University of Minho
School of Engineering

Machine Learning and Decision-Making

ADI @ LEI/3º, MiEI/4º - 2º Semestre
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Part IV – March 2022

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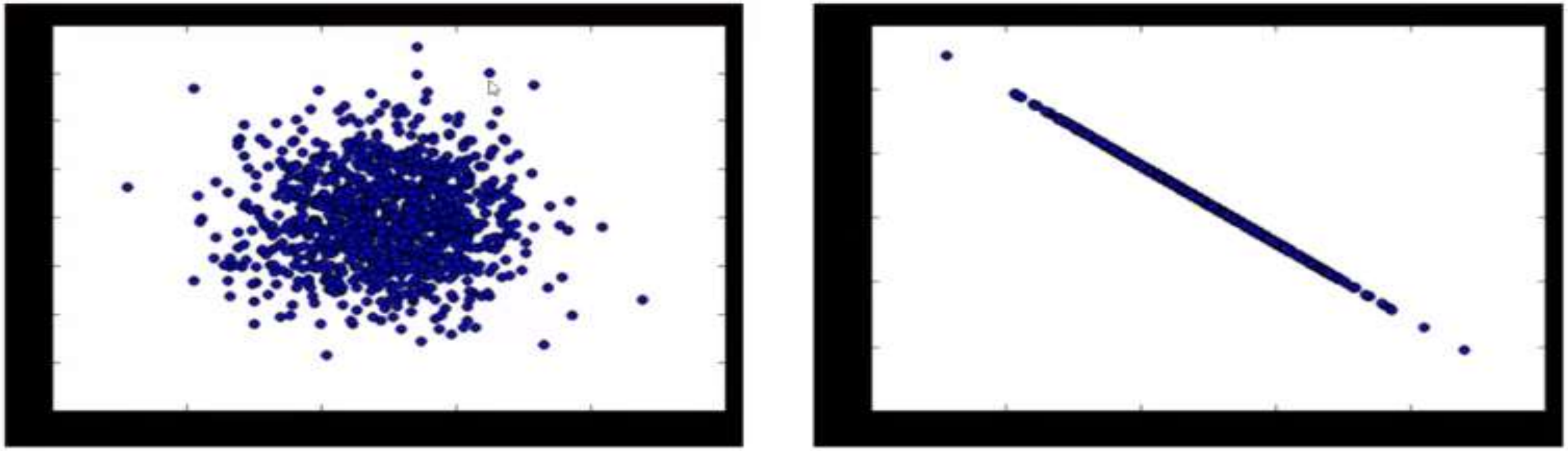
- Data Exploration
- Data Preparation
  - Join, Concatenation, Sorter, Filter and Aggregations
  - Feature Scaling, Outlier Detection, Feature Selection, Missing Values Treatment, Nominal Value Discretization, Binning and Feature Engineering
- Hands On

Covariance

Measures how two variables vary in tandem from their means, i.e., how 2 attributes depend on each other (left plot – low covariance / right plot – high covariance).



Covariance

Measuring covariance:

- Think of the datasets for the two variables as high-dimensional vectors
- Convert these to vectors of variances from the mean
- Take the dot product (cosine of the angle between them) of the two vectors
- Divide by the population size

Population Covariance Formula

$$Cov(x,y) = \frac{\Sigma(x_i-\bar{x})(y_i-\bar{y})}{N}$$

Sample Covariance

$$Cov(x,y) = \frac{\Sigma(x_i-\bar{x})(y_i-y)}{N-1}$$

Covariance & Correlation

Interpreting covariance is hard:

- Low covariance (close to 0) means there isn't much correlation between the two variables
- High covariance (far from 0 – can be negative for inverse relationships) means that there is a correlation

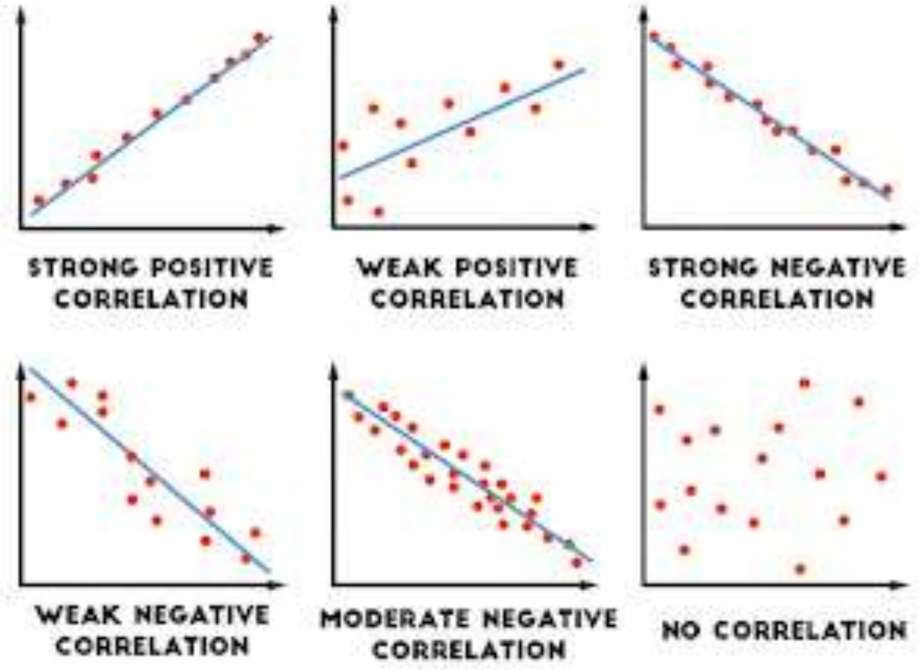
Interpreting correlation is easier:

- Normalization value of covariance divided by the standard deviations of both variables
    - Correlation of -1: perfect inverse correlation
    - Correlation of 0: no correlation
    - Correlation of 1: perfect correlation

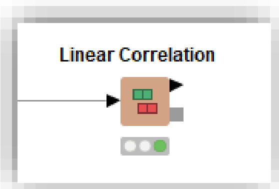
Covariance & Correlation

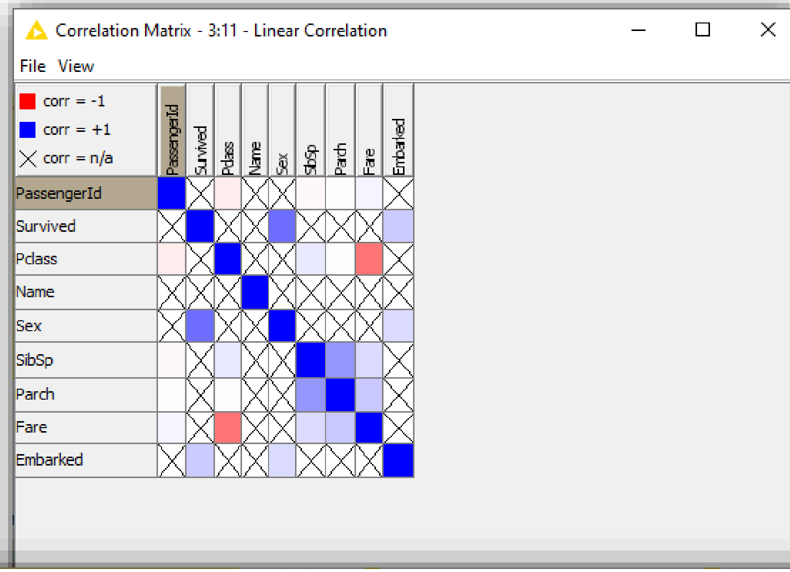
But… Correlation does not imply causation!!

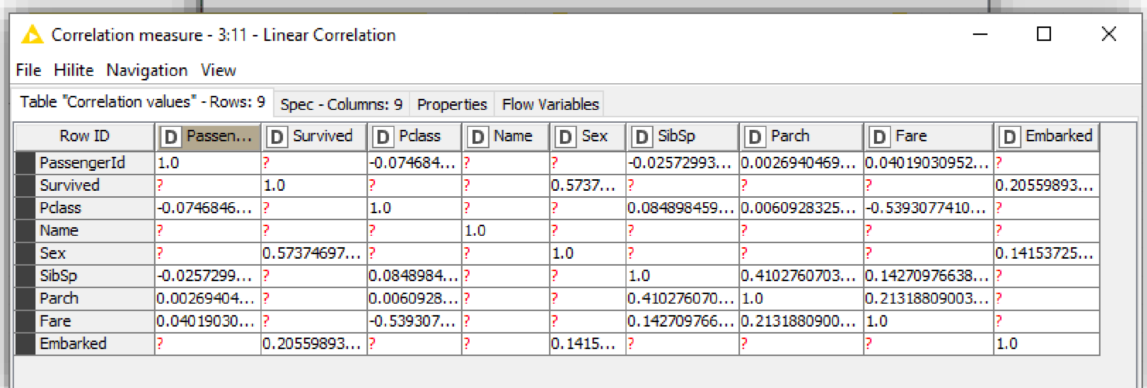
- Only a controlled, randomized experiment can give you insights on causation;
- Use correlation to decide what experiments to conduct.



Correlation Matrix






Correlation measure - 3:11 - Linear Correlation

File Hilite Navigation View

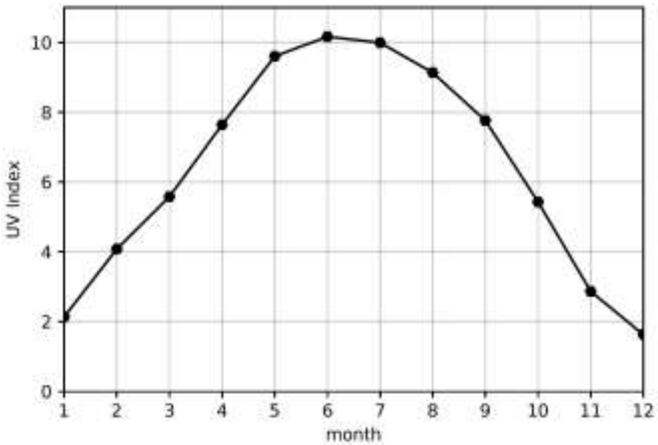
Table "Correlation values" - Rows: 9 | Spec - Columns: 9 | Properties | Flow Variables

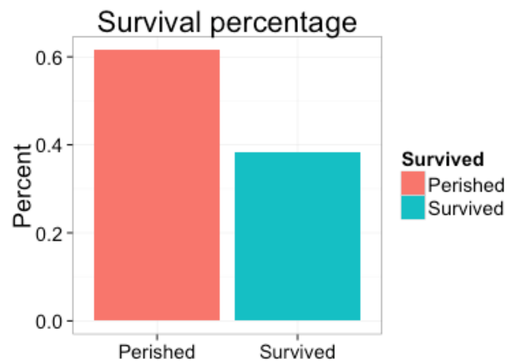
Row ID	Passen...	Survived	Pclass	Name	Sex	SibSp	Parch	Fare	Embarked
PassengerId	1.0	?	-0.074684...	?	?	-0.02572993...	0.0026940469...	0.04019030952...	?
Survived	?	1.0	?	?	0.5737...	?	?	?	0.20559893...
Pclass	-0.0746846...	?	1.0	?	?	0.084898459...	0.0060928325...	-0.5393077410...	?
Name	?	?	?	1.0	?	?	?	?	?
Sex	?	0.57374697...	?	?	1.0	?	?	?	0.14153725...
SibSp	-0.0257299...	?	0.0848984...	?	?	1.0	0.4102760703...	0.14270976638...	?
Parch	0.00269404...	?	0.0060928...	?	?	0.410276070...	1.0	0.21318809003...	?
Fare	0.04019030...	?	-0.539307...	?	?	0.142709766...	0.2131880900...	1.0	?
Embarked	?	0.20559893...	?	?	0.1415...	?	?	?	1.0

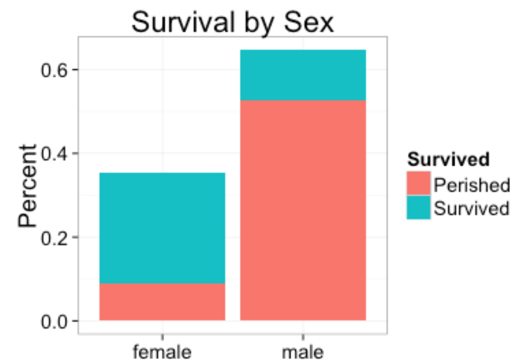
Correlation Matrix

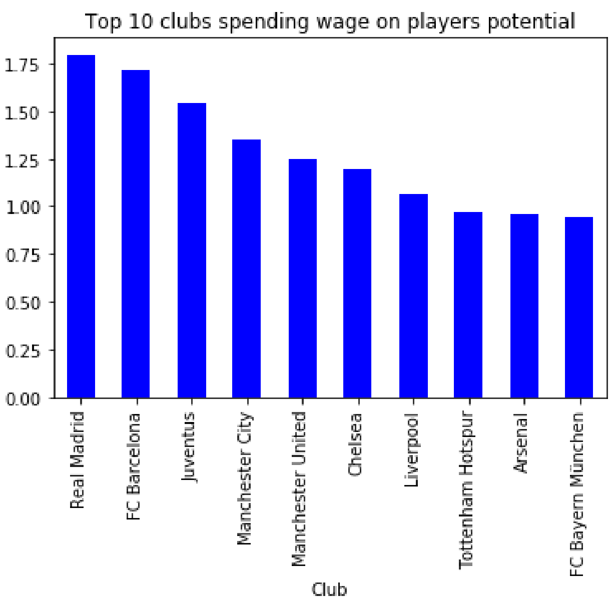
- Do we want to keep highly-correlated features?
- Both positive and negatively correlated ones?
- What about the correlation between the dependent and the independent features?
- …

