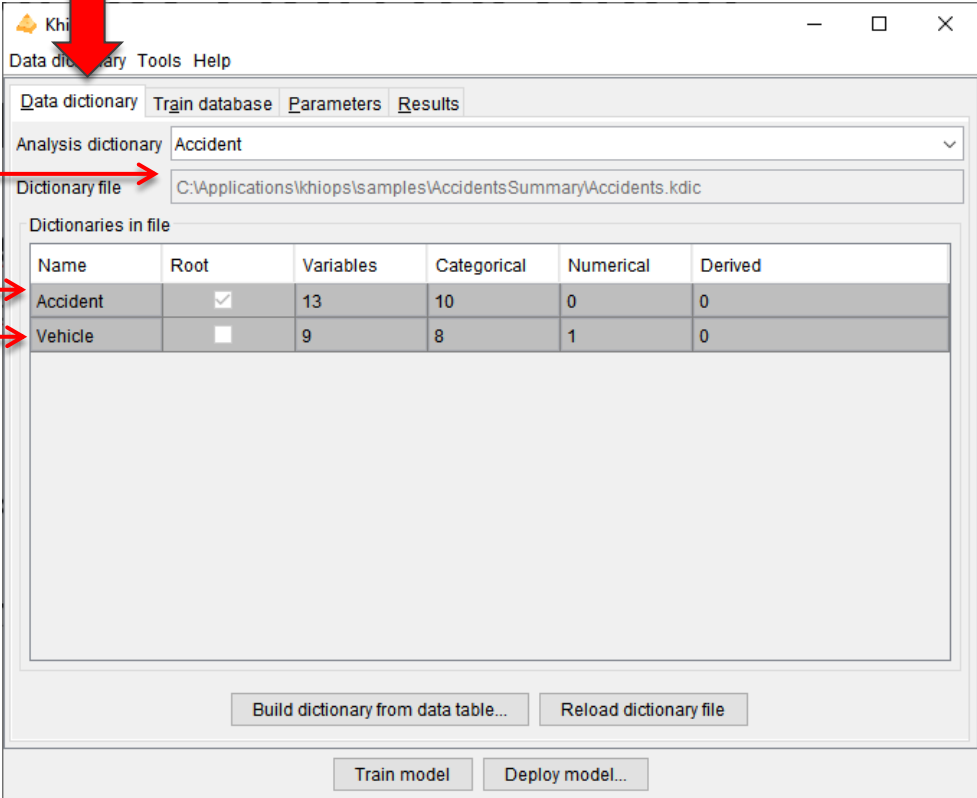
75

- **Step 1, bis** : Open the *Accidents.kdic* dictionary file

Analysis dictionary →

Root entity →

Secondary entity →



| Name | Root | Variables | Categorical | Numerical | Derived |
|----------|-------------------------------------|-----------|-------------|-----------|---------|
| Accident | <input checked="" type="checkbox"/> | 13 | 10 | 0 | 0 |
| Vehicle | <input type="checkbox"/> | 9 | 8 | 1 | 0 |

Buttons at the bottom: Build dictionary from data table..., Reload dictionary file, Train model, Deploy model...



Supervised classification

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- **Step 2 : Specify train and test databases**
 - Specify the root and secondary data table files

The screenshot shows the 'Train database' dialog box in the Khiops application. The 'Train database' tab is selected. The 'Database files' table contains the following data:

| Data root | Path | Dictionary | Data table file |
|-----------|----------|------------|--|
| Accident | | Accident | C:\Applications\khiops\samples\AccidentsSummary\Accident ... |
| Accident | Vehicles | Vehicle | C:\Applications\khiops\samples\AccidentsSummary\Vehicles ... |

Below the table, there are several settings:

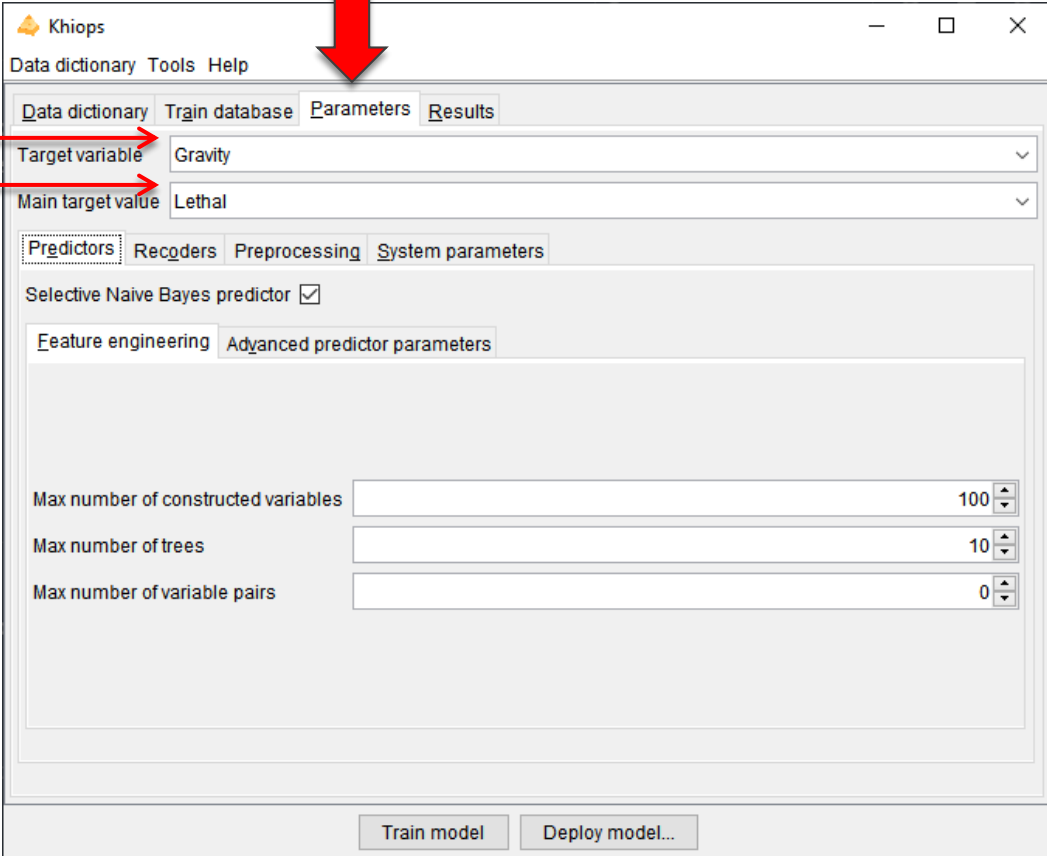
- Header line used: ☒
- Field separator:
- Sample percentage: 70
- Sampling mode: Include sample
- Selection variable:
- Selection value:
- Test database: Complementary

Buttons at the bottom include 'Train model' and 'Deploy model...'. A 'Detect file format' button is also present near the table.

Supervised classification

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- **Step 3 : Parameters**



Target variable

Main target value

Khops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Target variable Gravity

Main target value Lethal

Predictors Recorders Preprocessing System parameters

Selective Naive Bayes predictor ☒

Feature engineering Advanced predictor parameters

Max number of constructed variables 100

Max number of trees 10

Max number of variable pairs 0

Train model Deploy model...



Supervised classification

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- **Step 4 : Variable construction parameters**

Optional

Choice of construction rules

| Used | Family | Name | Label |
|-------------------------------------|-------------|--------------------|--|
| <input checked="" type="checkbox"/> | Entity | GetValue | Numerical value in a sub-entity |
| <input checked="" type="checkbox"/> | Entity | GetValueC | Categorical value in a sub-entity |
| <input checked="" type="checkbox"/> | Table | TableCount | Number of instances in a table |
| <input checked="" type="checkbox"/> | Table | TableCountDistinct | Number of distinct values in a table |
| <input checked="" type="checkbox"/> | Table | TableMax | Max of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMean | Mean of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMedian | Median of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMin | Min of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMode | Most frequent value in a table |
| <input checked="" type="checkbox"/> | Table | TableSelection | Selection from a table for a given selection criterion |
| <input checked="" type="checkbox"/> | Table | TableStdDev | Standard deviation of values in a table |
| <input checked="" type="checkbox"/> | Table | TableSum | Sum of values in a table |
| <input type="checkbox"/> | Date | Day | Day in a date |
| <input type="checkbox"/> | Date | DecimalYear | Year with decimal part for day in year |
| <input type="checkbox"/> | Date | WeekDay | Day in week in a date |
| <input type="checkbox"/> | Date | YearDay | Day in year in a date |
| <input type="checkbox"/> | Time | DecimalTime | Decimal hour in day |
| <input type="checkbox"/> | Timestamp | DecimalWeekDay | Week day with decimal part for fraction of days |
| <input type="checkbox"/> | Timestamp | DecimalYearTS | Year with decimal part for day in year, at timestamp precision |
| <input type="checkbox"/> | Timestamp | GetDate | Get date from timestamp |
| <input type="checkbox"/> | Timestamp | GetTime | Get time from timestamp |
| <input type="checkbox"/> | TimestampTZ | LocalTimestamp | Local timestamp from a timestampTZ |

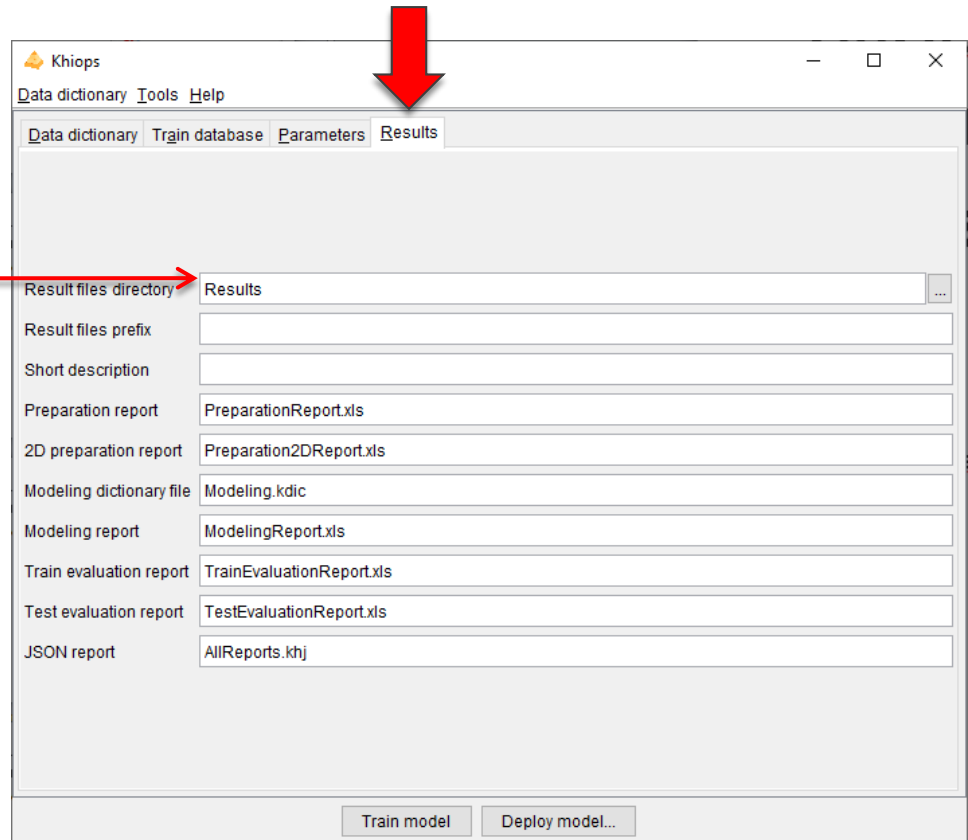
Default Select all Unselect all Close

Supervised classification

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- **Step 5 : Analysis results**

Results files directory



Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Result files directory Results

Result files prefix

Short description

Preparation report PreparationReport.xls

2D preparation report Preparation2DReport.xls

Modeling dictionary file Modeling.kdic

Modeling report ModelingReport.xls

Train evaluation report TrainEvaluationReport.xls

Test evaluation report TestEvaluationReport.xls

JSON report AllReports.khj

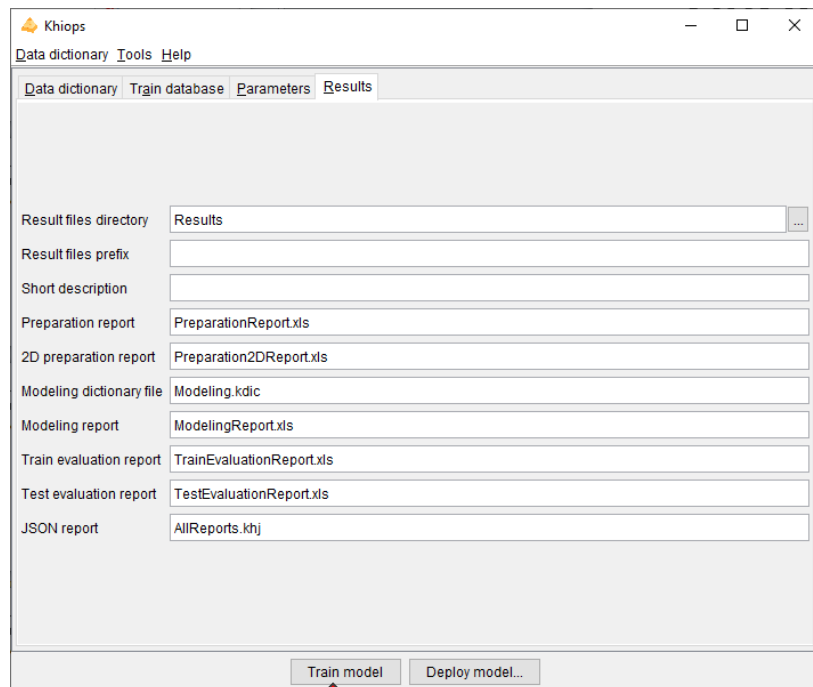
Train model Deploy model...



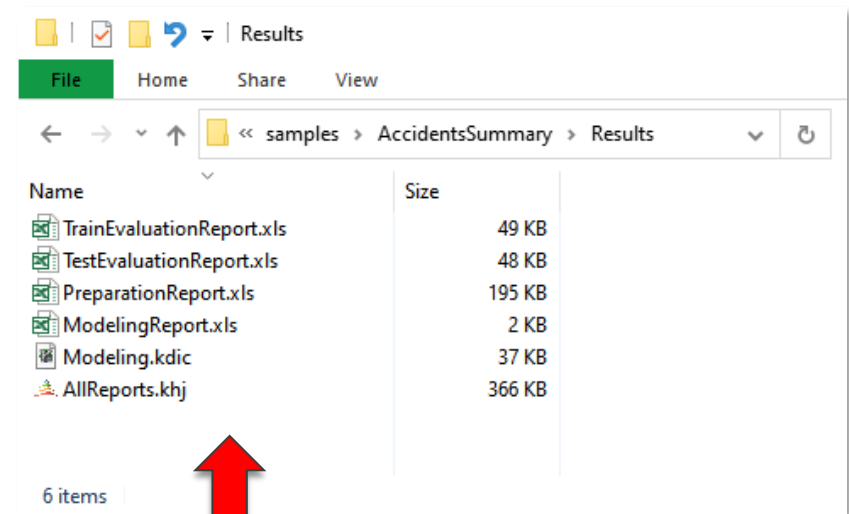
Supervised classification

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- Step 6 : Start the analysis**



1 - Train model



2 - Inspect the results using Khlops Visualization
(double-click on .khj file)





Exploratory of classification results using Khops Visualization

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Preparation ↓

Summary

Dictionary : Accident
Database : C:\Applications\khops\samples\AccidentsSummary\Accidents.txt
Target variable : Gravity
Instances : 40470
Learning task : Classification

Target variable stats

■ Lethal ■ NonLethal

109 Variables

| Rank | Name | Level | Parts | Val. | Type |
|-------------|---|---------------|----------|----------|------------------|
| R003 | CollisionType | 0.0360 | 3 | 8 | Categorical |
| R004 | Mode(Vehicles.FixedObstacle) | 0.0304 | 3 | 18 | Categorical |
| R005 | Commune | 0.0253 | 2 | 791 | Categorical |
| R006 | Light | 0.0234 | 4 | 5 | Categorical |
| R007 | Max(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 67 | Numerical |
| R008 | Mean(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 85 | Numerical |
| R009 | Median(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 69 | Numerical |
| R010 | Min(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 35 | Numerical |
| R011 | StdDev(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 76 | Numerical |
| R012 | Sum(Vehicles.PassengerNumber) where FixedObstacle = None | 0.0207 | 2 | 68 | Numerical |
| R013 | Count(Vehicles) where FixedObstacle = None | 0.0205 | 3 | 11 | Numerical |
| R014 | Count(Vehicles) where FixedObstacle <> None | 0.0203 | 2 | 9 | Numerical |
| R015 | Max(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0203 | 2 | 31 | Numerical |
| R016 | Mean(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0203 | 2 | 23 | Numerical |

Count(Vehicles) where FixedObstacle <> None

Internal Coverage

■ Coverage

Target distribution

■ Lethal ■ NonLethal

Current interval

Interval of Count(Vehicles... | [0,0.5]

Constructed variable name ↑

Constructed variable derivation rule ↑

Derivation rule

TableCount("Vehicles where FixedObstacle <> None")

Informations

Evaluated variables : 109
Constructed variables : 100
Informative variables : 66
Discretization : MODL
Value grouping : MODL



Example of a complex multi-table database

82

French road accidents database (full version)

This is the full version of the `AccidentsSummary` dataset.

It is described using the following **snowflake schema**:

```
Accident
|
| -- 1:n -- Vehicle
|           |
|           |-- 1:n -- User
|
| -- 1:1 -- Place
```



Each accident has associated one or more vehicles and one unique place. The vehicles involved in an accident have in turn associated one or more road users (passengers and pedestrians).

In the Khiops dictionary the Accident-Place relationship (1:1) is described with the `Entity` keyword, whereas the Accident-Vehicle and Vehicle-User relationships (1:n) with the `Table` keyword.

Objective: predict fatal traffic accidents (target variable: Gravity field of Accident table)

Supervised classification

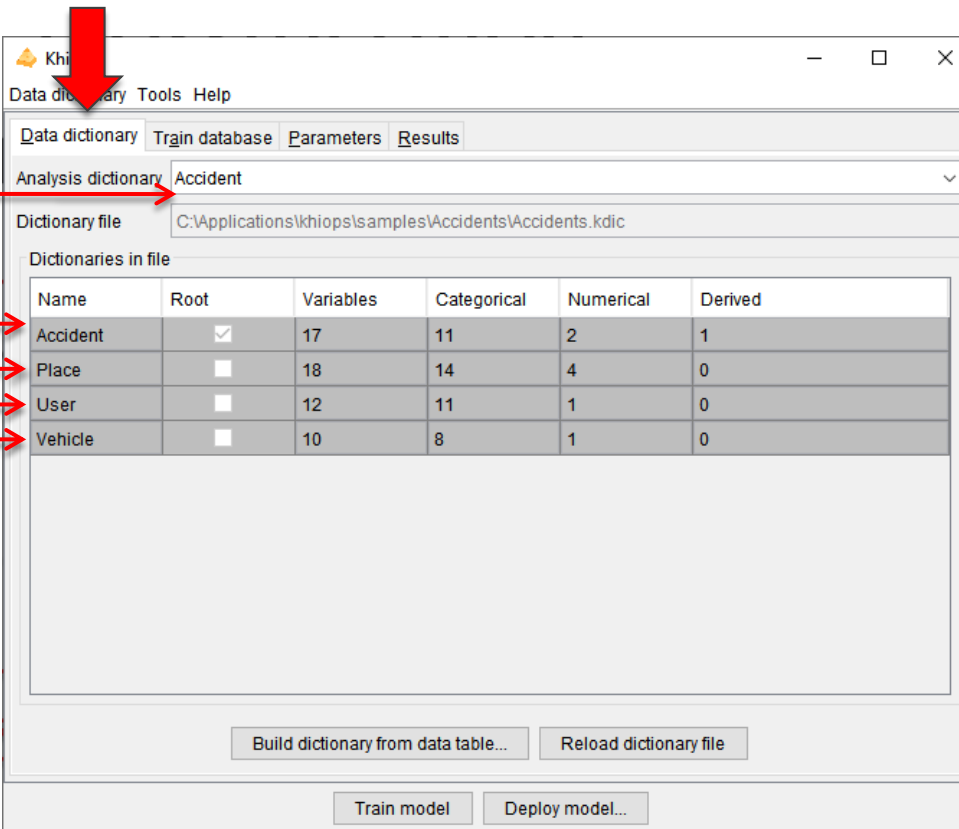
83

- **Step 1** : Open the *Accidents.kdic* dictionary file

Analysis dictionary →

Root entity →

Secondary entities →



Dictionary file: C:\Applications\khiops\samples\Accidents\Accidents.kdic

| Name | Root | Variables | Categorical | Numerical | Derived |
|----------|-------------------------------------|-----------|-------------|-----------|---------|
| Accident | <input checked="" type="checkbox"/> | 17 | 11 | 2 | 1 |
| Place | <input type="checkbox"/> | 18 | 14 | 4 | 0 |
| User | <input type="checkbox"/> | 12 | 11 | 1 | 0 |
| Vehicle | <input type="checkbox"/> | 10 | 8 | 1 | 0 |

Build dictionary from data table... Reload dictionary file

Train model Deploy model...