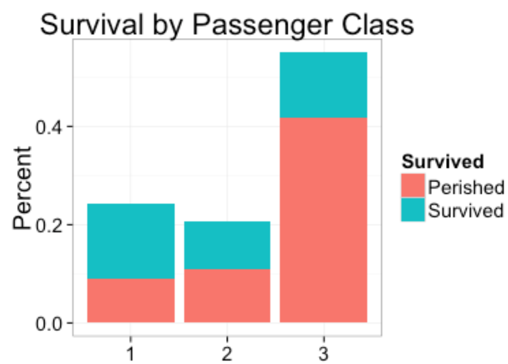
Data Viz. <- Often Neglected

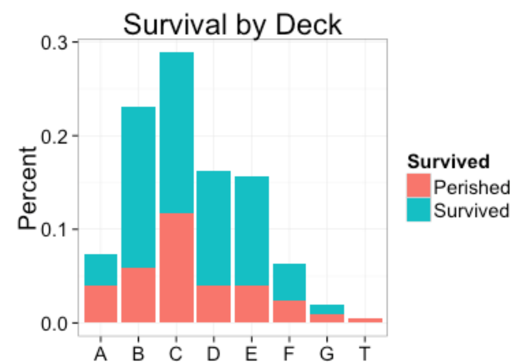




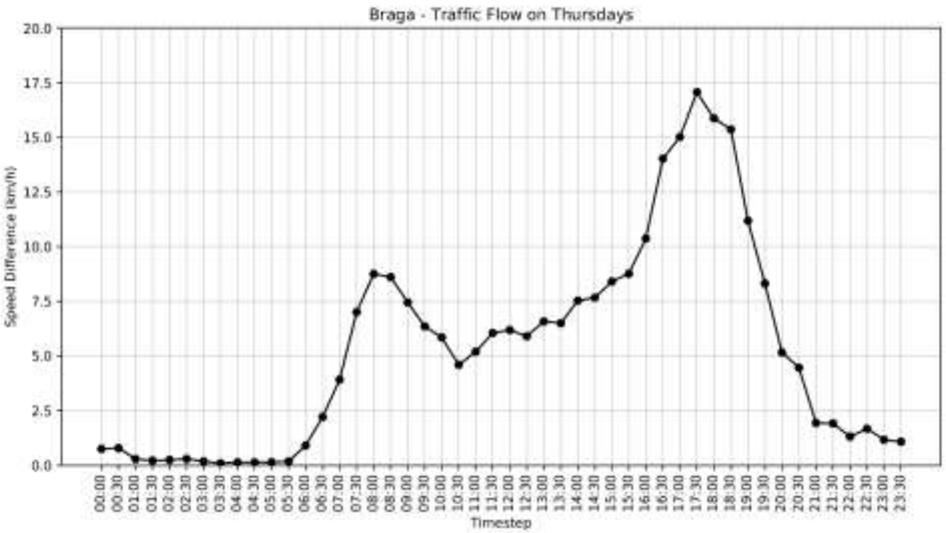


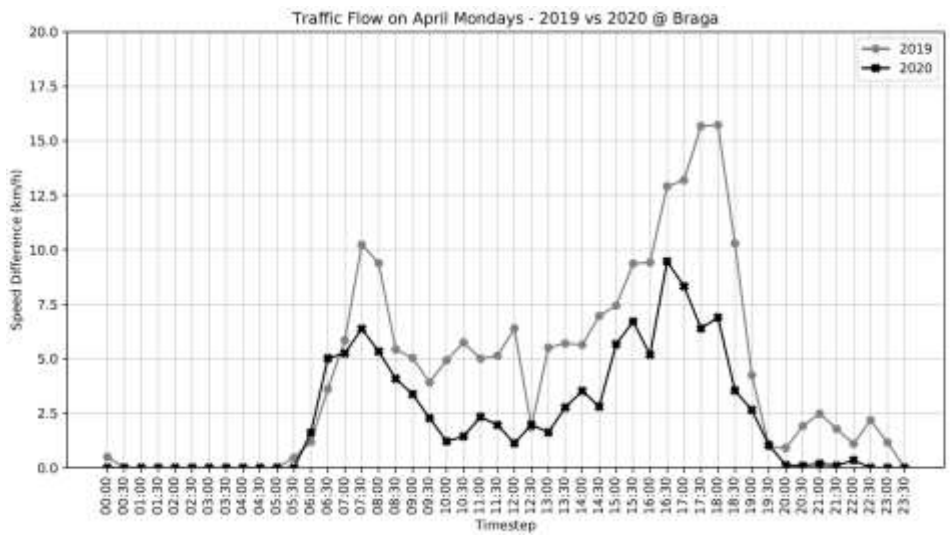






Data Viz. <- Often Neglected



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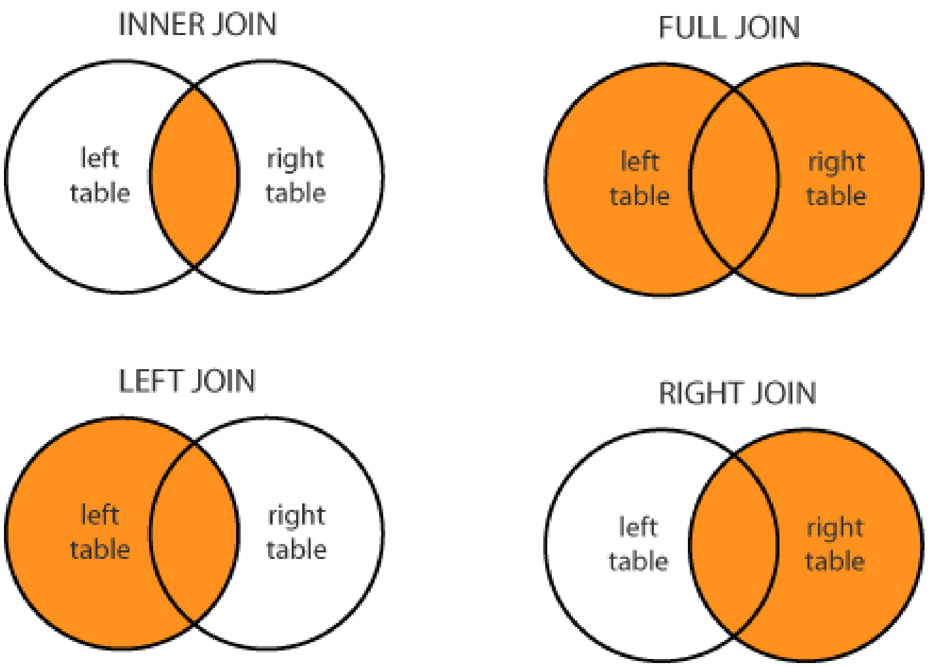
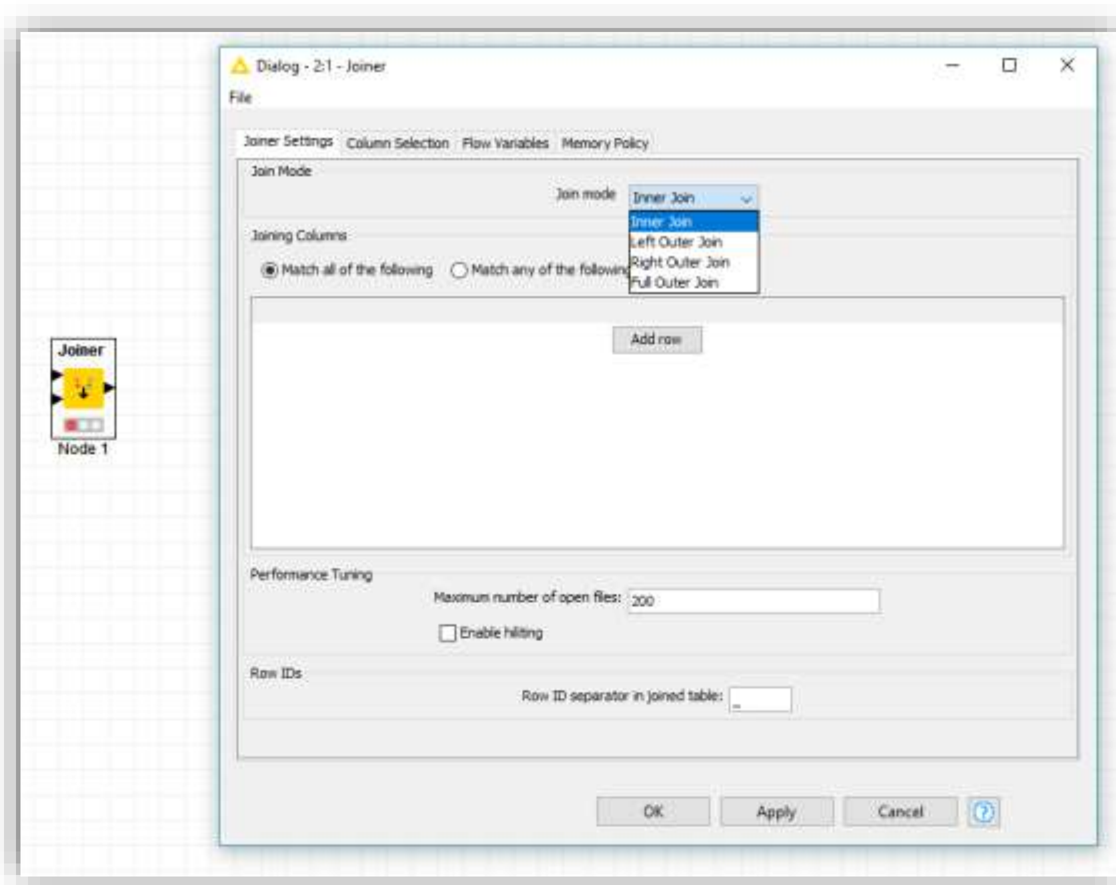
Join

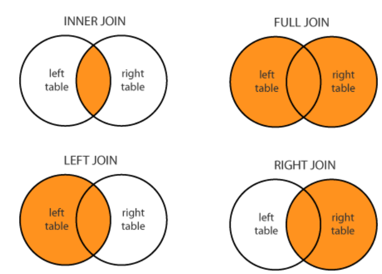
A Join is an operation that combines data from different tables



Join

Knime offers inner joins, right outer joins, left outer joins and full outer joins





Concatenation

Union of columns

Manually created table - 2:2 - Table Creator

File Hilite Navigation View

Table "default" - Rows: 2 | Spec - Columns: 3 | Properties | Flow Variables

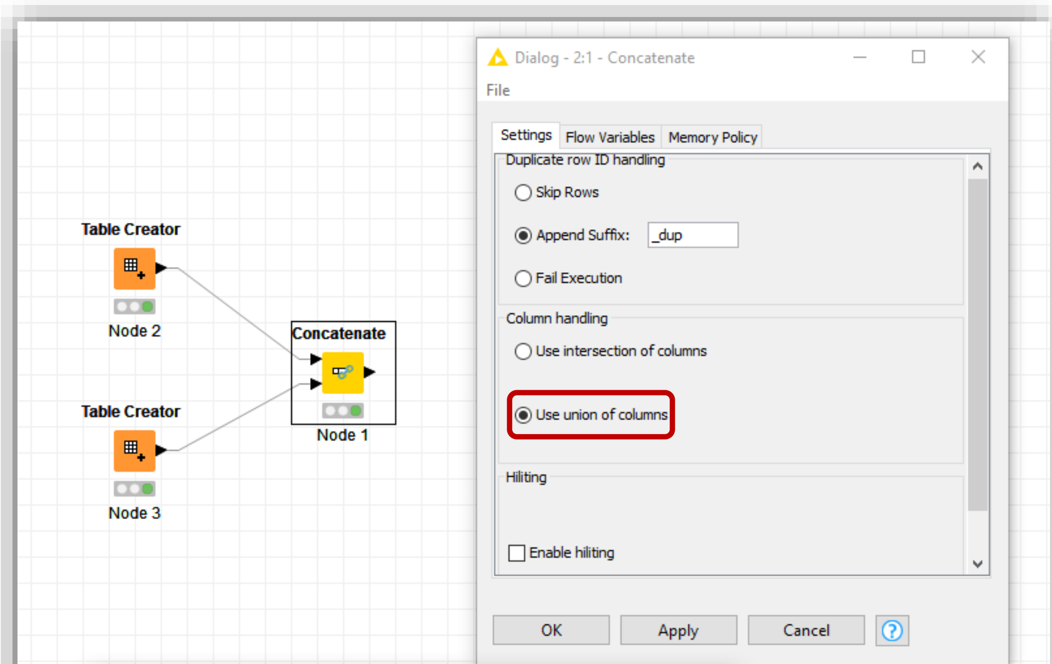
Row ID	S Id	S Name	S Age
Row0	1	Ze	19
Row1	2	Maria	22

Manually created table - 2:3 - Table Creator

File Hilite Navigation View

Table "default" - Rows: 3 | Spec - Columns: 4 | Properties | Flow Variables

Row ID	S Id	S Address	S Name	S Phone
Row0	3	Braga	Rui	543
Row1	4	Porto	Ana	345
Row2	5	Braga	João	324



Concatenated table - 2:1 - Concatenate

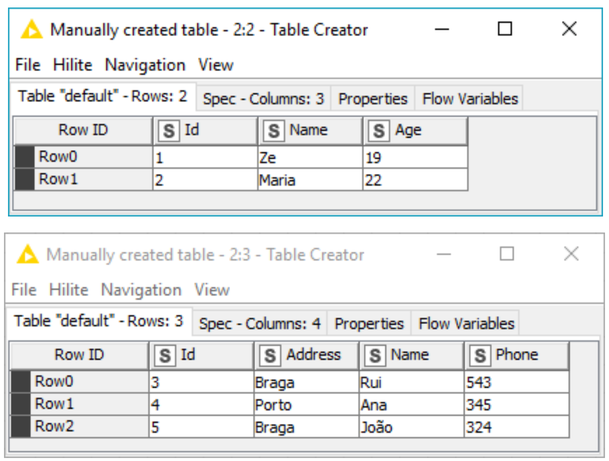
File Hilite Navigation View

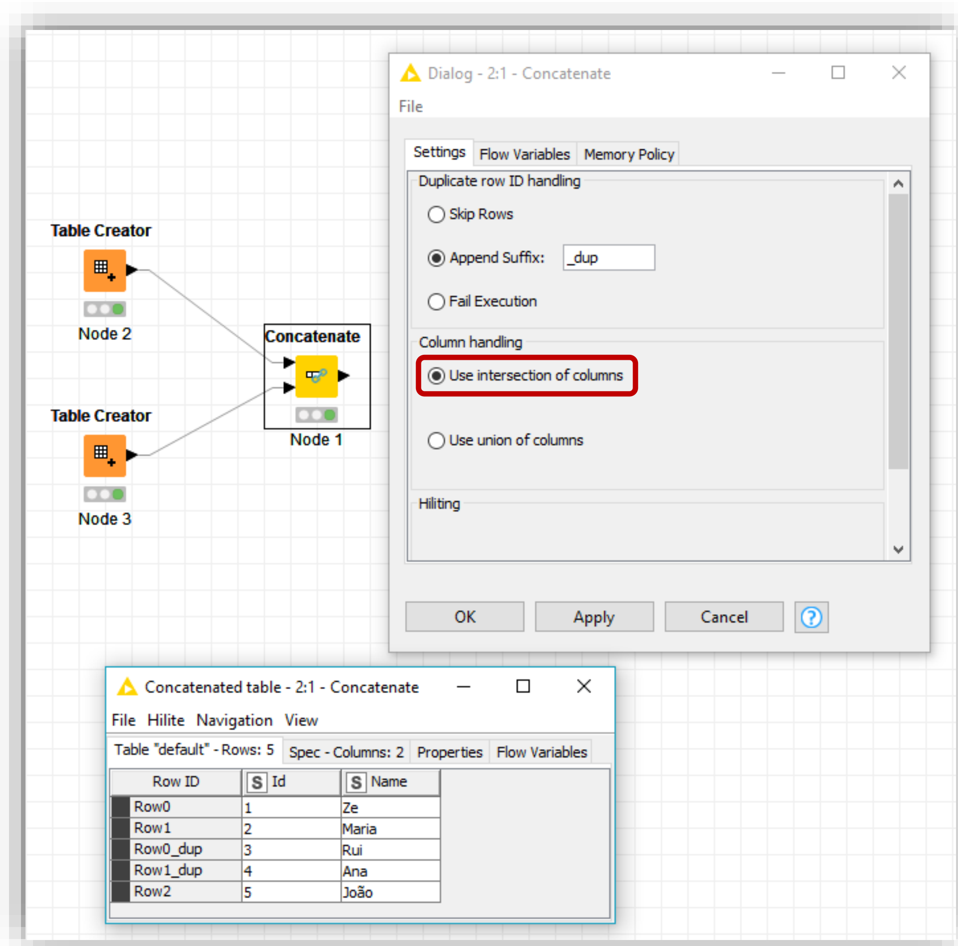
Table "default" - Rows: 5 | Spec - Columns: 5 | Properties | Flow Variables

Row ID	S Id	S Name	S Age	S Address	S Phone
Row0	1	Ze	19	?	?
Row1	2	Maria	22	?	?
Row0_dup	3	Rui	?	Braga	543
Row1_dup	4	Ana	?	Porto	345
Row2	5	João	?	Braga	324

Concatenation

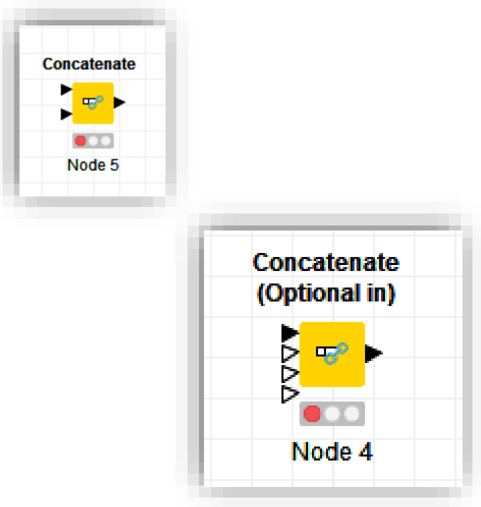
Intersection of columns



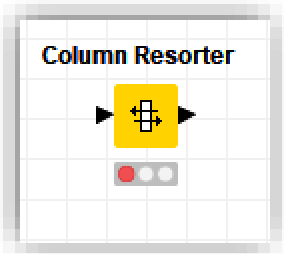


Concatenation

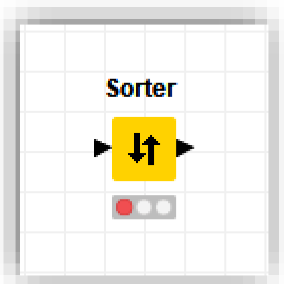
Concatenate (Optional in) works exactly like Concatenate but accepts up to 4 inputs!



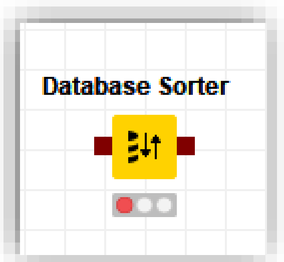
Sorter



Changes the order of the input columns, based on user defined settings

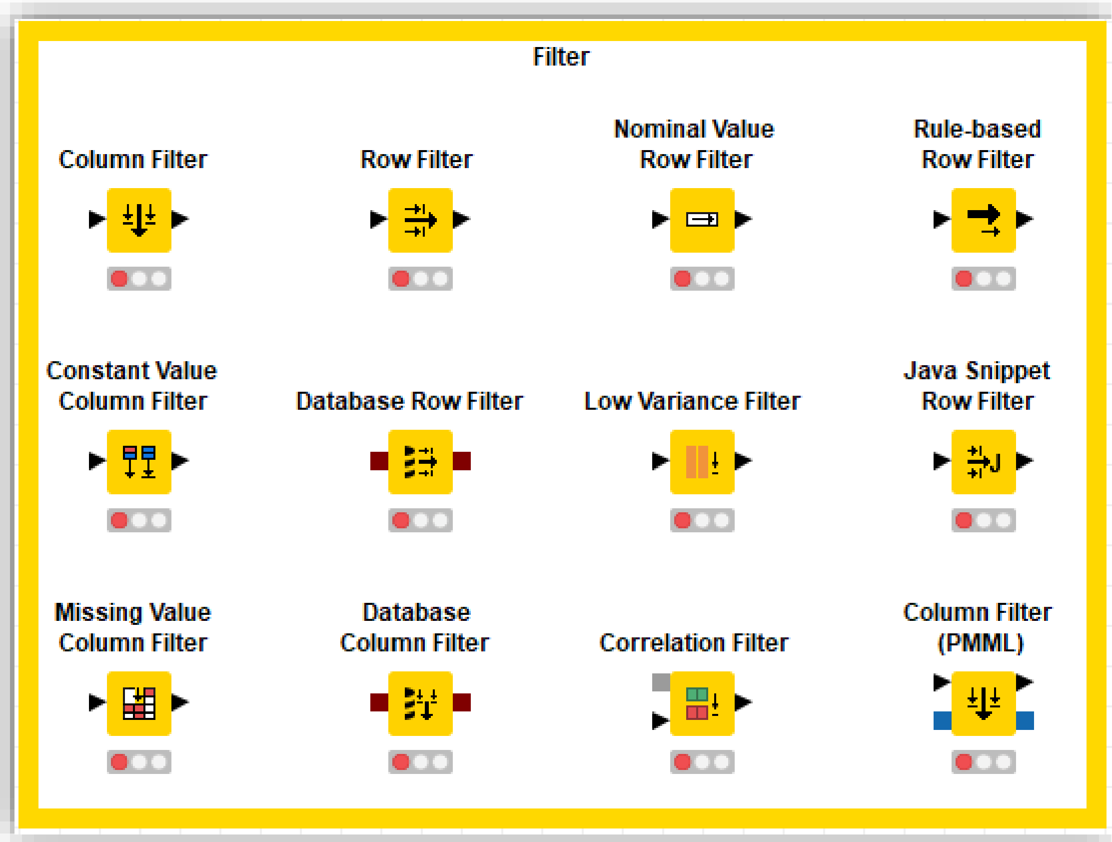


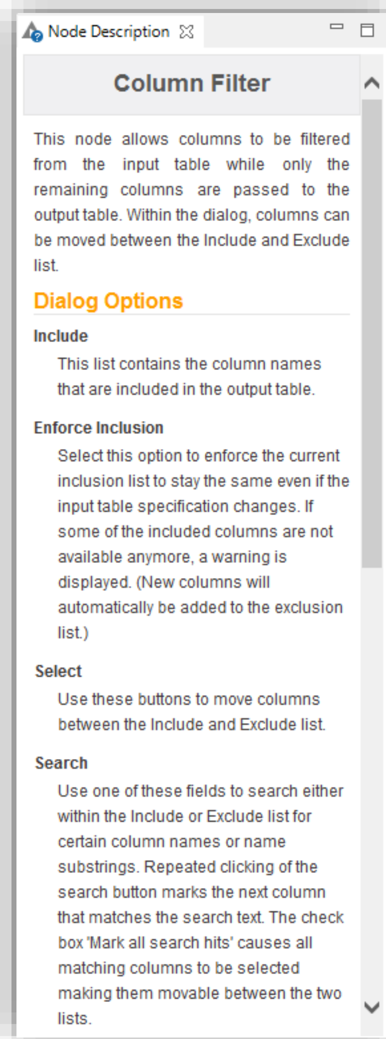
Sorts rows according to user-defined criteria



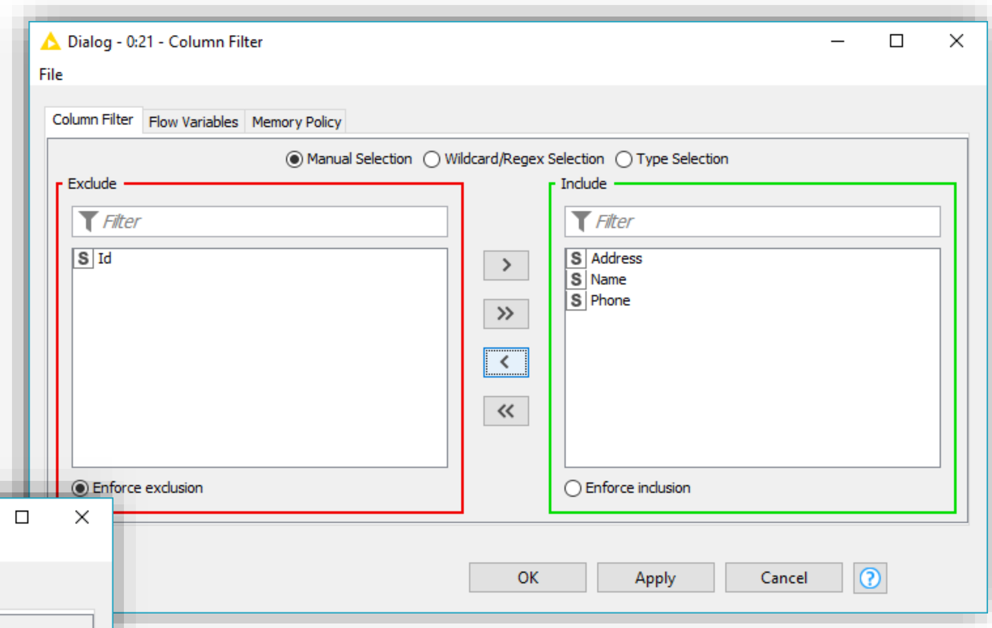
Allows rows to be sorted from the input database table (SQL ORDER BY clause)

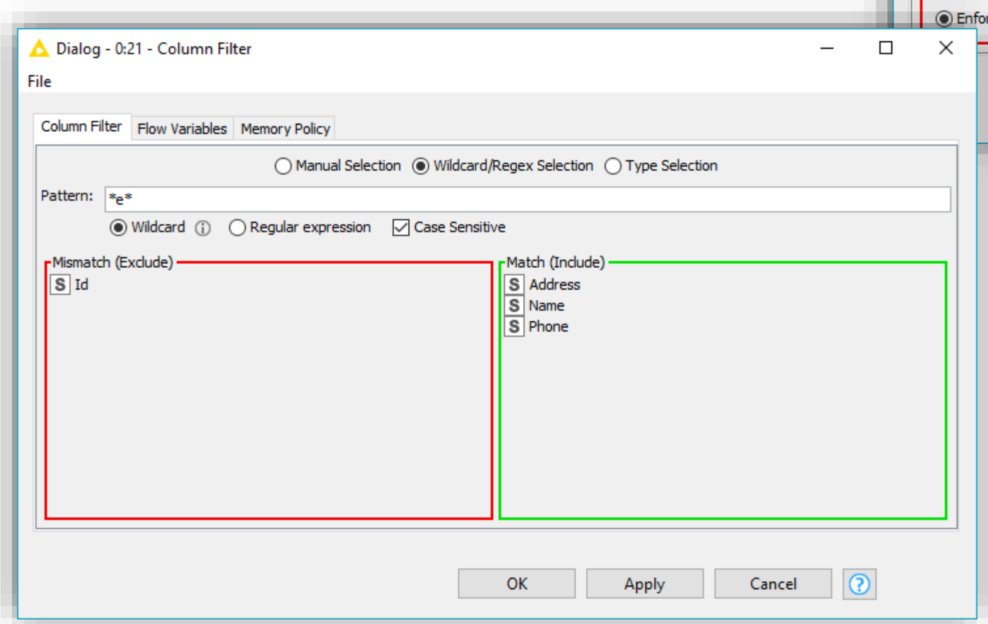
Filter


Filter
Column Filter
Row Filter
Nominal Value Row Filter
Rule-based Row Filter
Constant Value Column Filter
Database Row Filter
Low Variance Filter
Java Snippet Row Filter
Missing Value Column Filter
Database Column Filter
Correlation Filter
Column Filter (PMML)

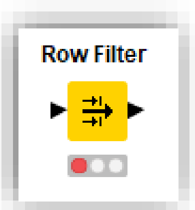

Node Description
Column Filter
This node allows columns to be filtered from the input table while only the remaining columns are passed to the output table. Within the dialog, columns can be moved between the Include and Exclude list.
Dialog Options
Include
This list contains the column names that are included in the output table.
Enforce Inclusion
Select this option to enforce the current inclusion list to stay the same even if the input table specification changes. If some of the included columns are not available anymore, a warning is displayed. (New columns will automatically be added to the exclusion list.)
Select
Use these buttons to move columns between the Include and Exclude list.
Search
Use one of these fields to search either within the Include or Exclude list for certain column names or name substrings. Repeated clicking of the search button marks the next column that matches the search text. The check box 'Mark all search hits' causes all matching columns to be selected making them movable between the two lists.

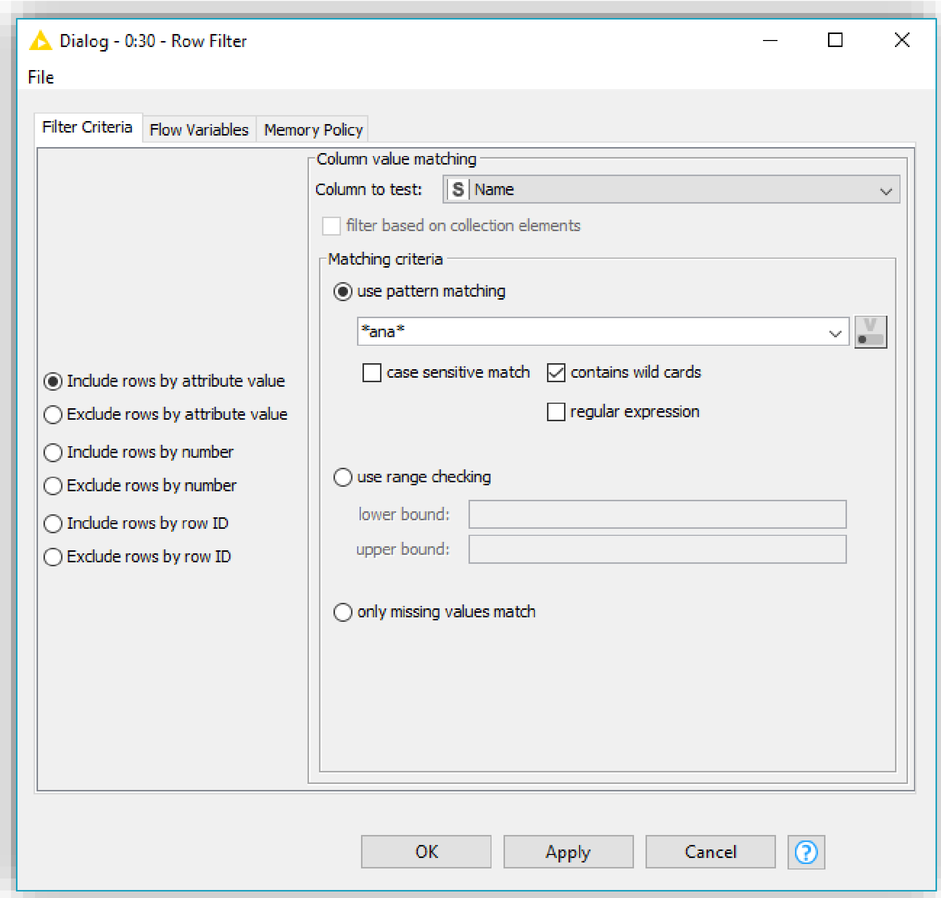
Column Filter



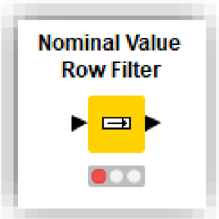


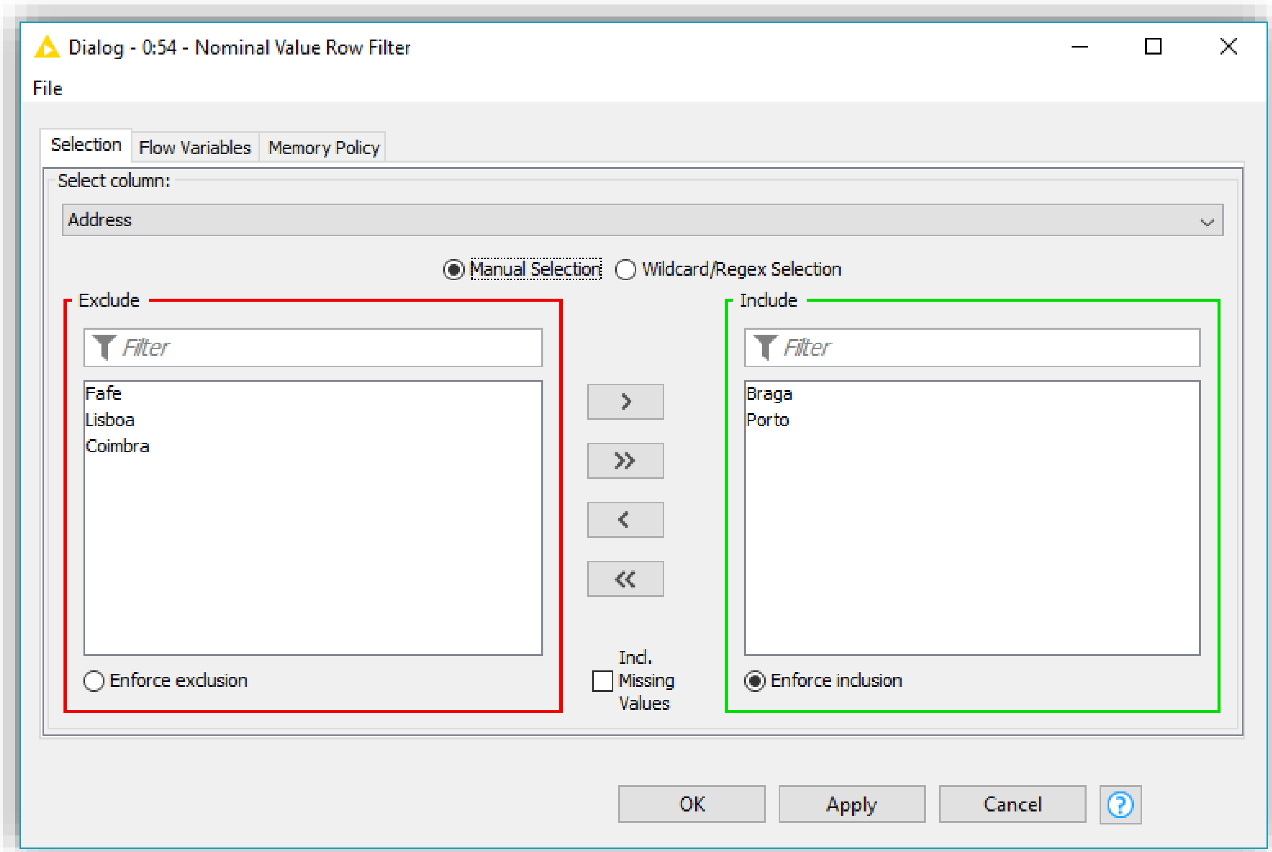
Row Filter


Row Filter

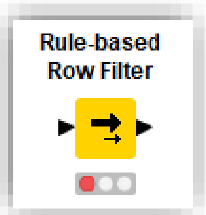

Dialog - 0:30 - Row Filter
File
Filter Criteria
Flow Variables
Memory Policy
Column value matching
Column to test:
S Name
filter based on collection elements
Matching criteria
use pattern matching
ana
case sensitive match
contains wild cards
regular expression
use range checking
lower bound:
upper bound:
only missing values match
Include rows by attribute value
Exclude rows by attribute value
Include rows by number
Exclude rows by number
Include rows by row ID
Exclude rows by row ID
OK
Apply
Cancel