Supervised classification

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- **Step 2 : Specify train and test databases**

- Root and other data table files have to be specified

Khlops

Data dictionary Tools

Data dictionary Train database Parameters Results

Database files

| Data root | Path | Dictionary | Data table file |
|-----------|-----------------|------------|--|
| Accident | | Accident | C:\Applications\khiops\samples\Accidents\Accidents.txt |
| Accident | Place | Place | C:\Applications\khiops\samples\Accidents\Places.txt |
| Accident | Vehicles | Vehicle | C:\Applications\khiops\samples\Accidents\Vehicles.txt |
| Accident | Vehicles' Users | User | C:\Applications\khiops\samples\Accidents\Users.txt |

Detect file format

Header line used ☒

Field separator

Sample percentage 70

Sampling mode Include sample

Selection variable

Selection value

Test database Complementary

Inspect test database settings...

Train model Deploy model...

Root data table files

Secondary data table files

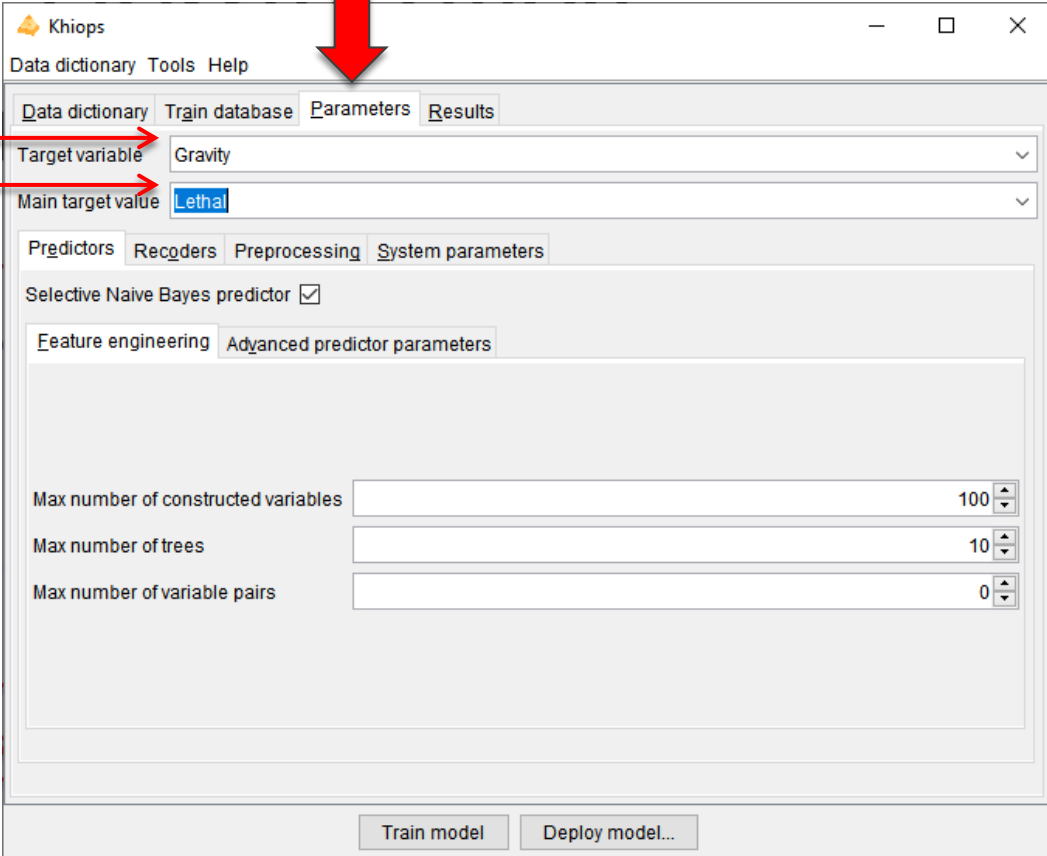
Supervised classification

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- **Step 3 : Parameters**

Target variable →

Main target value →



The screenshot shows the 'Khiops' window with the 'Parameters' tab selected. The 'Target variable' is set to 'Gravity' and the 'Main target value' is set to 'Lethal'. The 'Predictors' tab is also visible, showing the 'Selective Naive Bayes predictor' checked. The 'Feature engineering' and 'Advanced predictor parameters' tabs are also present. The 'Max number of constructed variables' is set to 100, 'Max number of trees' is set to 10, and 'Max number of variable pairs' is set to 0. The 'Train model' and 'Deploy model...' buttons are at the bottom.

Max number of constructed variables 100

Max number of trees 10

Max number of variable pairs 0

Train model Deploy model...

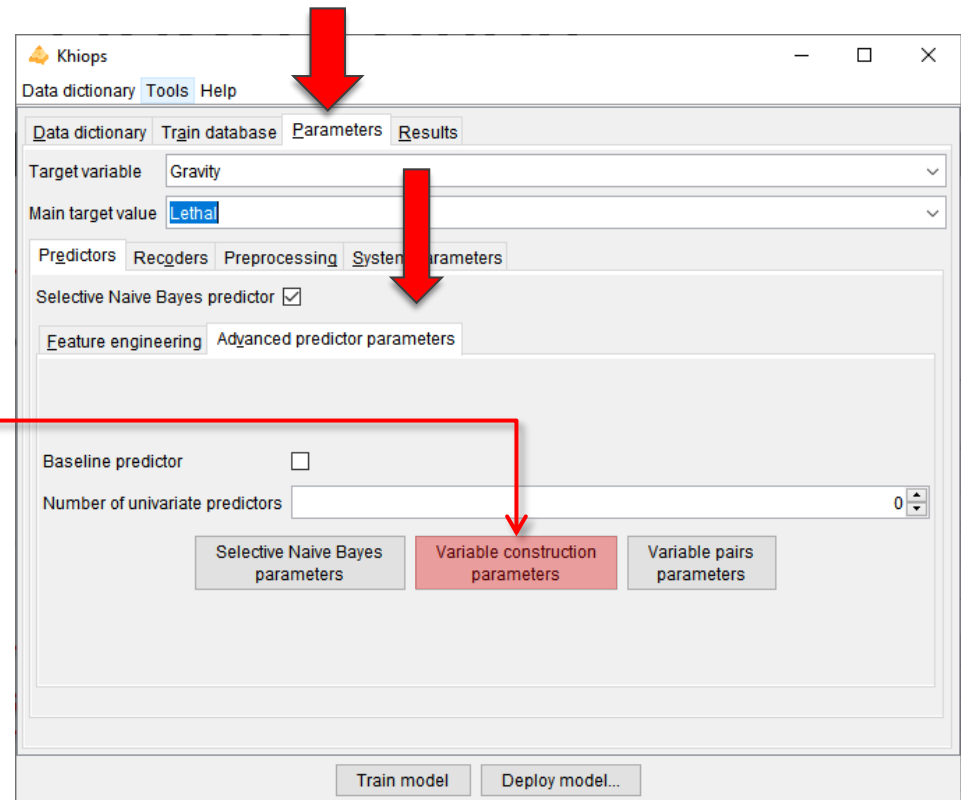
Supervised classification

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- **Step 4 : Variable construction parameters**

Optional

Choice of construction rules



The screenshot shows the 'Khiops' application window with the 'Parameters' tab selected. The 'Target variable' is set to 'Gravity' and the 'Main target value' is 'Lethal'. The 'Predictors' sub-tab is active, showing the 'Selective Naive Bayes predictor' checked. The 'Advanced predictor parameters' sub-tab is also visible. At the bottom, there are three buttons: 'Selective Naive Bayes parameters', 'Variable construction parameters' (highlighted in red), and 'Variable pairs parameters'. The 'Train model' and 'Deploy model...' buttons are at the very bottom.



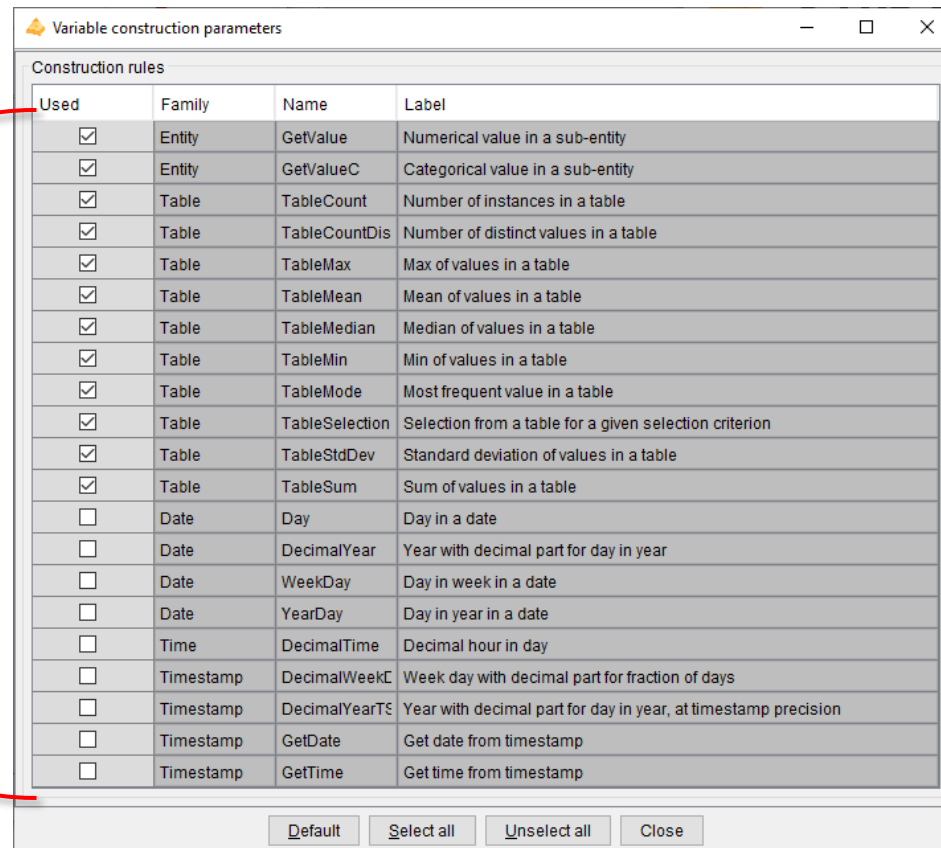
Supervised classification

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- **Step 4 : Variable construction parameters**