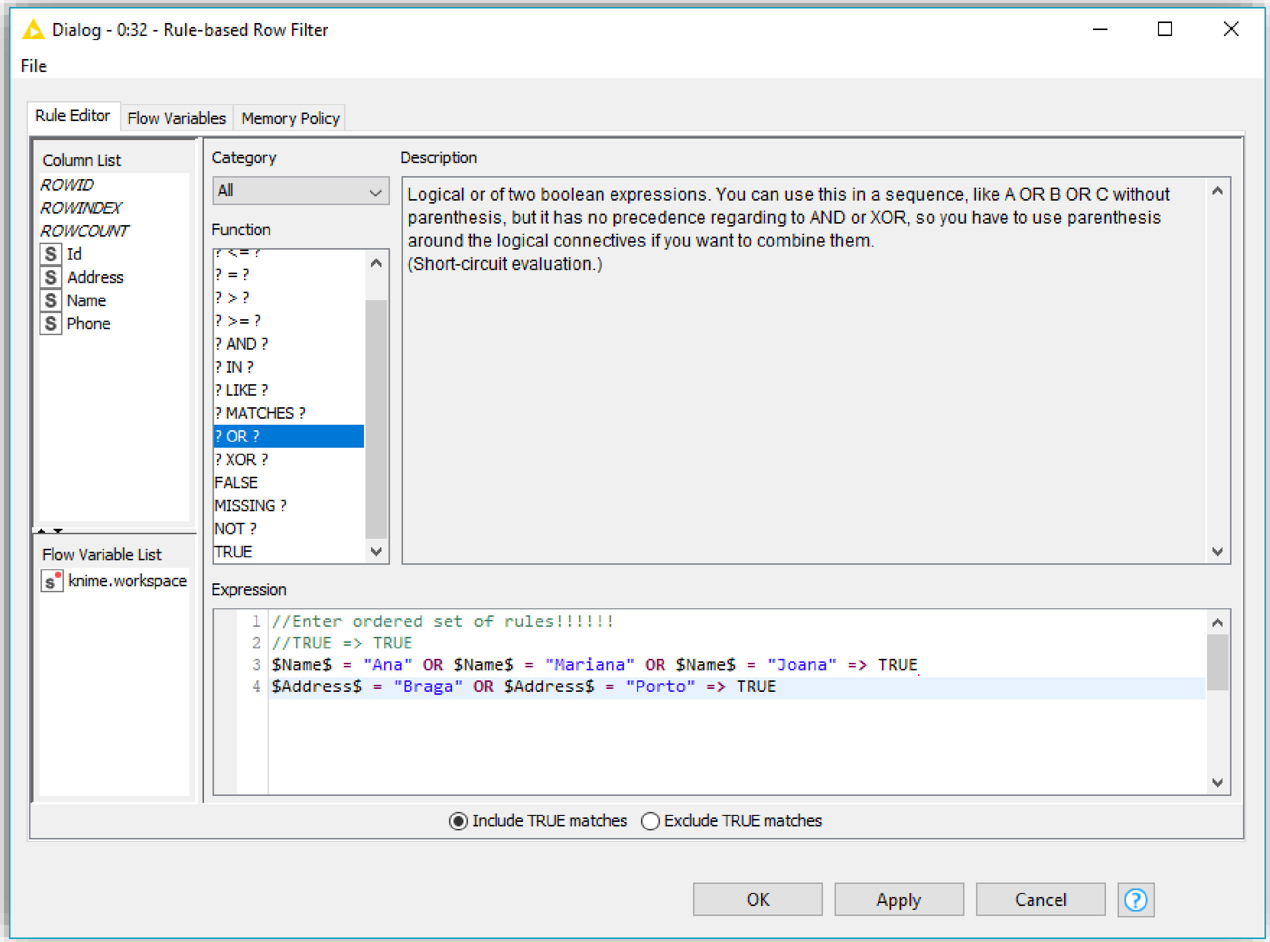
Nominal Value Row Filter



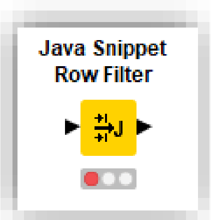


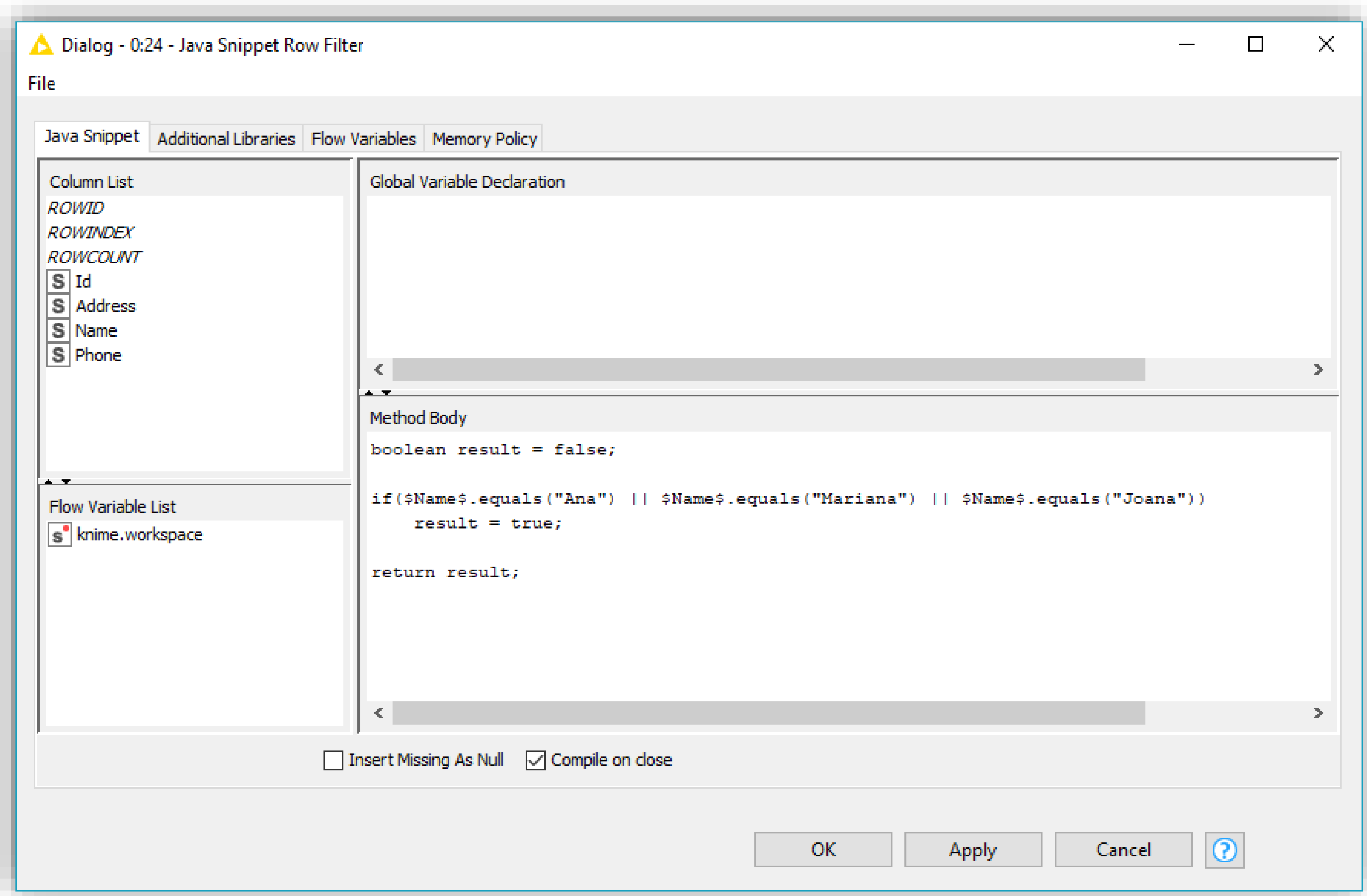
Rule-based Row Filter



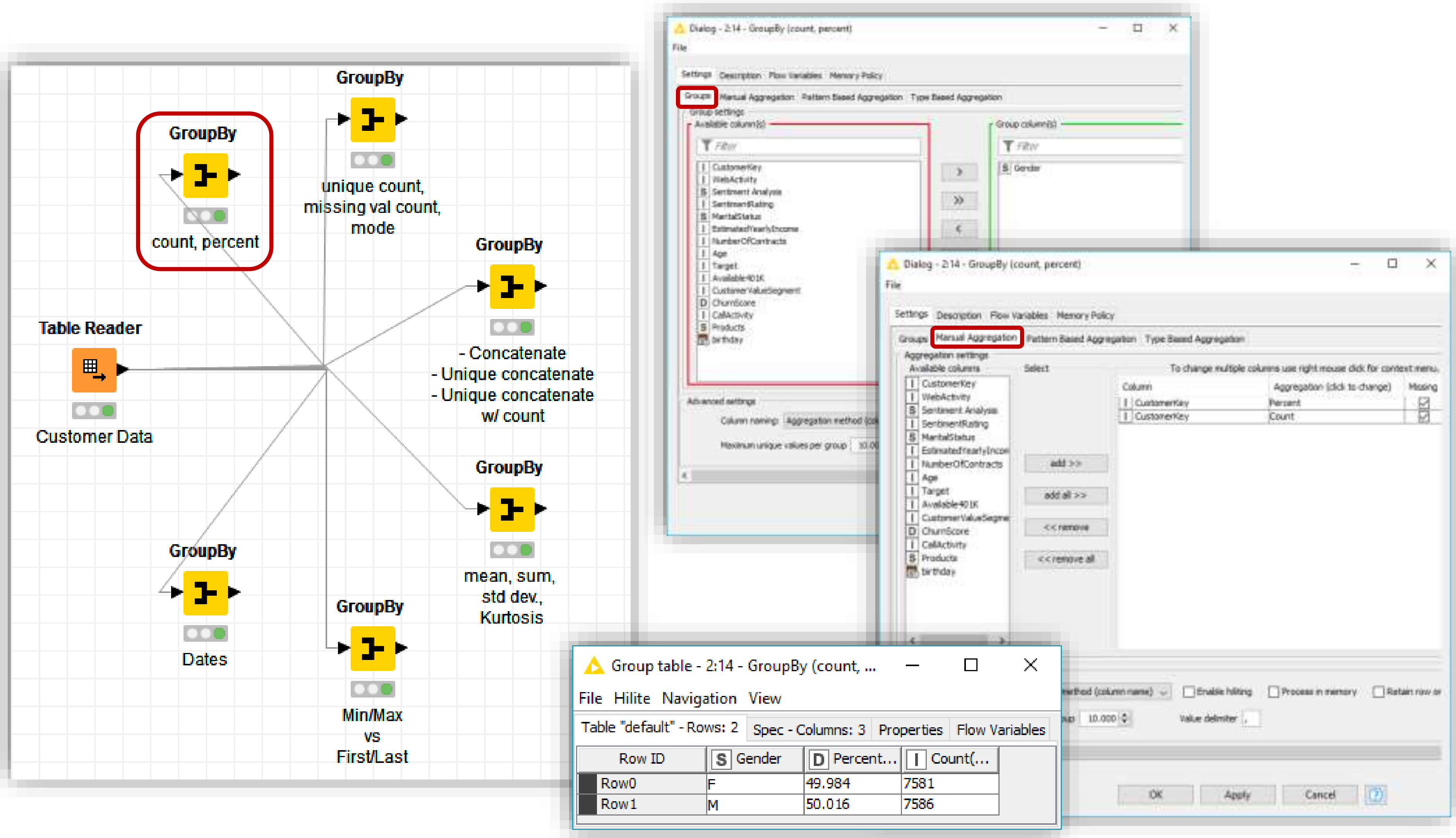


Java Snippet Row Filter

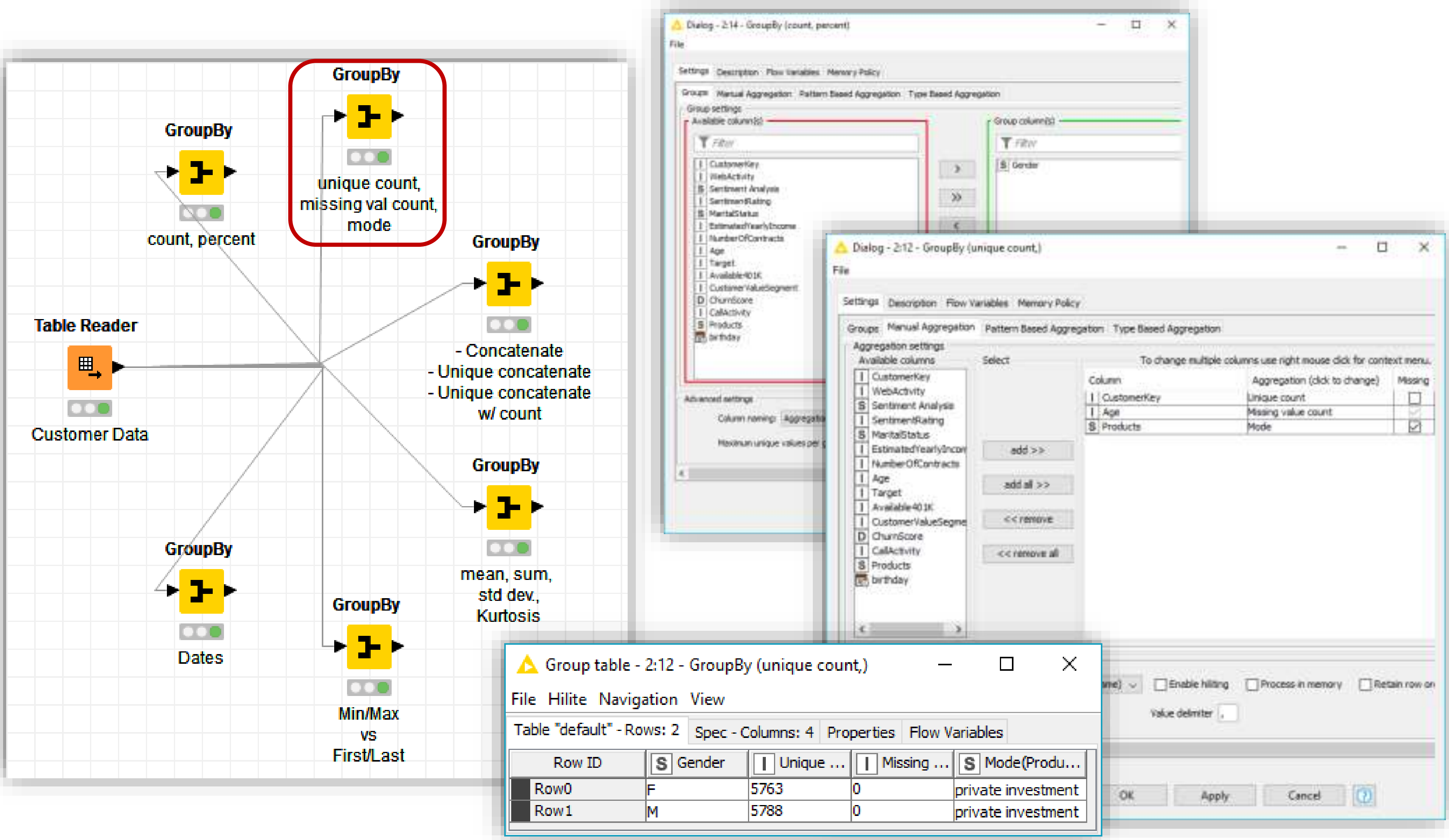




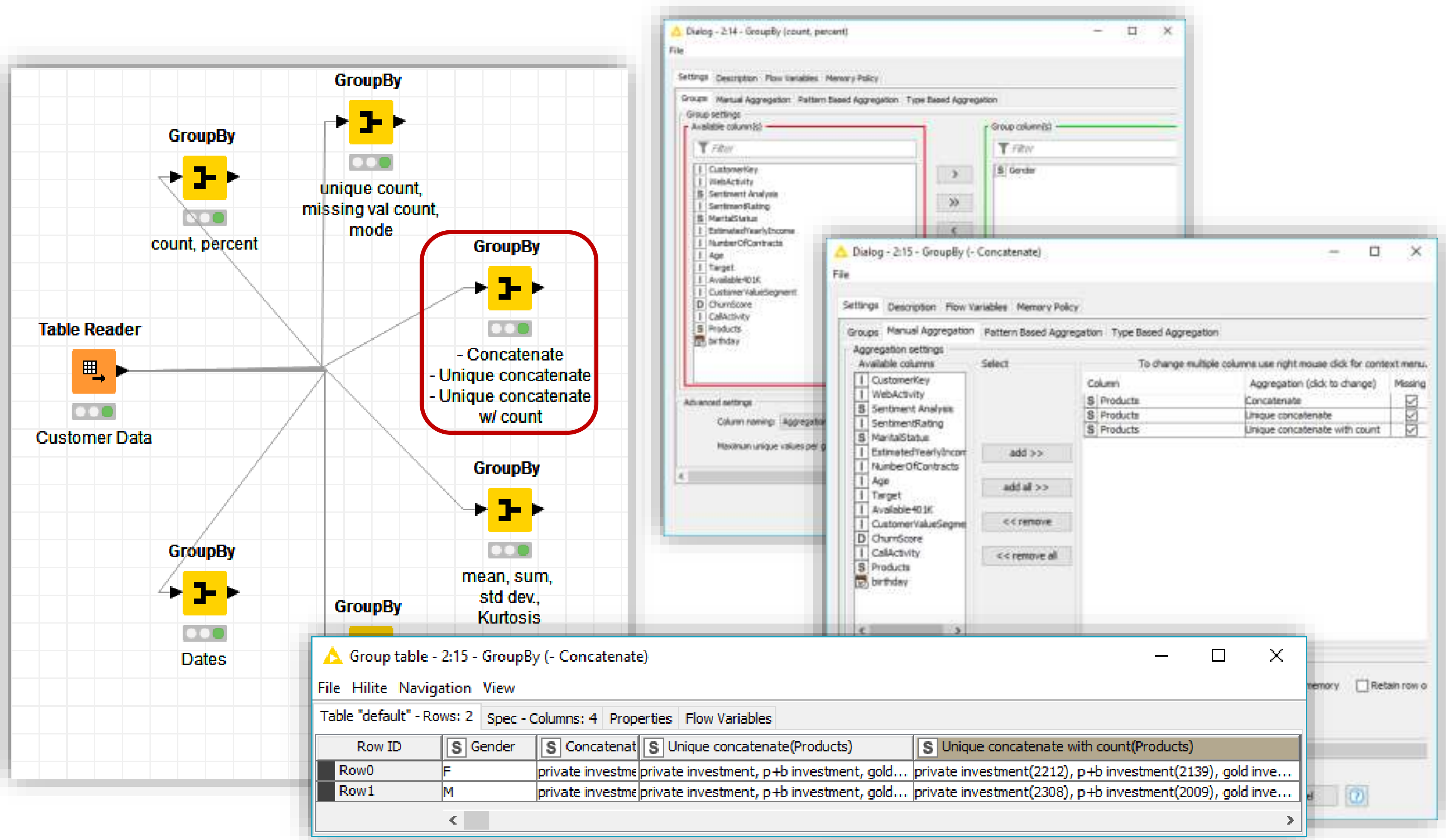
Basic Aggregations
Count and Percent



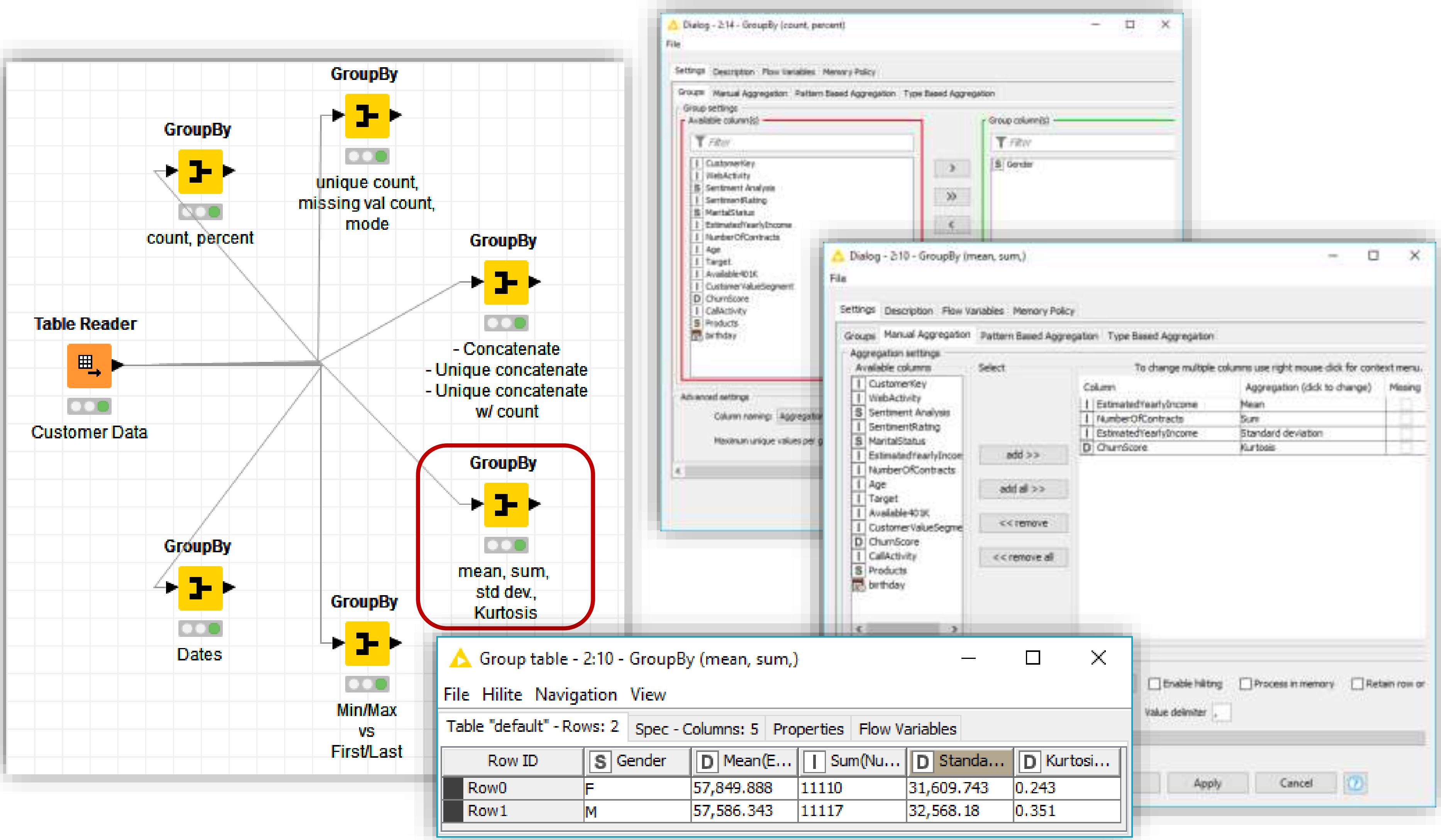
Basic Aggregations
Unique Count, Missing Values Count and Mode



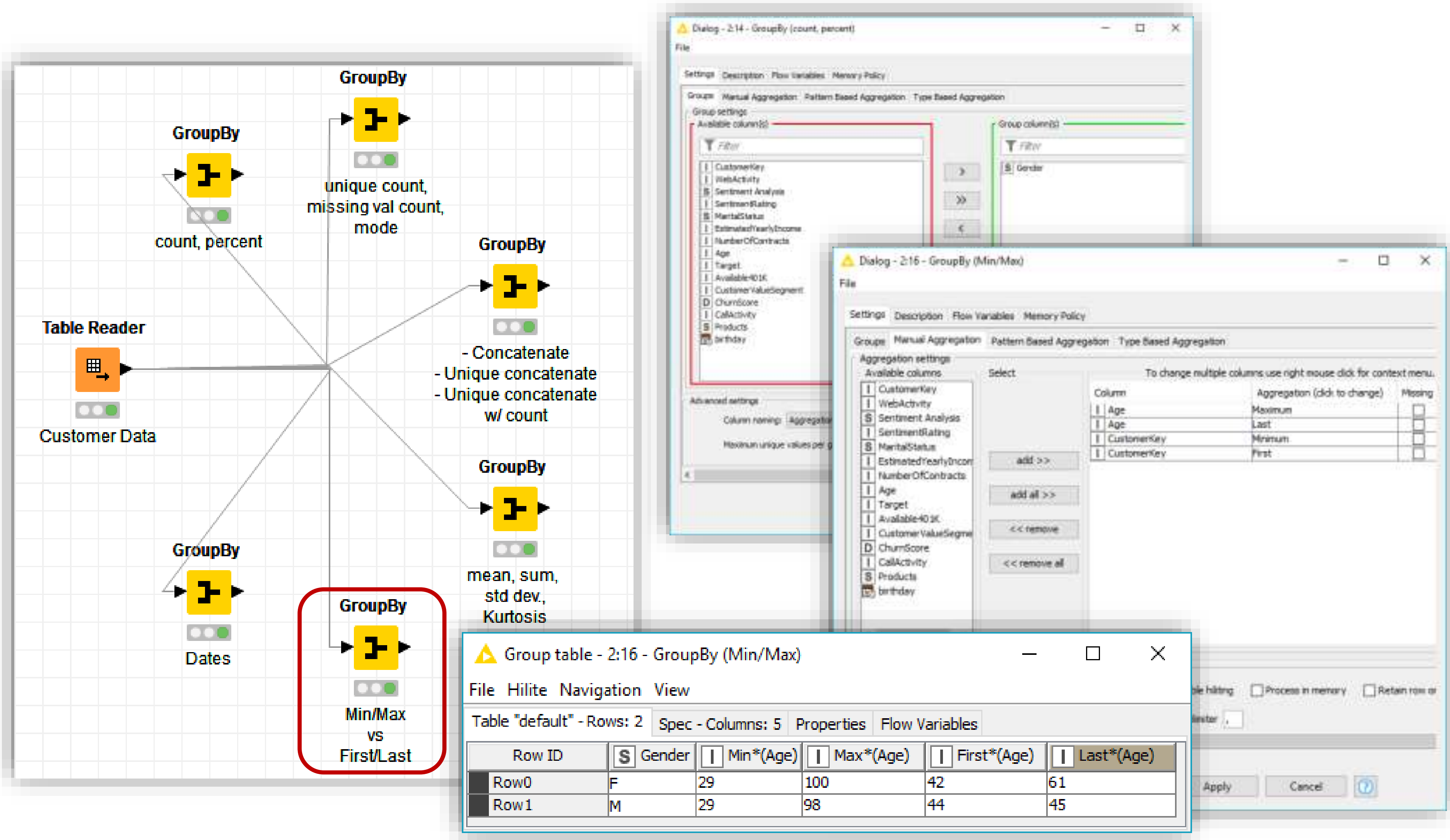
Basic Aggregations
Concatenate



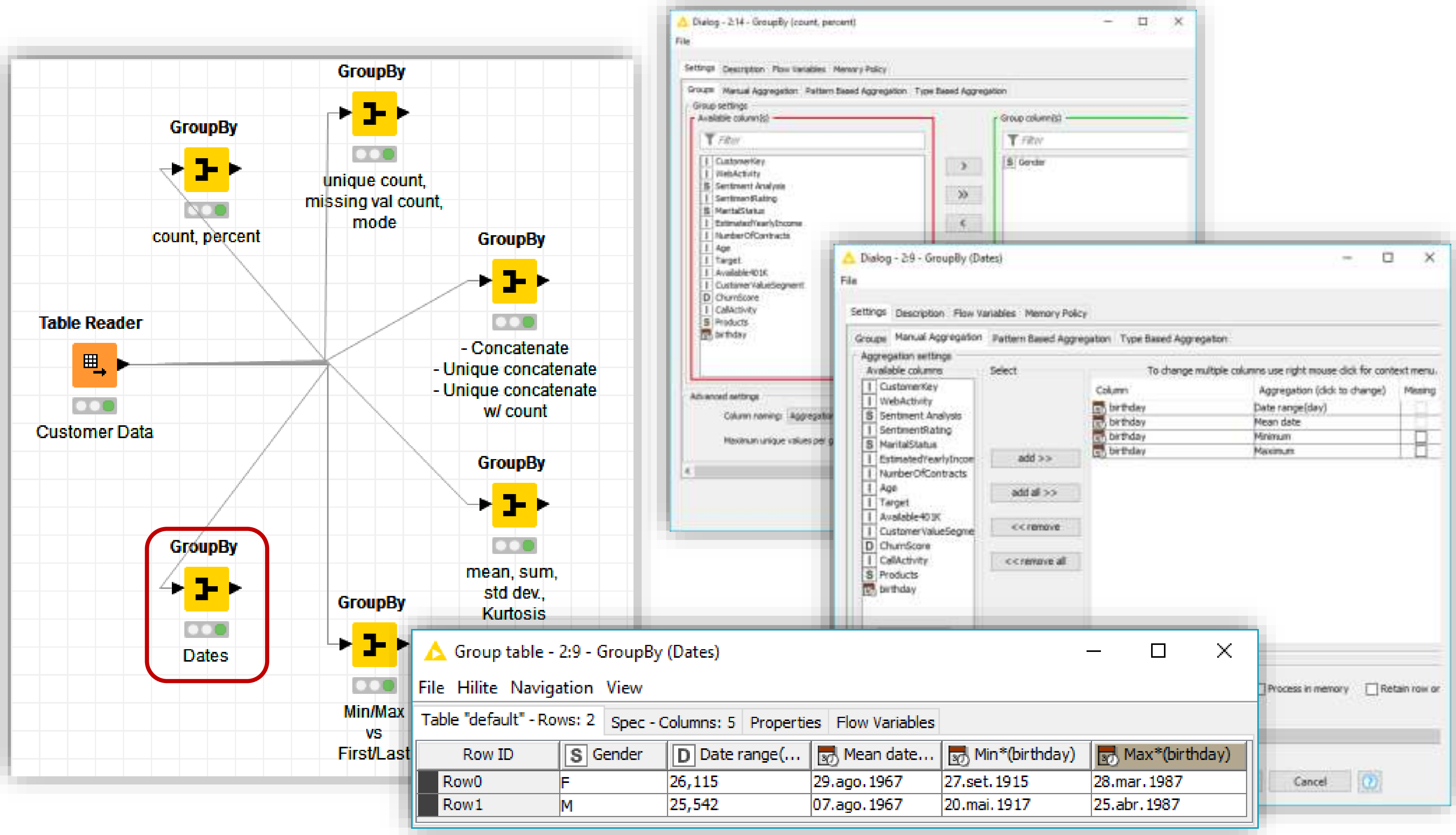
Basic Aggregations
Mean, Sum, Standard Deviation and Kurtosis



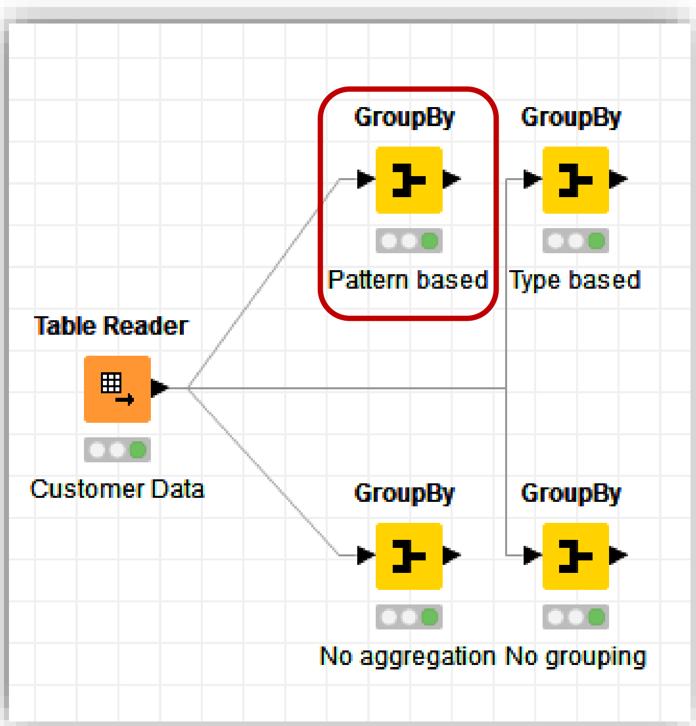
Basic Aggregations
Min/Max vs First/Last