Optional

Choice of construction rules



The dialog box titled "Variable construction parameters" contains a table of construction rules. A red bracket on the left side of the table indicates that the selection of rules is optional.

| Used | Family | Name | Label |
|-------------------------------------|-----------|----------------|--|
| <input checked="" type="checkbox"/> | Entity | GetValue | Numerical value in a sub-entity |
| <input checked="" type="checkbox"/> | Entity | GetValueC | Categorical value in a sub-entity |
| <input checked="" type="checkbox"/> | Table | TableCount | Number of instances in a table |
| <input checked="" type="checkbox"/> | Table | TableCountDis | Number of distinct values in a table |
| <input checked="" type="checkbox"/> | Table | TableMax | Max of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMean | Mean of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMedian | Median of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMin | Min of values in a table |
| <input checked="" type="checkbox"/> | Table | TableMode | Most frequent value in a table |
| <input checked="" type="checkbox"/> | Table | TableSelection | Selection from a table for a given selection criterion |
| <input checked="" type="checkbox"/> | Table | TableStdDev | Standard deviation of values in a table |
| <input checked="" type="checkbox"/> | Table | TableSum | Sum of values in a table |
| <input type="checkbox"/> | Date | Day | Day in a date |
| <input type="checkbox"/> | Date | DecimalYear | Year with decimal part for day in year |
| <input type="checkbox"/> | Date | WeekDay | Day in week in a date |
| <input type="checkbox"/> | Date | YearDay | Day in year in a date |
| <input type="checkbox"/> | Time | DecimalTime | Decimal hour in day |
| <input type="checkbox"/> | Timestamp | DecimalWeekI | Week day with decimal part for fraction of days |
| <input type="checkbox"/> | Timestamp | DecimalYearTE | Year with decimal part for day in year, at timestamp precision |
| <input type="checkbox"/> | Timestamp | GetDate | Get date from timestamp |
| <input type="checkbox"/> | Timestamp | GetTime | Get time from timestamp |

Buttons: Default, Select all, Unselect all, Close

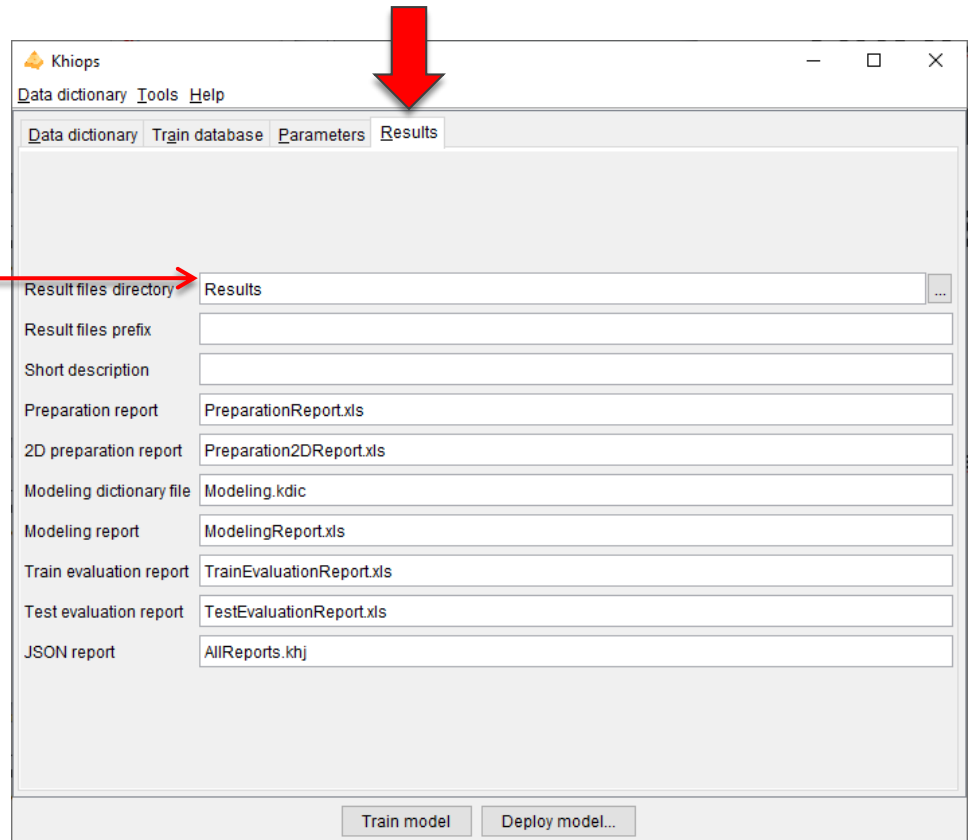


Supervised classification

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- **Step 5 : Analysis results**

Results files directory



Khiops

Data dictionary Tools Help

Data dictionary Train database Parameters Results

Result files directory Results

Result files prefix

Short description

Preparation report PreparationReport.xls

2D preparation report Preparation2DReport.xls

Modeling dictionary file Modeling.kdic

Modeling report ModelingReport.xls

Train evaluation report TrainEvaluationReport.xls

Test evaluation report TestEvaluationReport.xls

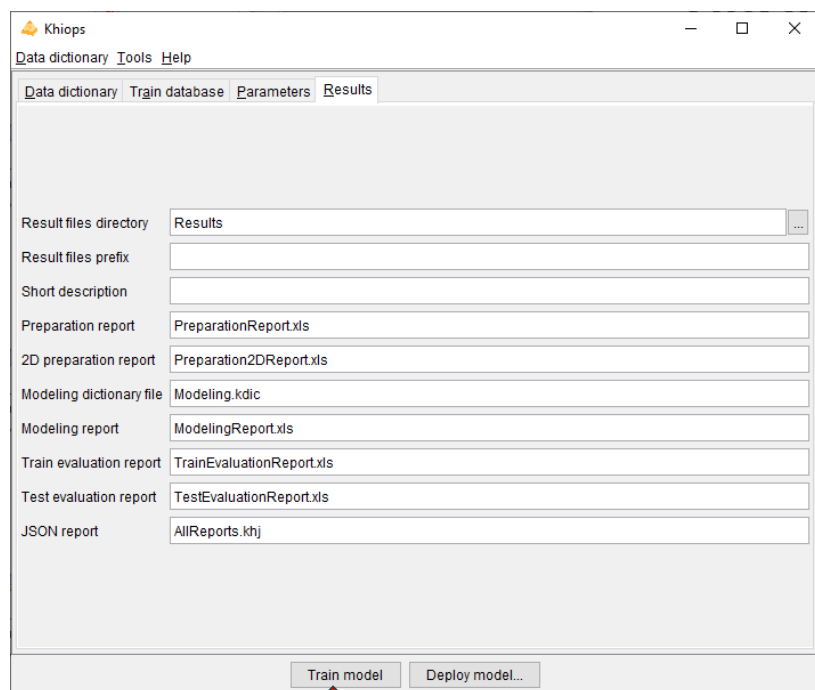
JSON report AllReports.khj

Train model Deploy model...

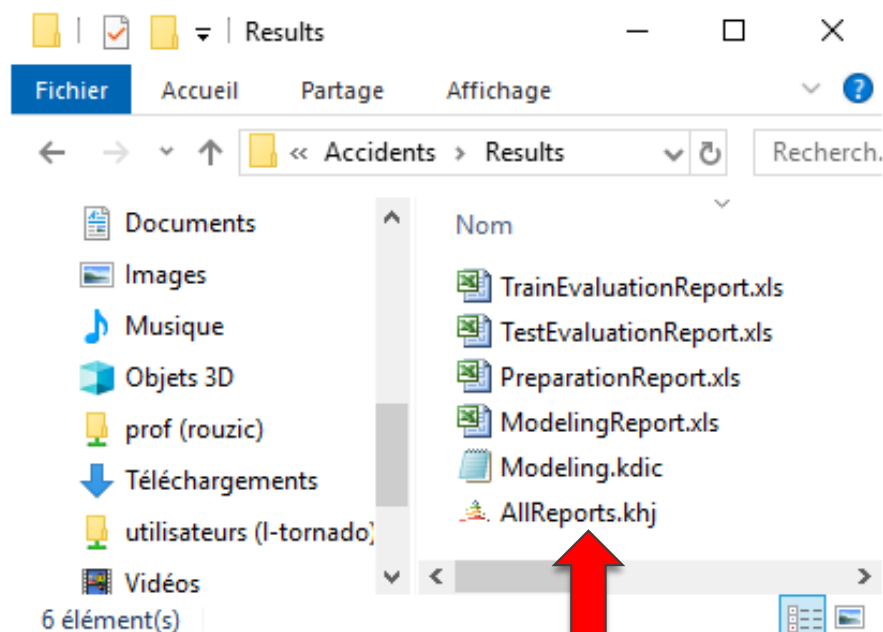
Supervised classification

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- Step 6 : Start the analysis**



1 - Train model



2 - Inspect the results using Khlops Visualization
(double-click on .khj file)



Exploratory of classification results using Khiops Visualization

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Khiops Visualization
File View Help Report a bug

KHIOPS Visualization

Project **Preparation** Tree preparation Modeling Evaluation

Summary
Dictionary : Accident
Database : C:\Applications\khiops\samples\Accidents\Accidents.txt
Target variable : Gravity
Instances : 40470

Target variable stats
Lethal NonLethal

Informations
Evaluated variables : 112
Constructed variables : 100
Informative variables : 84
Discretization : MODL
Value grouping : MODL