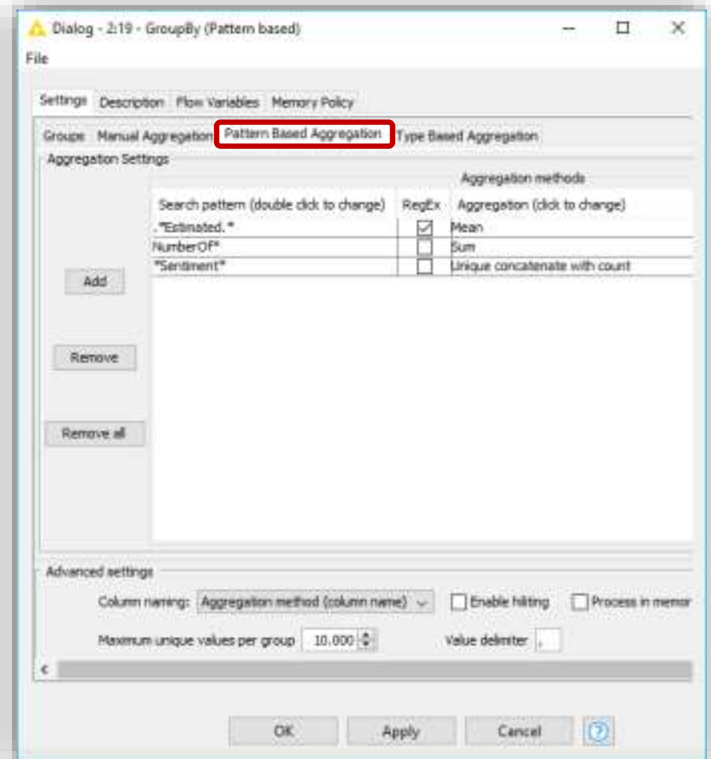


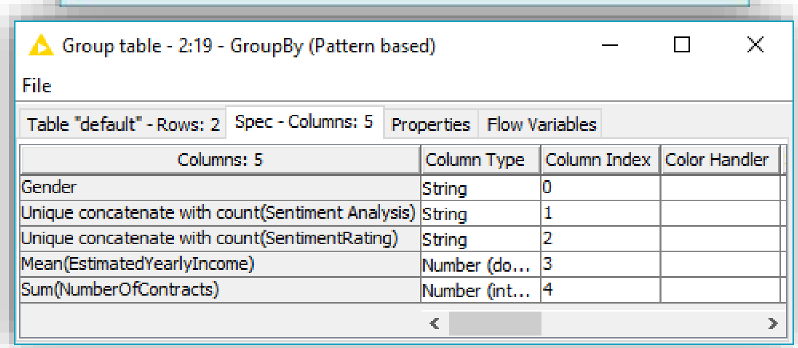
Basic Aggregations
Dates



Advanced Aggregations
Pattern Based

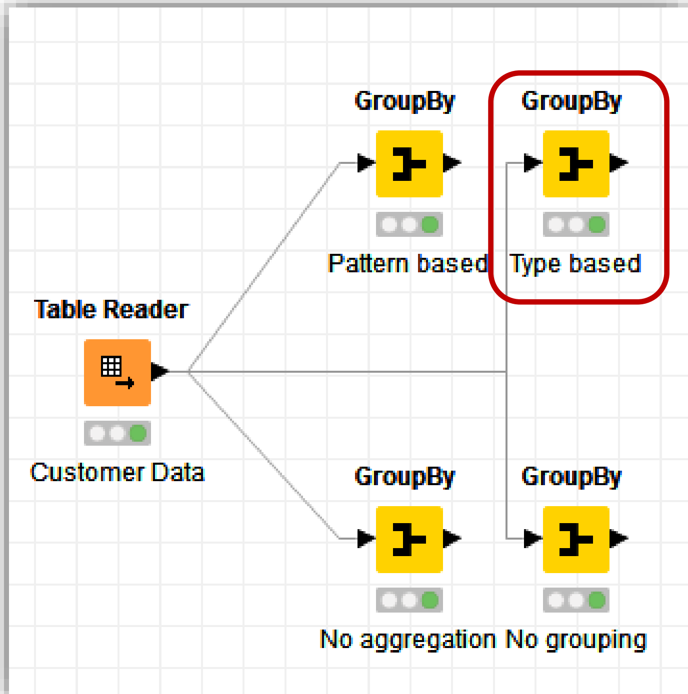


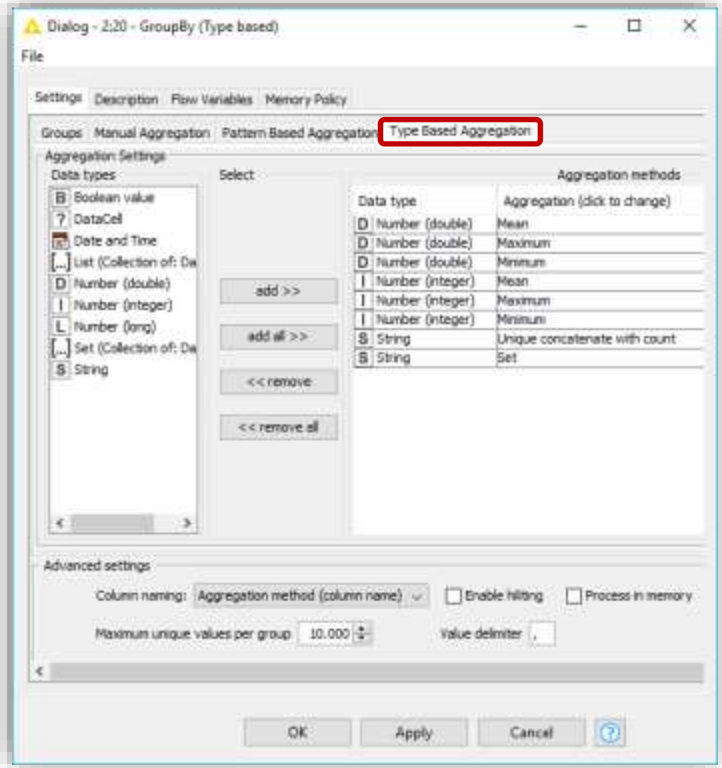


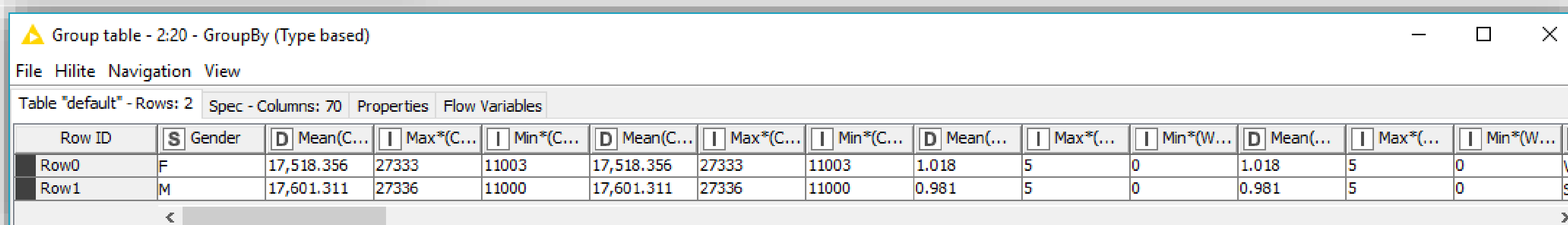


Columns: 5	Column Type	Column Index	Color Handler
Gender	String	0	
Unique concatenate with count(Sentiment Analysis)	String	1	
Unique concatenate with count(SentimentRating)	String	2	
Mean(EstimatedYearlyIncome)	Number (do…	3	
Sum(NumberOfContracts)	Number (int…	4	

Advanced Aggregations
Data Type Based

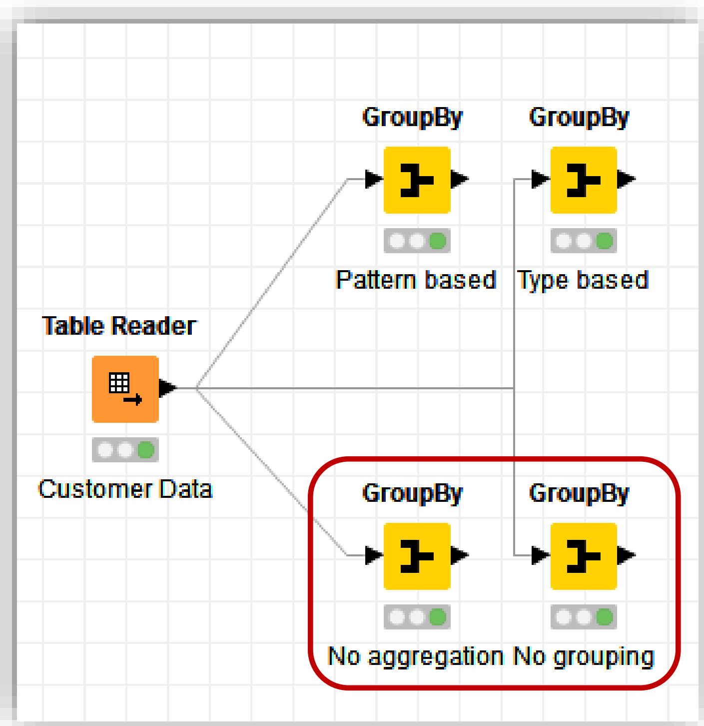


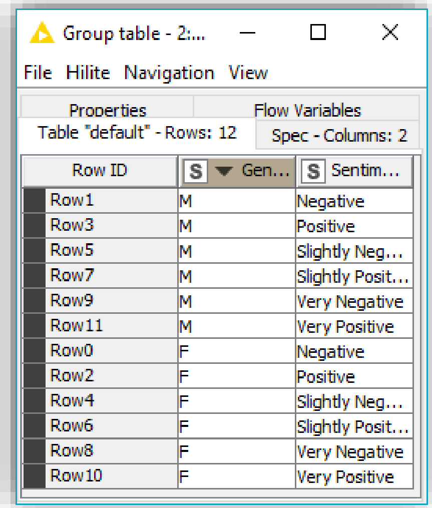




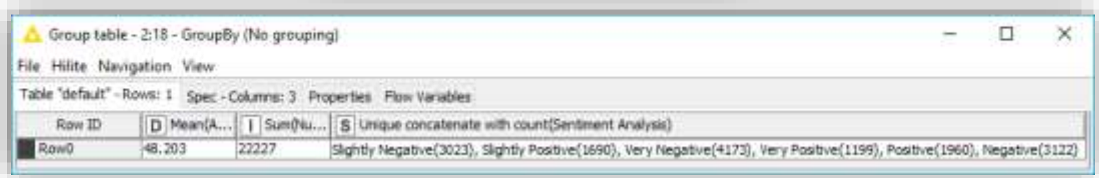
Row ID	Gender	Mean(C...	Max*(C...	Min*(C...	Mean(C...	Max*(C...	Min*(C...	Mean(...	Max*(...	Min*(W...	Mean(...	Max*(...	Min*(W...
Row0	F	17,518.356	27333	11003	17,518.356	27333	11003	1.018	5	0	1.018	5	0
Row1	M	17,601.311	27336	11000	17,601.311	27336	11000	0.981	5	0	0.981	5	0

Advanced Aggregations
No Aggregation vs No Grouping





Row ID	Gen...	Sentim...
Row1	M	Negative
Row3	M	Positive
Row5	M	Slightly Neg...
Row7	M	Slightly Posit...
Row9	M	Very Negative
Row11	M	Very Positive
Row0	F	Negative
Row2	F	Positive
Row4	F	Slightly Neg...
Row6	F	Slightly Posit...
Row8	F	Very Negative
Row10	F	Very Positive

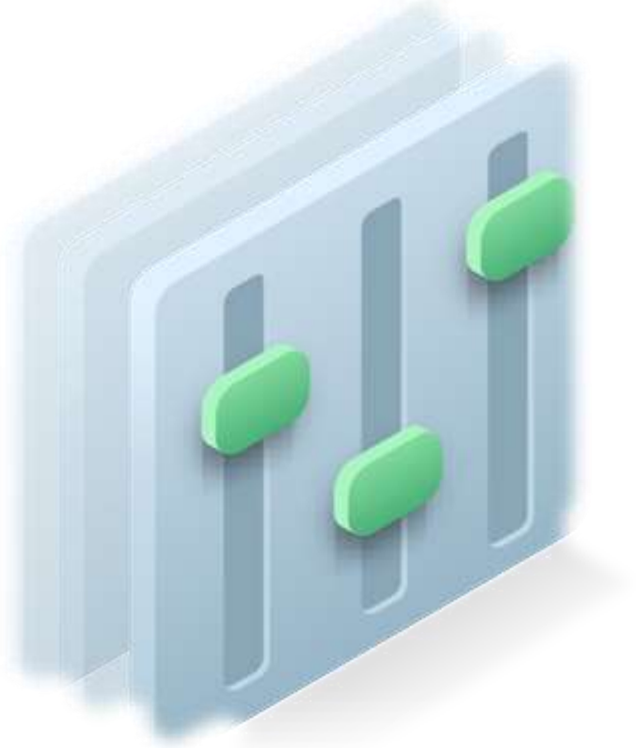


Row ID	Mean(A...	Sum(Nu...	Unique concatenate with count(Sentiment Analysis)
Row0	48.203	22227	Slightly Negative(3023), Slightly Positive(1690), Very Negative(4173), Very Positive(1199), Positive(1960), Negative(3122)

Advanced Data Preparation

How?

1. Feature scaling
2. Outlier detection
3. Feature selection
4. Missing Values treatment
5. Nominal value discretization
6. Binning
7. Feature Engineering



Feature scaling

1. Normalizing the range of the independent features

   Rationale:

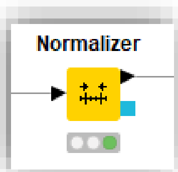
   Many classifiers use distance metrics (ex.: Euclidean distance) and, if one feature has a broad range of values, the distance will be governed by this particular feature. Hence, the range should be normalized so that each feature may contribute proportionately to the final distance.

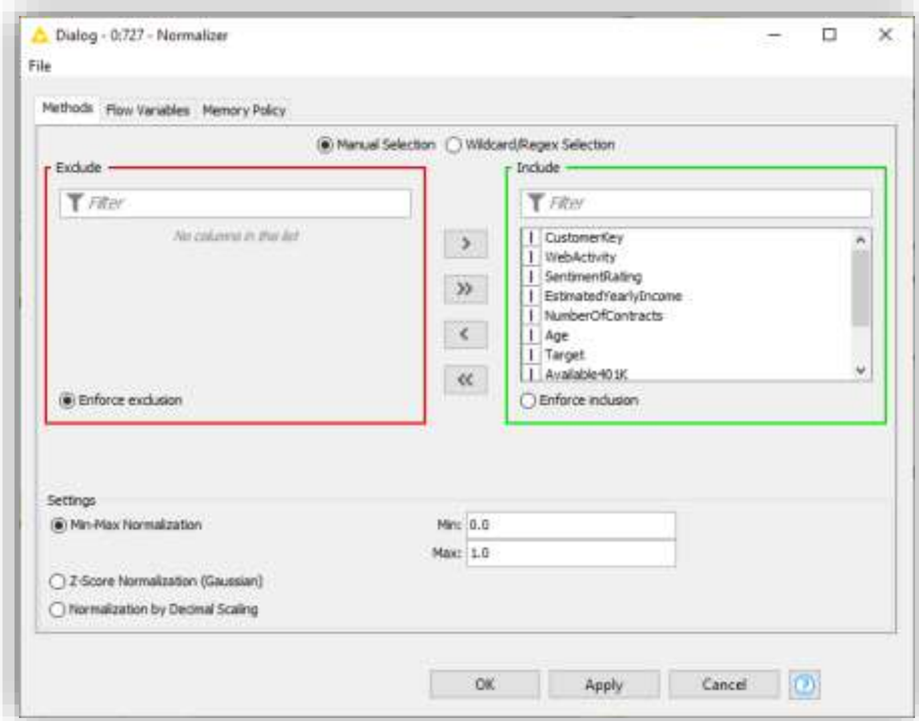
Feature scaling

1. Normalize the range of the independent features:

   i. **Normalization**

   Rescaling data so that all values fall within the range of 0 and 1, for example.