112 Variables
Level distribution

| Rank | Name | Level ↓ | Parts | Values | Type |
|-------------|---|---------------|----------|-----------|------------|
| R009 | Mode(Vehicles.FixedObstacle) | 0.0304 | 3 | 18 | Cate |
| R010 | Latitude | 0.0297 | 11 | 33911 | Num |
| R011 | Commune | 0.0253 | 2 | 791 | Cate |
| R012 | Light | 0.0234 | 4 | 5 | Cate |
| R013 | Mean(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0206 | 2 | 85 | Num |
| R014 | Median(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0206 | 2 | 69 | Num |
| R015 | Count(Vehicles) where FixedObstacle = None | 0.0204 | 3 | 11 | Num |
| R016 | Mean(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0202 | 2 | 33 | Num |
| R017 | Median(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0202 | 2 | 32 | Num |
| R018 | Min(Vehicles.PassengerNumber) where FixedObstacle <> None | 0.0202 | 2 | 28 | Num |

Mean(Vehicles.PassengerNumber) where FixedObstacle <> None
Scale chart

Internal Coverage
Coverage

Target distribution
Lethal NonLethal
Values Lift

Current interval
Interval of Mean(Vehicles.PassengerNumber) where FixedObstacle <> None
Missing

Constructed variable name
Mean(Vehicles.PassengerNumber) where FixedObstacle <> None

Constructed variable derivation rule
TableMean("Vehicles where FixedObstacle <> None", PassengerNumber)

Khops multi-table

91

- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond



- Impact on Khops Coclustering
 - Deployment of coclustering models
 - Given a text*word coclustering model, assign new texts (with their words) to their closest cluster
 - Given a cookie*page coclustering model, assign new cookies (with their pages) to their closest cluster
 - Given a curve*X*Y triclustering model, assign new curves (with their X*Y points) to their closest cluster

- In this tutorial



- Build a triclustering model on the SpliceJunctionDNA data table

- Clusters of sequence samples
- Intervals of positions in the sequences
- Clusters of DNA chars



- Prepare a deployment model

- Build a deployment dictionary



- Deploy the model on the multi-table SpliceJunction database

- Assign new DNA sequences to trained clusters of sequences

Splice junction multi-table database

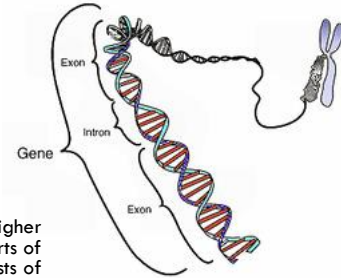
92

- **Molecular Biology (Splice-junction Gene Sequences)**

- **Objective:**

- **Recognition of boundaries between exons and introns in DNA sequences**

- Splice junctions are points on a DNA sequence at which 'superfluous' DNA is removed during the process of protein creation in higher organisms. The problem posed in this dataset is to recognize, given a sequence of DNA, the boundaries between exons (the parts of the DNA sequence retained after splicing) and introns (the parts of the DNA sequence that are spliced out). This problem consists of two subtasks: recognizing exon/intron boundaries (referred to as EI sites), and recognizing intron/exon boundaries (IE sites). (In the biological community, IE borders are referred to as "acceptors" while EI borders are referred to as "donors".)



- **Database dictionary**

- **Root entity: splice junction**

- SampleId
 - Class (EI, IE, NEG)
 - Sequence of DNA

- **Secondary entity: DNA**

- SampleId:
 - Pos: position in the sequence
 - Char (A, C, G, T)

- **Database files**

- SpliceJunction.txt
 - SpliceJunctionDNA.txt

SpliceJunction.txt

| SampleId | Class |
|----------------------|-------|
| AGMKPNRSB-NEG-1 | N |
| AGMORS12A-NEG-181 | N |
| AGMORS9A-NEG-481 | N |
| AGMRSPNI-NEG-1141 | N |
| ATRINS-ACCEPTOR-1678 | IE |
| ATRINS-ACCEPTOR-701 | IE |
| ATRINS-DONOR-521 | EI |
| ATRINS-DONOR-905 | EI |
| ... | |

SpliceJunctionDNA.txt

| SampleId | Pos | Char |
|-------------------|-----|------|
| AGMKPNRSB-NEG-1 | 1 | C |
| AGMKPNRSB-NEG-1 | 2 | A |
| ... | | |
| AGMKPNRSB-NEG-1 | 58 | A |
| AGMKPNRSB-NEG-1 | 59 | C |
| AGMKPNRSB-NEG-1 | 60 | A |
| AGMORS12A-NEG-181 | 1 | A |
| AGMORS12A-NEG-181 | 2 | G |
| ... | | |
| AGMORS12A-NEG-181 | 59 | G |
| AGMORS12A-NEG-181 | 60 | G |
| AGMORS9A-NEG-481 | 1 | T |
| AGMORS9A-NEG-481 | 2 | G |
| AGMORS9A-NEG-481 | 3 | G |
| ... | | |

Exploratory analysis of DNA sequences:

- . find clusters of similar DNA sequences
- . using a triclustering SampleId x Pos x Char

Orange Restricted

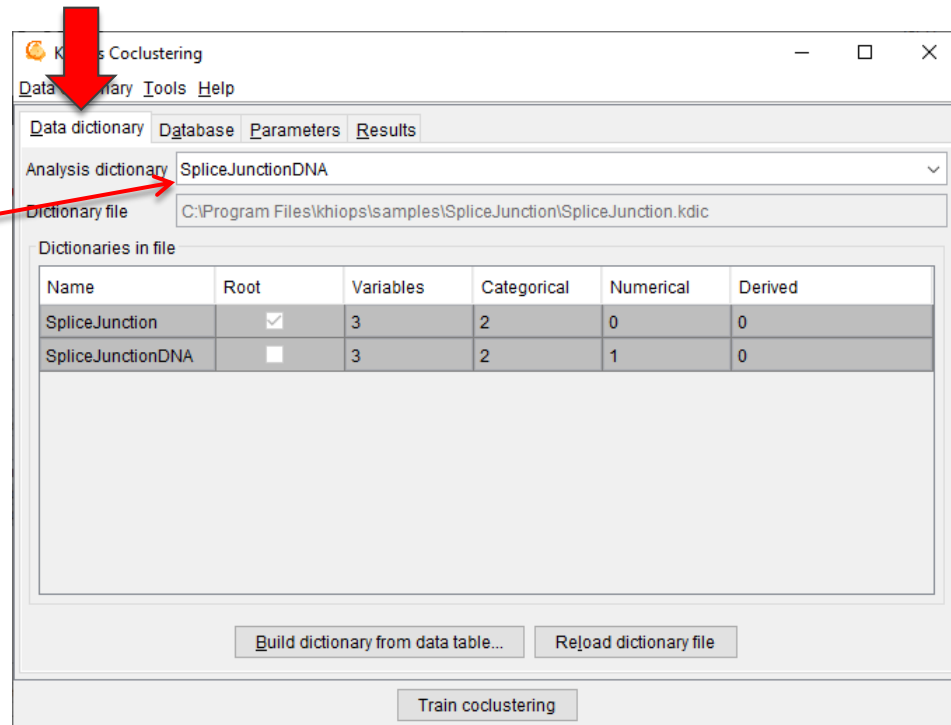


Train a triclustering model

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- **Step 1 : Open an existing dictionary**
(ex: sample SpliceJunction.kdic)

Analysis dictionary
(secondary entity)





Train a triclustering model

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- **Step 2 : Specification of used database**

Data table file

(one single file for analysis of the secondary entity)

Khiops Coclustering

Data dictionary Tools Help

Data dictionary Database Parameters Results

Database files

| Data root | Path | Dictionary | Data table file |
|-------------------|------|-------------------|--|
| SpliceJunctionDNA | | SpliceJunctionDNA | C:\Program Files\khiops\samples\SpliceJunction\SpliceJunctionDNA.txt ... |

Detect file format

Header line used ☒

Field separator

Sample percentage

Sampling mode

Selection variable

Selection value

Train coclustering



Train a triclustering model

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- **Step 3 : Specification of triclustering variables**

Triclustering
variables

The screenshot shows the 'Khiops Coclustering' window with the 'Parameters' tab selected. Under the 'Coclustering parameters' sub-tab, the 'Coclustering variables' section contains a list of variables: 'Name', 'SampleId', 'Pos', and 'Char'. Each variable has a dropdown arrow to its right. A red arrow points from the 'Triclustering variables' text to this list. Below the list are 'Insert variable' and 'Remove variable' buttons. At the bottom, there is a 'Frequency variable' dropdown and a 'Train coclustering' button.



Train a triclustering model

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- **Step 4 : Analysis results**

Result files directory

The screenshot shows the 'Khiops Coclustering' application window. The 'Results' tab is selected, indicated by a red arrow. The 'Result files directory' field is highlighted with a red arrow and the text 'Result files directory'. The field contains the text 'TriclusteringResults'. Other fields include 'Result files prefix', 'Short description', 'Coclustering report' (set to 'Coclustering.khc'), and 'Export JSON' (checked). A 'Train coclustering' button is at the bottom.

Khiops Coclustering

Data dictionary Tools Help

Data dictionary Database Parameters Results

Result files directory TriclusteringResults

Result files prefix

Short description

Coclustering report Coclustering.khc

Export JSON ☒

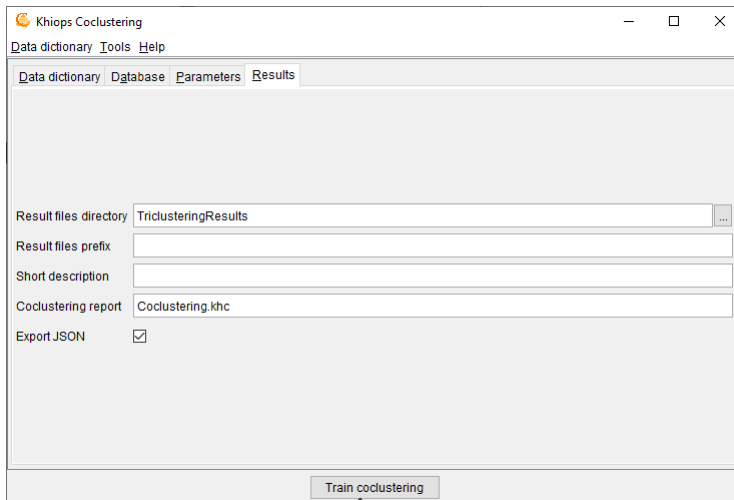
Train coclustering



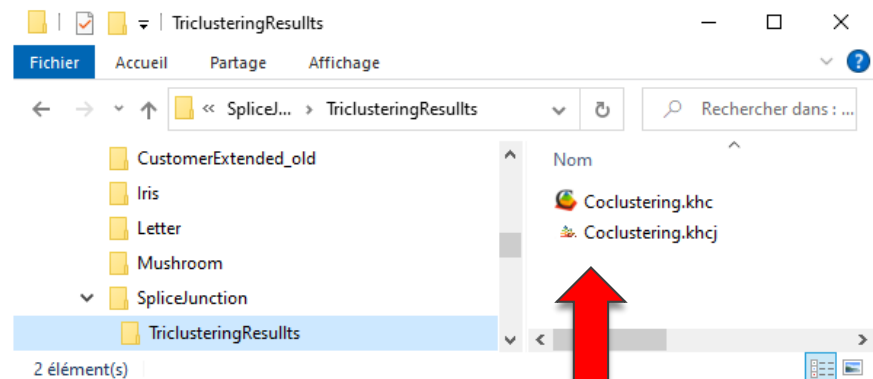
Train a triclustering model

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- **Step 5 : Start the analysis**



1 – Start the analysis



2 - Inspect the results using Khiops Covisualization
(double-click on .khcj file)



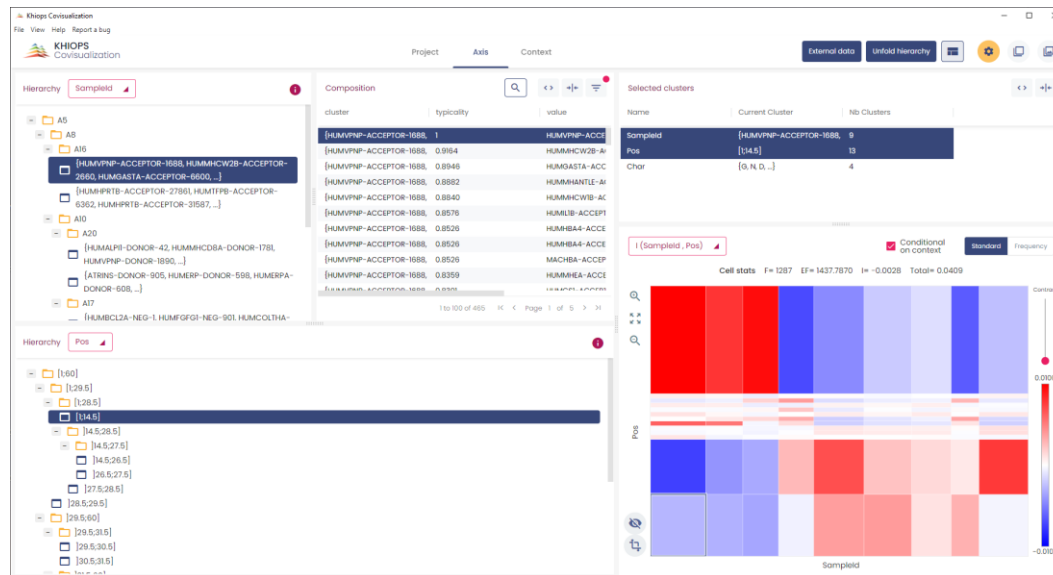
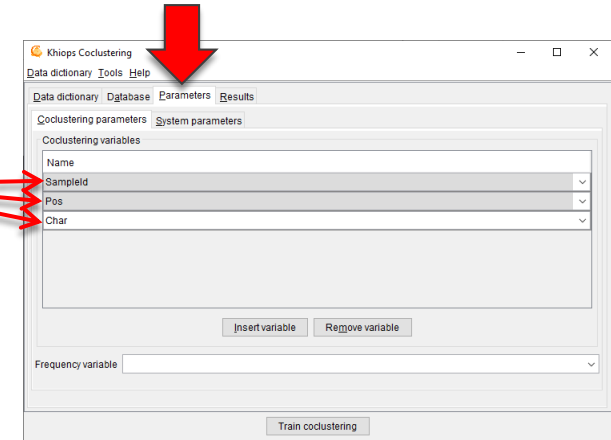


Khiops covisualisation: base SpliceJunctionDNA

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- With Khiops Coclustering
 - Analysis of correlation between variables
SampleId*Pos*Char



With Khiops Covisualization

- Exploratory analysis of the results

Khops multi-table

99

- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond



- Impact on Khops Coclustering
 - Deployment of coclustering models
 - Given a text*word coclustering model, assign new texts (with their words) to their closest cluster
 - Given a cookie*page coclustering model, assign new cookies (with their pages) to their closest cluster
 - Given a curve*X*Y triclustering model, assign new curves (with their X*Y points) to their closest cluster

• In this tutorial



- Train a triclustering model on the SpliceJunctionDNA data table
 - Clusters of sequence samples
 - Intervals of positions in the sequences
 - Clusters of DNA chars



• Prepare a deployment model

- Build a deployment dictionary



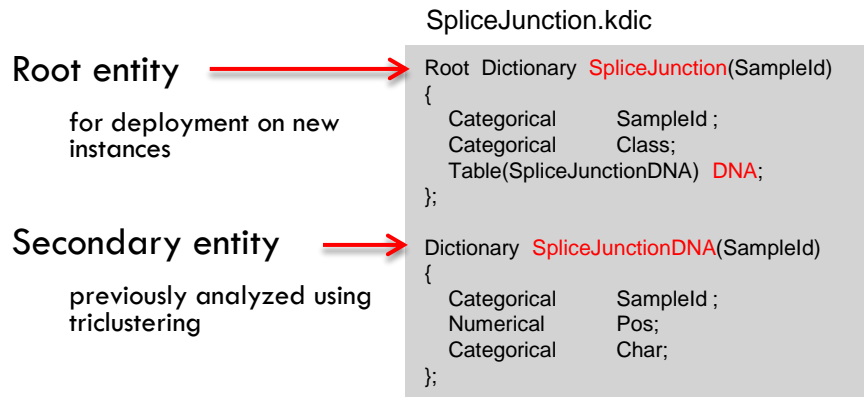
- Deploy the model on the multi-table SpliceJunction database
 - Assign new DNA sequences to trained clusters of sequences



Prepare a deployment model

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- **Prerequisite : a multi-table database**
 - dictionary file
 - data files(ex: sample SpliceJunction)



SpliceJunction.txt

| SampleId | Class |
|----------------------|-------|
| AGMKPNRSB-NEG-1 | N |
| AGMORS12A-NEG-181 | N |
| AGMORS9A-NEG-481 | N |
| AGMRSPNI-NEG-1141 | N |
| ATRINS-ACCEPTOR-1678 | IE |
| ATRINS-ACCEPTOR-701 | IE |
| ATRINS-DONOR-521 | EI |
| ATRINS-DONOR-905 | EI |
| ... | |

SpliceJunctionDNA.txt

| SampleId | Pos | Char |
|-------------------|-----|------|
| AGMKPNRSB-NEG-1 | 1 | C |
| AGMKPNRSB-NEG-1 | 2 | A |
| ... | | |
| AGMKPNRSB-NEG-1 | 58 | A |
| AGMKPNRSB-NEG-1 | 59 | C |
| AGMKPNRSB-NEG-1 | 60 | A |
| AGMORS12A-NEG-181 | 1 | A |
| AGMORS12A-NEG-181 | 2 | G |
| ... | | |
| AGMORS12A-NEG-181 | 59 | G |
| AGMORS12A-NEG-181 | 60 | G |
| AGMORS9A-NEG-481 | 1 | T |
| AGMORS9A-NEG-481 | 2 | G |
| AGMORS9A-NEG-481 | 3 | G |
| ... | | |



Prepare a deployment model

101

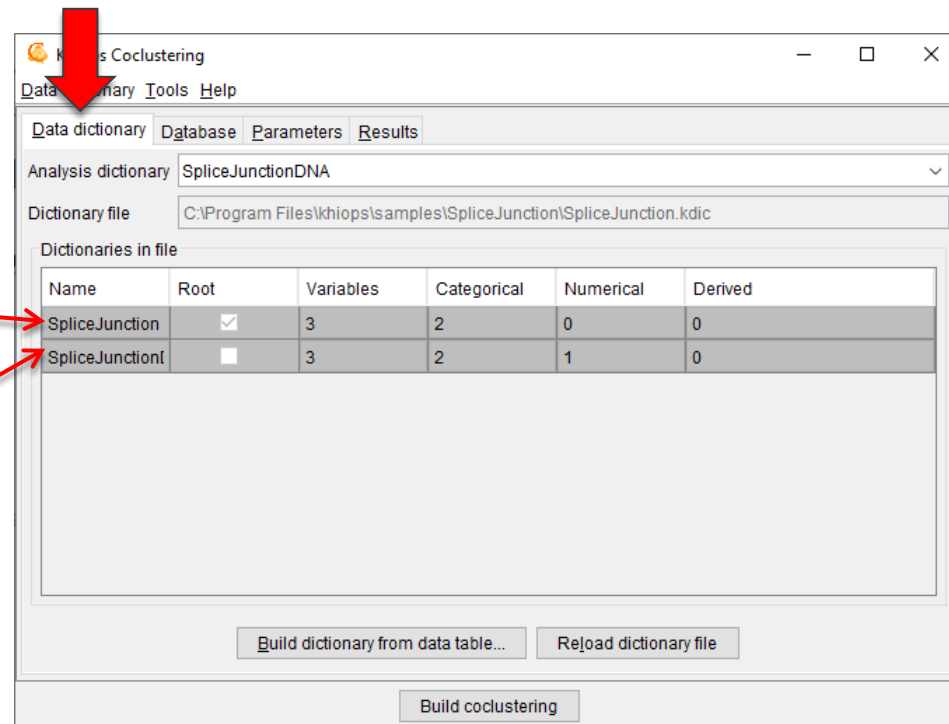
- **Step 1 : Open an existing dictionary**
(ex: sample SpliceJunction.kdic)