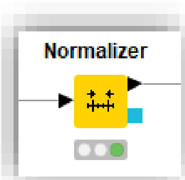
$$z = (b - a)\frac{x - \min(x)}{\max(x) - \min(x)} + a$$

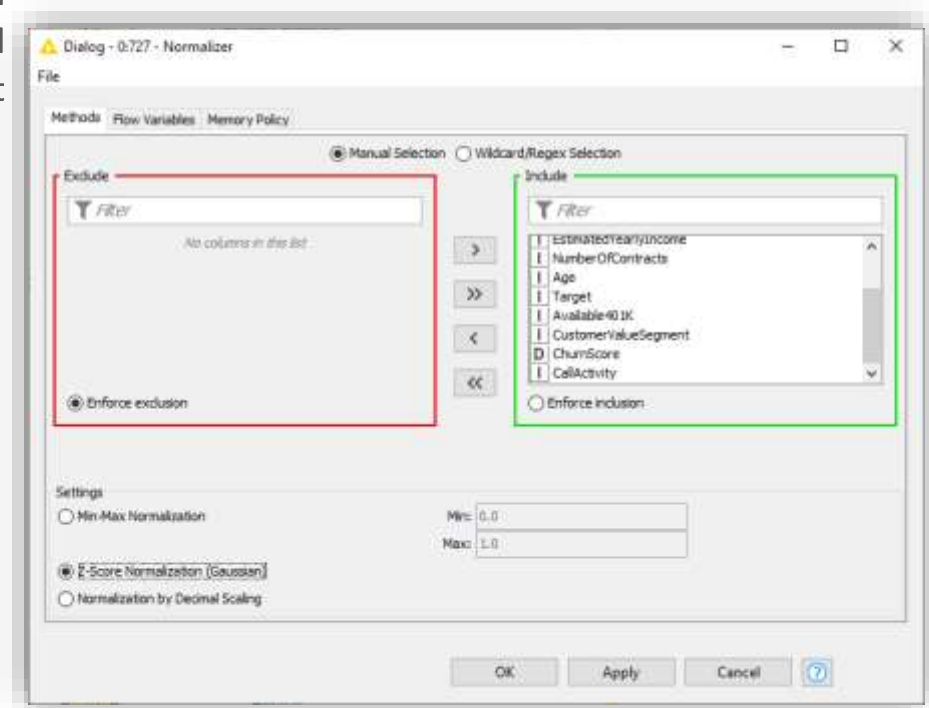
Feature scaling

1. Normalize the range of the independent features:

   ii. Standardization (or Z-score Normalization)

   Rescaling the distribution of values so that the mean of observed values is 0 and the standard deviation is 1. Assumes observations fit a Gaussian distribution with a well-behaved mean and standard deviation, which may not always be the case.





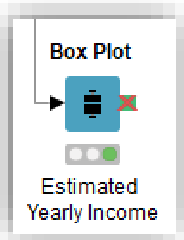
$$z = \frac{x_i - \mu}{\sigma}$$

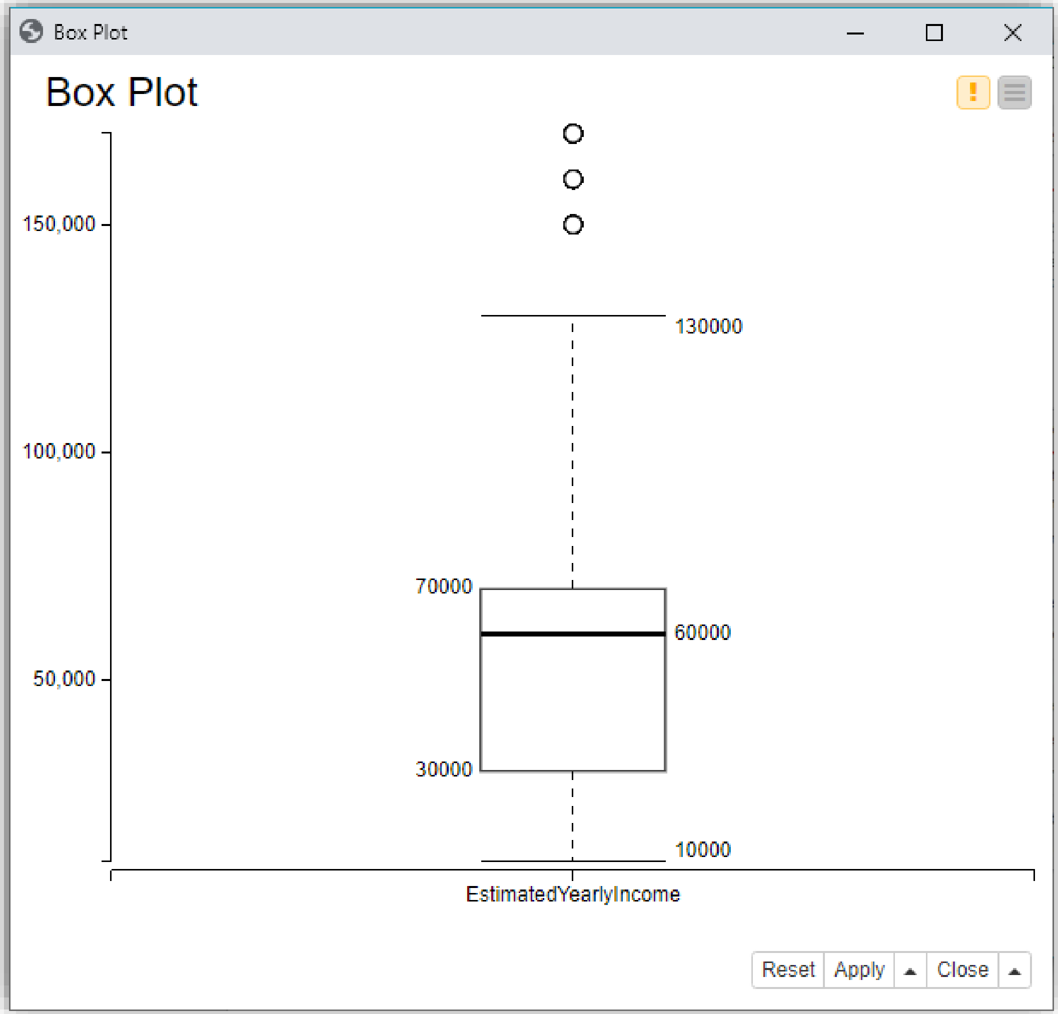
Outlier Detection

2. Outlier detection:

   i. Statistical-based strategy

      - Box Plots
      - Z-Score (std. dev)

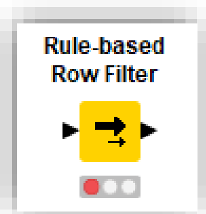


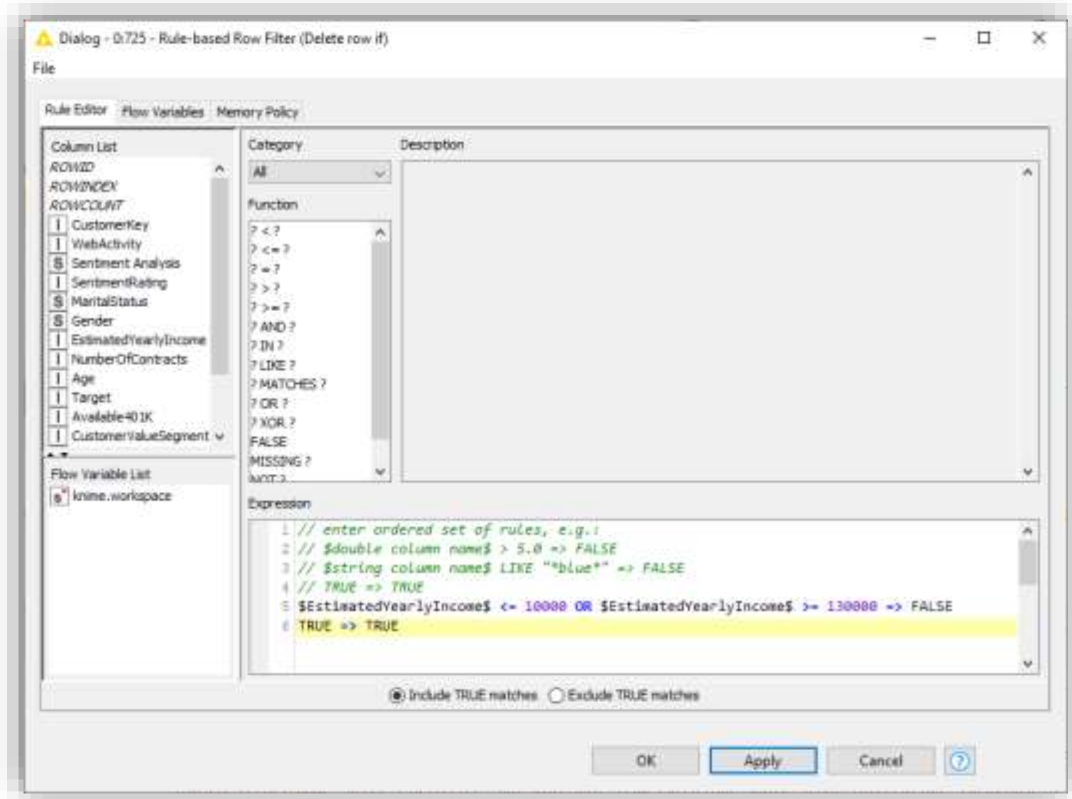


Outlier Detection

2. Outlier detection:

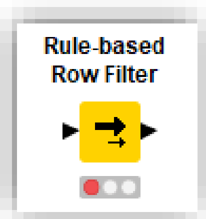
   ii. Knowledge-based strategy

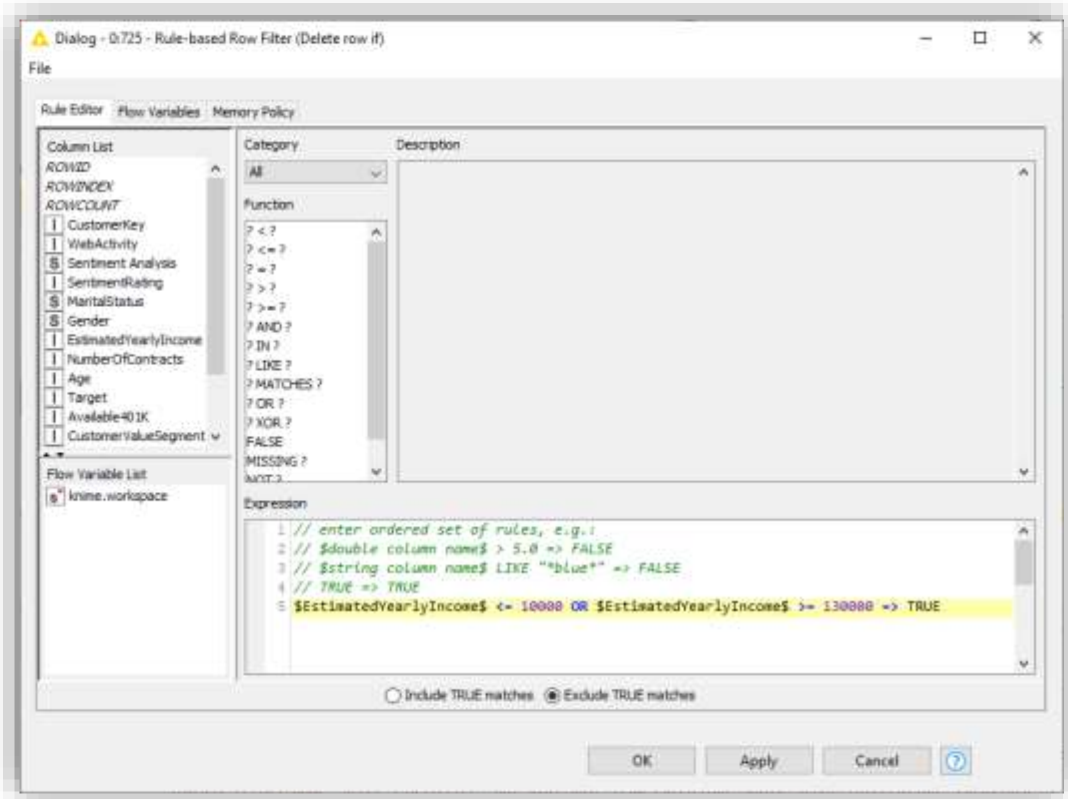




Outlier Detection

2. Outlier detection:
   - ii. Knowledge-based strategy



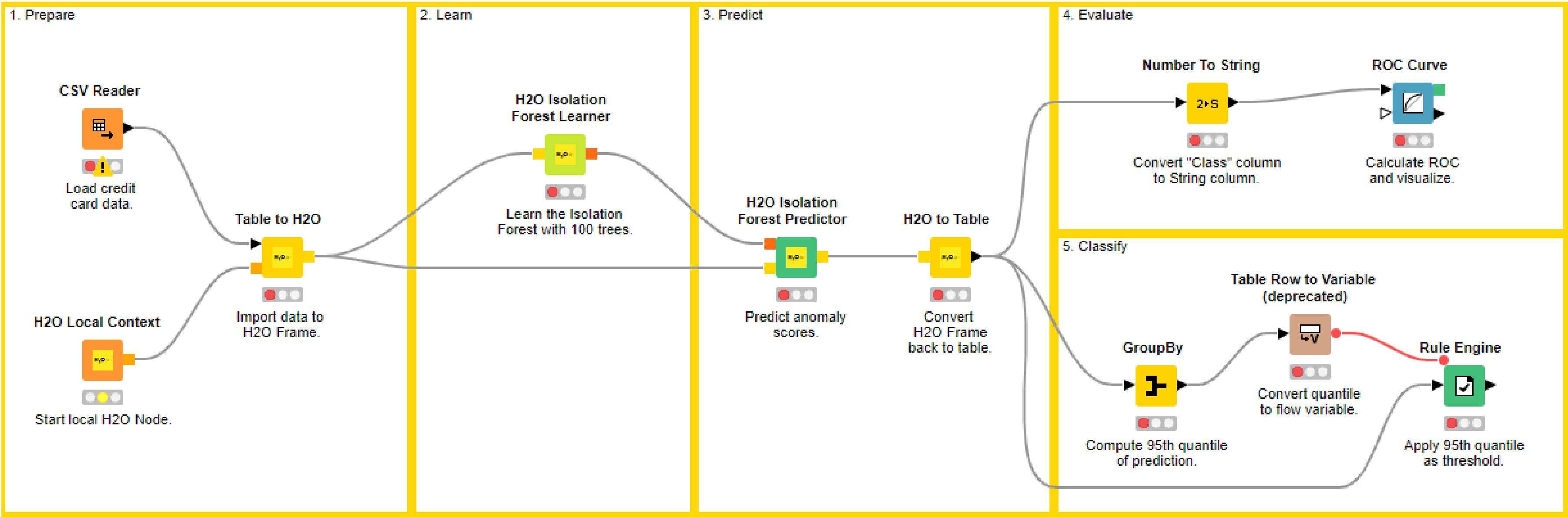


Outlier Detection

2. Outlier detection:

   iii. Model-based strategy

   - Isolation Forest
   - One-Class SVM
   - Minimum Covariance Determinant
   - …



Outlier Detection

2. Outlier detection:

   i. Statistical-based strategy

   ii. Knowledge-based strategy

   iii. Model-based strategy

The Outlier Dilemma: Drop or Cap?

To keep the dataset size we may want to cap outliers instead of dropping them. However, it can affect the distribution of data!

Feature Selection

3. Feature Selection (or dimensionality reduction)

Rationale:

Which features should we use to create a predictive model? Select a sub-set of the most important features to reduce dimensionality.