Root entity

for deployment on new
instances

Secondary entity

previously analyzed using
triclustering

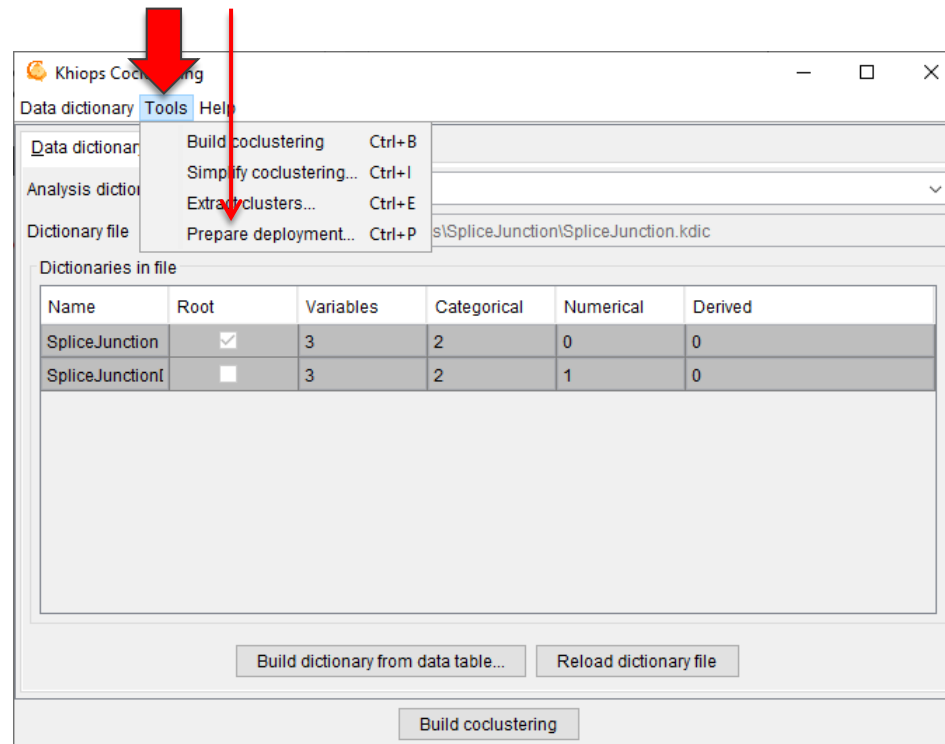




Prepare a deployment model

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- **Step 2 :** *Start « Tools – Prepare deployment »*

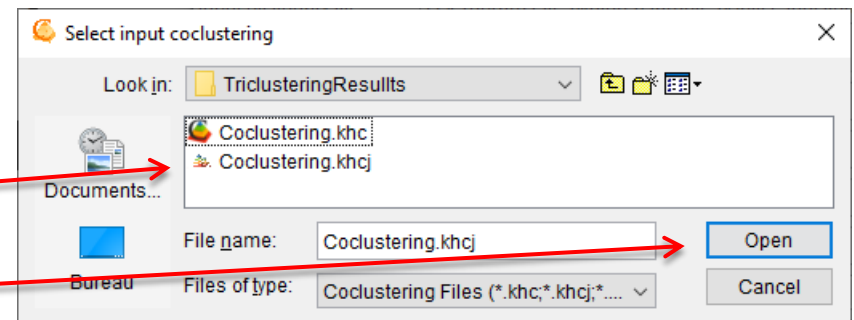
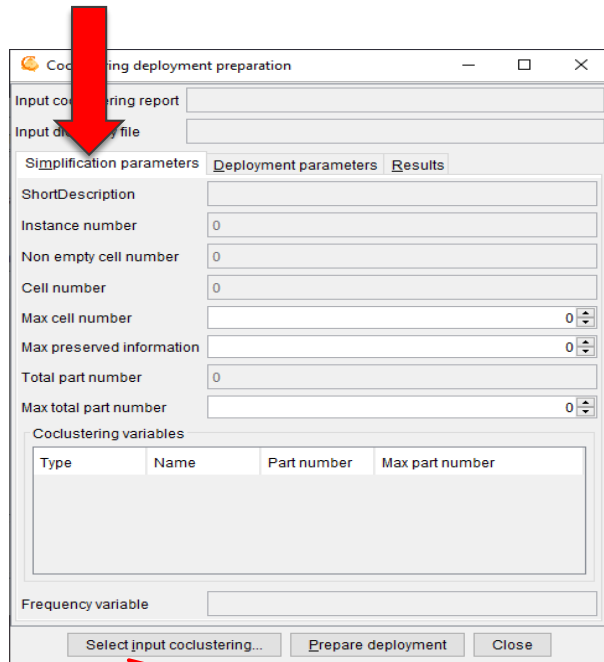




Prepare a deployment model

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- **Step 3 : Select input coclustering file**
 - (ex: previously trained triclustering model)



1. click on button
2. select a triclustering model file
3. open



Prepare a deployment model

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- **Step 4** : The triclustering model is summarized in the first pane
 - if necessary, specify simplification parameters

Simplification
parameters

Coclustering deployment preparation

Input coclustering report: C:\Program Files\khiops\samples\SpliceJunction\Triclusterir

Input dictionary file: C:\Program Files\khiops\samples\SpliceJunction\SpliceJunc

Simplification parameters | Deployment parameters | Results

ShortDescription:

Instance number: 190680

Non empty cell number: 453

Cell number: 468

Max cell number: 0

Max preserved information: 0

Total part number: 26

Max total part number: 0

Coclustering variables

| Type | Name | Part number | Max part number |
|-------------|----------|-------------|-----------------|
| Categorical | SampleId | 9 | 0 |
| Numerical | Pos | 13 | 0 |
| Categorical | Char | 4 | 0 |

Frequency variable:

Select input coclustering... Prepare deployment Close



Prepare a deployment model

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- Step 5 : Specify deployment parameters**

Specification of input dictionary to enrich

```
Root Dictionary SpliceJunction(SampleId)
{
  Categorical    SampleId ;
  Categorical    Class;
  Table(SpliceJunctionDNA) DNA;
};

Dictionary SpliceJunctionDNA(SampleId)
{
  Categorical    SampleId ;
  Numerical      Pos;
  Categorical    Char;
};
```

Coclustering deployment preparation

Input coclustering report: C:\Program Files\khio...mples\SpliceJunction\TricoclusteringResults\Coclustering.khc

Input dictionary file: C:\Program Files\khio...mples\SpliceJunction\SpliceJunction.kdic

Input dictionary: SpliceJunction

Input table variable: DNA

Coclustering deployed variable: SampleId

Build predicted cluster variable: ☒

Build inter-cluster distance variables: ☐

Build frequency recoding variables: ☐

Output variables prefix: P_

Select input coclustering... Prepare deployment Close

Specification of deployment variables to build

One variable to assign closest cluster

. closest cluster of *SampleId*

Several variables for distance to each cluster

. distance to each cluster of *SampleId*

Several variables for secondary record number per interval/group of the other dimensions of the triclustering

. frequency per interval of *Pos*

. frequency per group of *Char*



Prepare a deployment model

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- **Step 6 : Specify result parameters**

Result files directory

Deployment dictionary file
(to deploy cluster information
on new data)

Coclustering deployment preparation

Input coclustering report: C:\Program Files\khiops\samples\SpliceJunction\TricoclusteringResults\Coclustering.khc

Input dictionary file: C:\Program Files\khiops\samples\SpliceJunction\SpliceJunction.kdic

Simplification parameters | Deployment parameters | **Results**

Result files directory: Deployment

Result files prefix:

Coclustering dictionary file: Coclustering.kdic

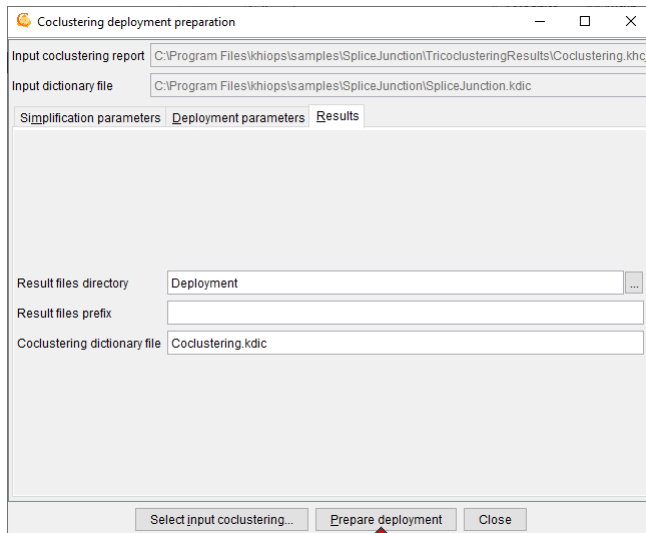
Select input coclustering... Prepare deployment Close



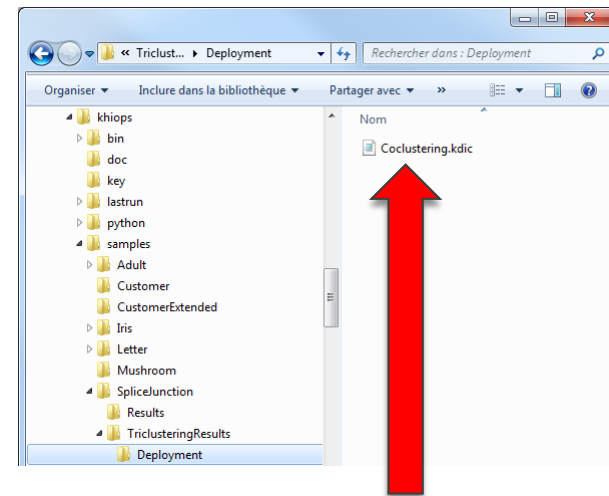
Prepare a deployment model

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- **Step 7 : Build the deployment dictionary**



1 – Build the deployment dictionary



2 – The deployment dictionary is ready for use with Khiops « *Transfer database* » functionality

Khops multi-table

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- Khops can deal with multi-table databases
 - star schema: one root entity and several 0-1 or 0-n secondary entities
 - snowflake schemas and beyond

• Impact on Khops Coclustering

- Deployment of coclustering models
 - Given a text*word coclustering model, assign new texts (with their words) to their closest cluster
 - Given a cookie*page coclustering model, assign new cookies (with their pages) to their closest cluster
 - Given a curve*X*Y triclustering model, assign new curves (with their X*Y points) to their closest cluster

• In this tutorial

- Train a triclustering model on the SpliceJunctionDNA data table
 - Clusters of sequence samples
 - Intervals of positions in the sequences
 - Clusters of DNA chars
- Prepare a deployment model
 - Build a deployment dictionary
- **Deploy the model on the multi-table SpliceJunction database**
 - Assign new DNA sequences to trained clusters of sequences



Deploy the model

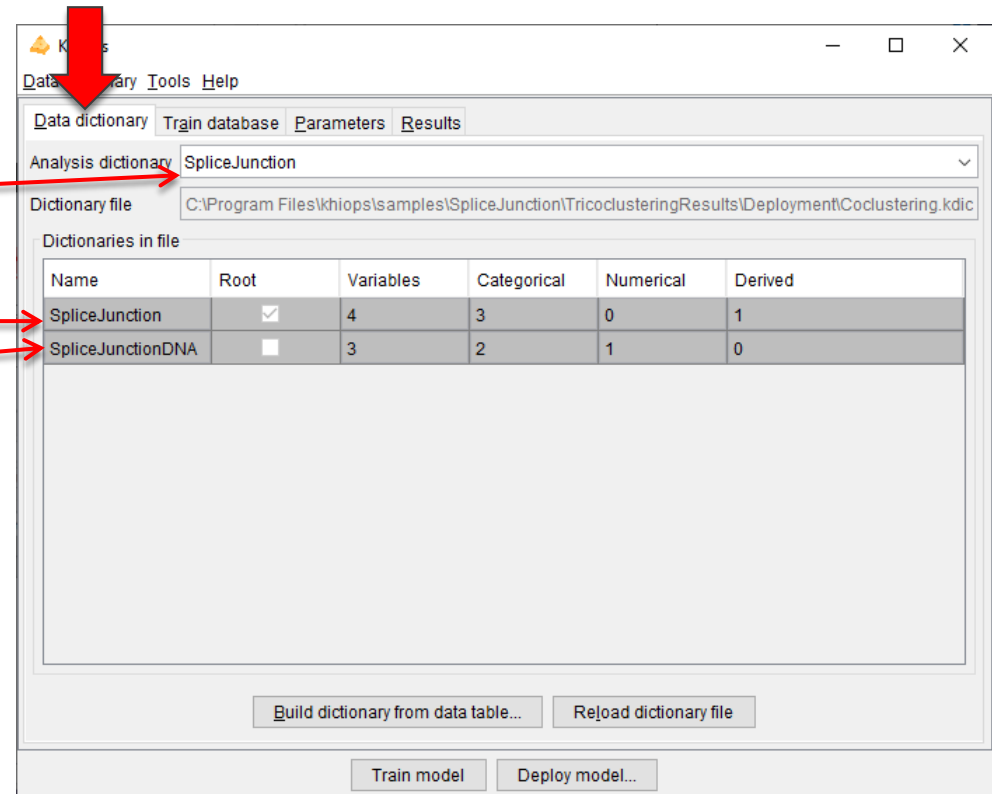
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- **Step 1** : Open the deployment dictionary file with Khiops
(ex: Samples\SpliceJunction\TriclusteringResults\Deployment\Coclustering.kdic)

Deployment dictionary

Root entity

Secondary entity





Deploy the model

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- **Step 2 : If necessary, select deployment variables**

(use « Inspect current dictionary » by right-click on dictionary SpliceJunction)

Initial variables

Used by default

Model variables

(technical variables)

Deployment variables

Cluster index (unused by default)

Cluster label (used by default)

The screenshot shows the 'Dictionary' window in Orange software. The 'Name' field is 'SpliceJunction', 'Root' is checked, and 'Key' is 'SampleId'. The 'Variables' section contains a table with columns: Used, Type, Name, Derived, Meta-data, and Label. The table lists 11 variables. The first three variables (SampleId, Class, DNA) are marked as 'Used' and are 'Initial variables'. The next six variables (P_Coclustering, P_SampleIdLabels, P_PosSet, P_CharSet, P_DeployedCoclusteringAtSampleId, P_SampleIdIndex) are not marked as 'Used' and are 'Model variables'. The last two variables (P_SampleIdPredictedLabel) are marked as 'Used' and are 'Deployment variables'. The 'Cluster index' (P_SampleIdIndex) is unused by default, and the 'Cluster label' (P_SampleIdPredictedLabel) is used by default.

| Used | Type | Name | Derived | Meta-data | Label |
|-------------------------------------|-------------------------------|----------------------------------|-------------------------------------|-----------|---|
| <input checked="" type="checkbox"/> | Categorical | SampleId | <input type="checkbox"/> | | |
| <input checked="" type="checkbox"/> | Categorical | Class | <input type="checkbox"/> | | |
| <input checked="" type="checkbox"/> | Table(SpliceJunctionDNA) | DNA | <input type="checkbox"/> | | |
| <input type="checkbox"/> | Structure(DataGrid) | P_Coclustering | <input checked="" type="checkbox"/> | | DataGrid(SampleId, Pos, Char) |
| <input type="checkbox"/> | Structure(VectorC) | P_SampleIdLabels | <input checked="" type="checkbox"/> | | Cluster labels for variable SampleId |
| <input type="checkbox"/> | Structure(Vector) | P_PosSet | <input checked="" type="checkbox"/> | | Value distribution for variable Pos |
| <input type="checkbox"/> | Structure(VectorC) | P_CharSet | <input checked="" type="checkbox"/> | | Value distribution for variable Char |
| <input type="checkbox"/> | Structure(DataGridDeployment) | P_DeployedCoclusteringAtSampleId | <input checked="" type="checkbox"/> | | Deployed coclustering for variable SampleId |
| <input type="checkbox"/> | Numerical | P_SampleIdIndex | <input checked="" type="checkbox"/> | | Predicted cluster index for variable SampleId |
| <input checked="" type="checkbox"/> | Categorical | P_SampleIdPredictedLabel | <input checked="" type="checkbox"/> | | Predicted label for variable SampleId |

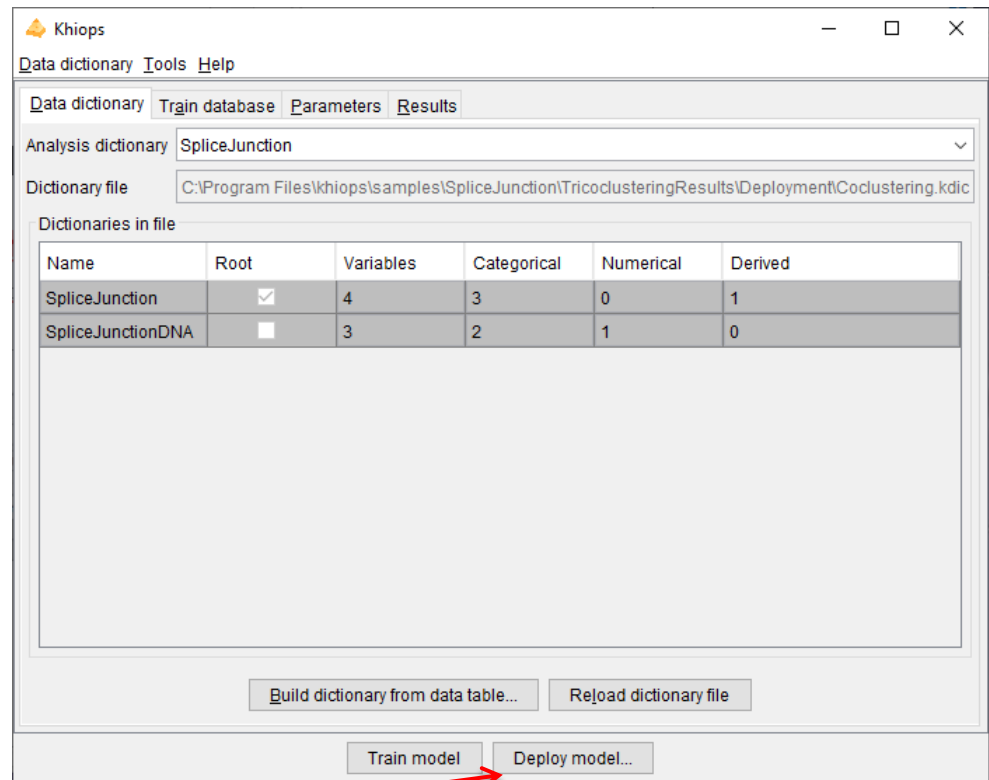
Buttons: Select all, Unselect all, Close



Deploy the model

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- **Step 3 :** Open the « *Deploy model* » dialog box



click on button



Deploy the model

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- **Step 4 : Specify the file transfer parameters**

Deployment dictionary: SpliceJunction

Input database

Database files

| Data root | Path | Dictionary | Data table file |
|----------------|------|-------------------|--|
| SpliceJunction | | SpliceJunction | C:\Program Files\khiops\samples\SpliceJunction\SpliceJunction.txt |
| SpliceJunction | DNA | SpliceJunctionDNA | C:\Program Files\khiops\samples\SpliceJunction\SpliceJunctionDNA.txt |

Detect file format

Header line used ☒

Field separator

Sample percentage 100

Sampling mode Include sample

Selection variable

Selection value

Output database

Database files

| Data root | Path | Dictionary | Data table file |
|----------------|------|-------------------|--|
| SpliceJunction | | SpliceJunction | C:\Program Files\khiops\samples\SpliceJunctionID_SpliceJunction.txt |
| SpliceJunction | DNA | SpliceJunctionDNA | C:\Program Files\khiops\samples\SpliceJunctionID_SpliceJunctionDNA.txt |

Header line used ☒

Field separator

Output format tabular

Deploy model Build deployed dictionary... Close

1 Specify the deployment dictionary

2 Specify the input data table files

- splice junction samples with their DNA sequence
- all files are mandatory

3 Specify the output data table files

- secondary files are optional

4 Deploy

- The output files are enriched with new fields derived from the triclustering analysis

End of tutorial: summary

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- **Khiops**
 - Optimal data preparation based on discretization and value grouping
 - Scoring models for classification and regression
 - Correlation analysis between pairs of variables



- **Khiops Visualization**
 - Analysis of Khiops results using an interactive visualization tool



- **Khiops Coclustering**
 - Correlation analysis of two or more variables using a hierarchical coclustering model



- **Khiops Covisualization**
 - Exploratory analysis of Khiops Coclustering results using an interactive visualization tool



- **Multi-table functionalities**
 - Multi-table database
 - Automatic feature construction
 - Multi-table functionalities in Khiops and Khiops Coclustering