The removal of unimportant features:

- May affect significantly the performance of a model
- Reduces overfitting (less opportunity to make decisions based on noise)
- Improves accuracy
- Helps reducing the complexity of a model (reduces training time)

Feature Selection

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The removal of unimportant features:

- May affect significantly the performance of a model
- Reduces overfitting (less opportunity to make decisions based on noise)
- Improves accuracy
- Helps reducing the complexity of a model (reduces training time)

What can we remove:

- Redundant features (duplicate)
- Irrelevant and unneeded features (non-useful)

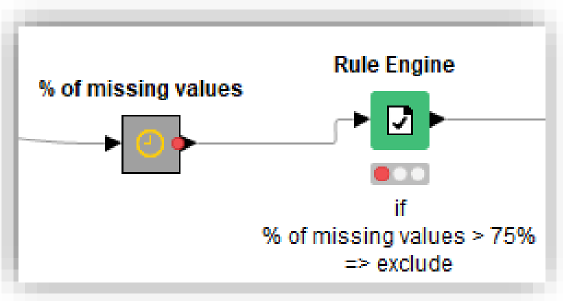
Feature Selection Methods:

- Filter methods
- Wrapper methods
- Embedded methods

Feature Selection

3. Filter Methods:

   i. Remove a feature if the percentage of missing values is higher than a threshold



   ii. Use the chi-square test to measure the degree of dependency between a feature and the target class

   - For each feature calculate X^2
   - Normalize X^2 and sort in descending order
   - Select *n* features with the highest importance (or those that are above the threshold)

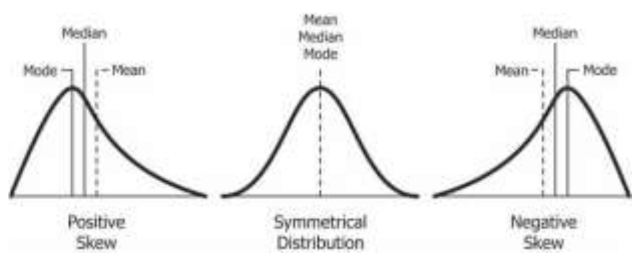
Feature Selection

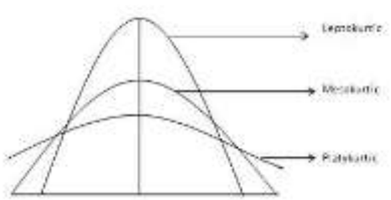
3. Filter Methods:

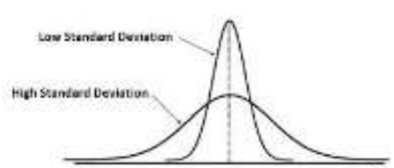
   iii. Remove feature if low standard deviation

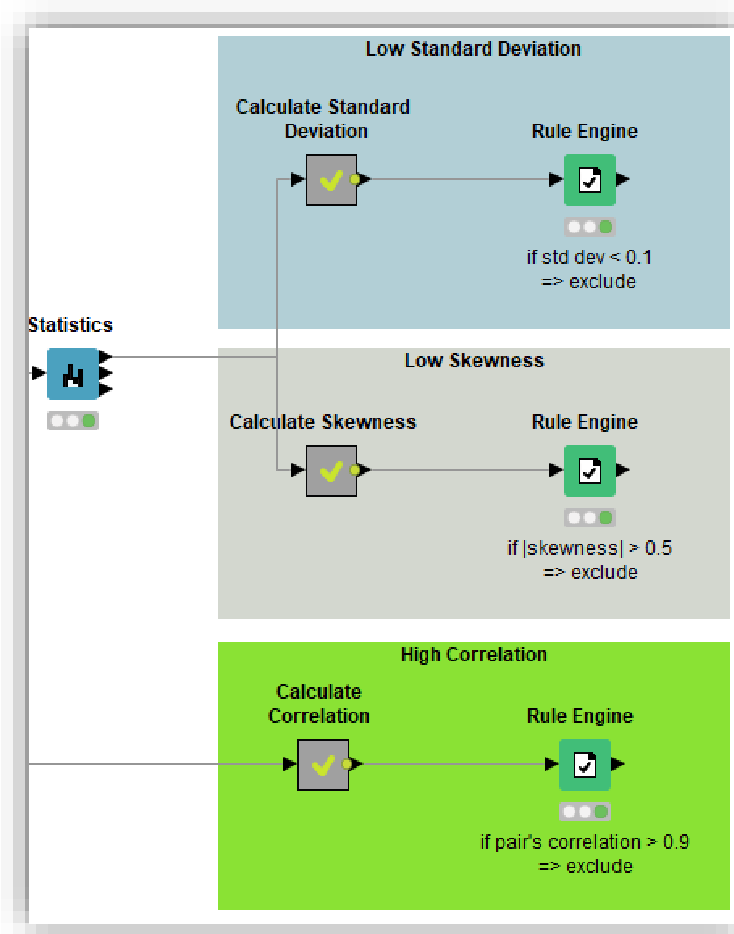
   iv. Remove feature if data are highly skewed

   v. Remove features that are highly correlated between each other







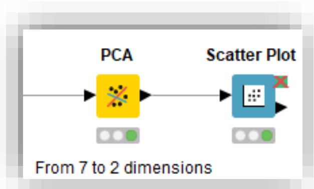


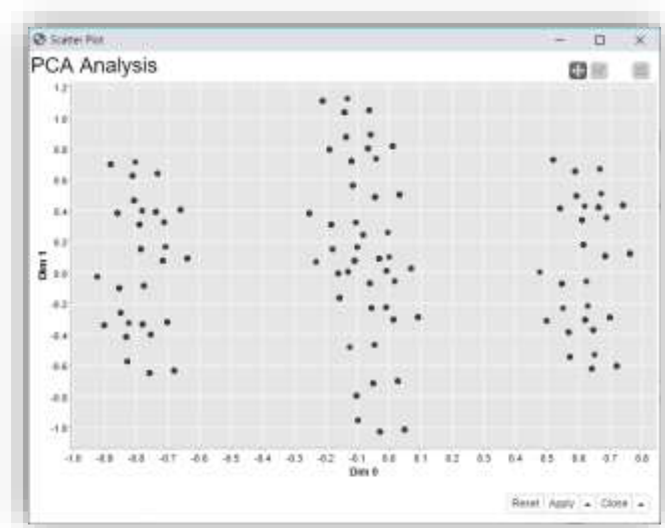
Feature Selection

3. Filter Methods:

   vi. Principal Component Analysis (PCA)

   A technique to reduce the dimension of the feature space. The goal is to reduce the number of features without losing too much information. A popular application of PCA is for visualizing higher dimensional data.



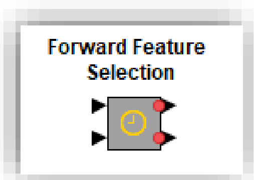


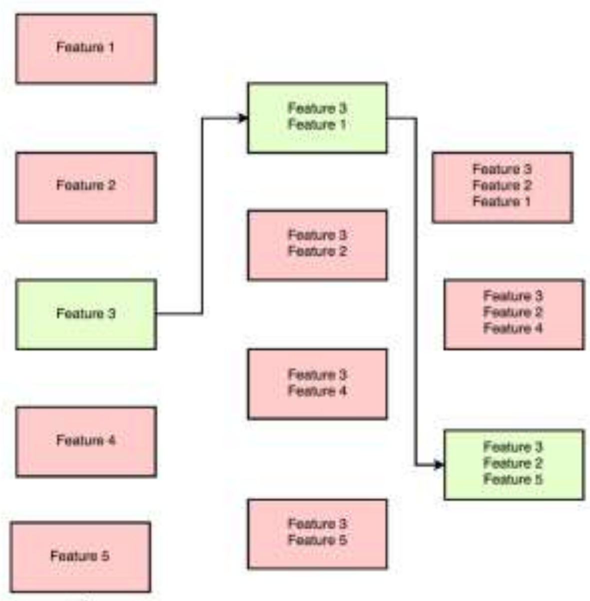
Feature Selection

3. Wrapper Methods:

   Use a ML algorithm to select the most important features! Select a set of features as a search problem, prepare different combinations, evaluate and compare them!
   Measure the “usefulness” of features based on the classifier performance.

   vii. Sequential Forward Selection



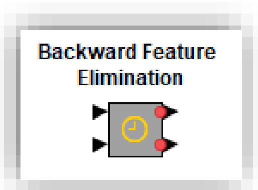


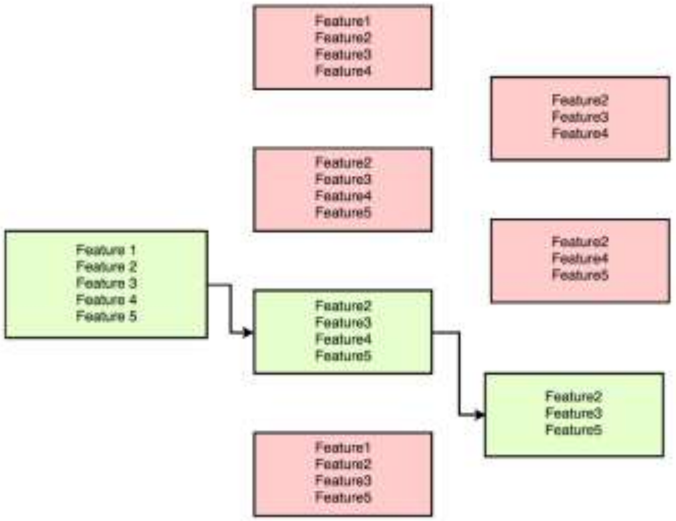
Feature Selection

3. Wrapper Methods:

Use a ML algorithm to select the most important features! Select a set of features as a search problem, prepare different combinations, evaluate and compare them!
Measure the “usefulness” of features based on the classifier performance.

vii. Backward Feature Elimination





Feature Selection

3. Embedded Methods:

Algorithms that already have built-in feature selection methods.

Lasso, for example, has their own feature selection methods.
For example, if a feature's weight is zero than it has no importance!

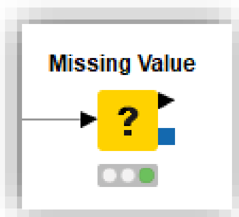
Regularization - constrain/regularize or shrink the coefficient estimates towards zero!

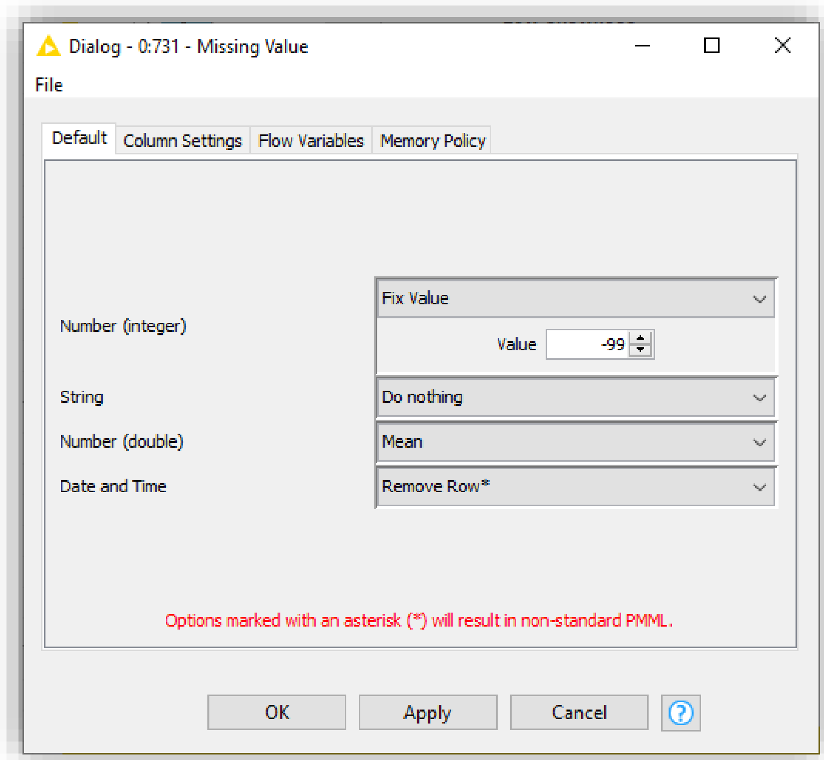
Missing Values

4. Missing Values treatment:

   i. First analyse each feature in regard to the number and percentage of missing values

   ii. Then decide what to do:
      - Remove
      - Mean
      - (Linear/…) Interpolation
      - Mask
      - …





Nominal Value Discretization/Encoding

5. Nominal value discretization:

   Rationale:

   Categorical data often called nominal data, are variables that contain label values rather than numeric ones. Several methods may be applied:

   - One-Hot Encoding
   - Label Encoding
   - Binary Encoding

Nominal Value Discretization/Encoding

Movie	Genre
Jumanji	Adventure
American Pie	Comedy
Braveheart	Drama
…	…

Nominal Value Discretization/Encoding

Movie	Genre
Jumanji	Adventure
American Pie	Comedy
Braveheart	Drama
…	…

Label Encoded

Movie	Genre	Category
Jumanji	Adventure	0
American Pie	Comedy	1
Braveheart	Drama	2
…	…	

Nominal Value Discretization/Encoding

Movie	Genre
Jumanji	Adventure
American Pie	Comedy
Braveheart	Drama
…	…

One-Hot Encoded

Movie	Adventure	Comedy	Drama
Jumanji	1	0	0
American Pie	0	1	0
Braveheart	0	0	1
…	…		

Nominal Value Discretization/Encoding

Movie	Genre
Jumanji	Adventure
American Pie	Comedy
Braveheart	Drama
…	…

Label Encoded

Movie	Genre	Category
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…	…	

One-Hot Encoded

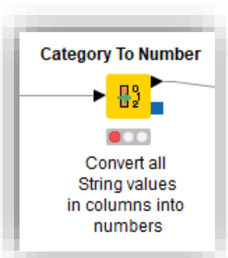
Movie	Adventure	Comedy	Drama
Jumanji	1	0	0
American Pie	0	1	0
Braveheart	0	0	1
…	…		

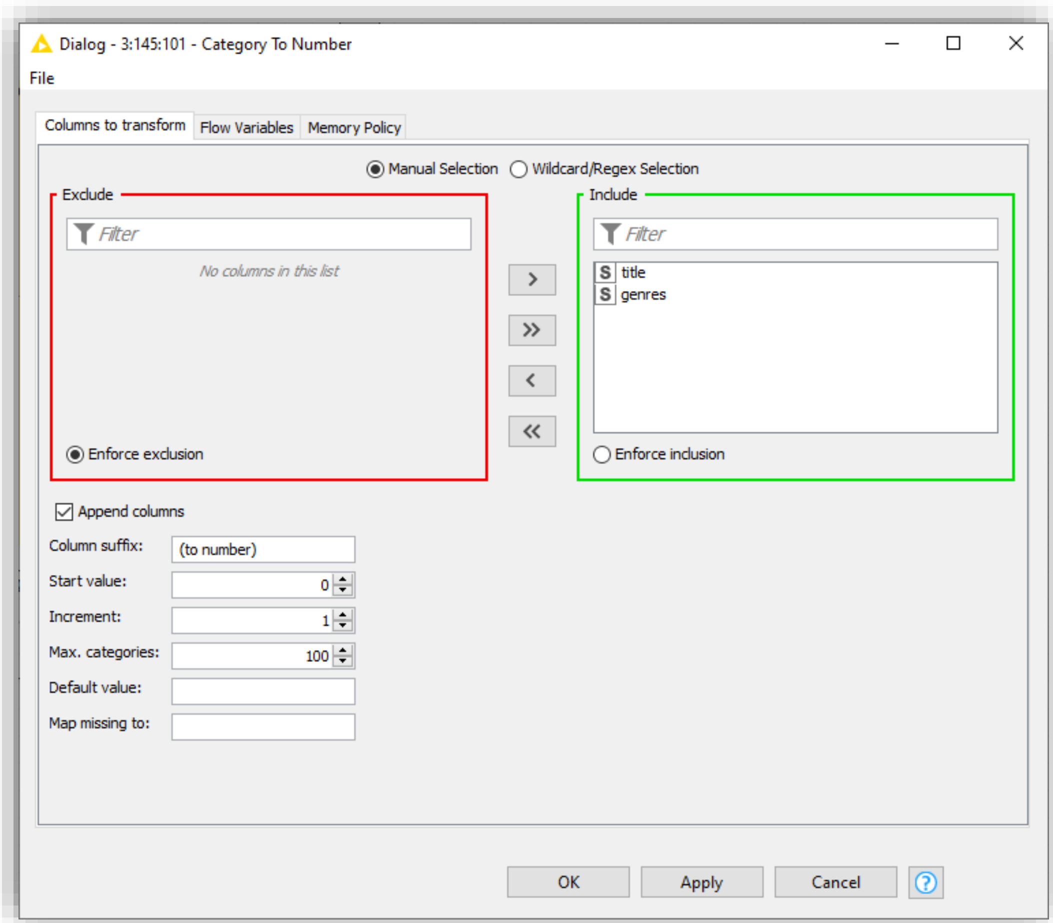
Integer values have a natural ordered relationship between each other. ML models may be able to understand such relationships.

Categorical features where no such ordinal relationship exists. However, for a huge number of categories…

Nominal Value Discretization/Encoding

5. Nominal value discretization:





Nominal Value Discretization/Encoding

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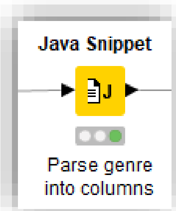
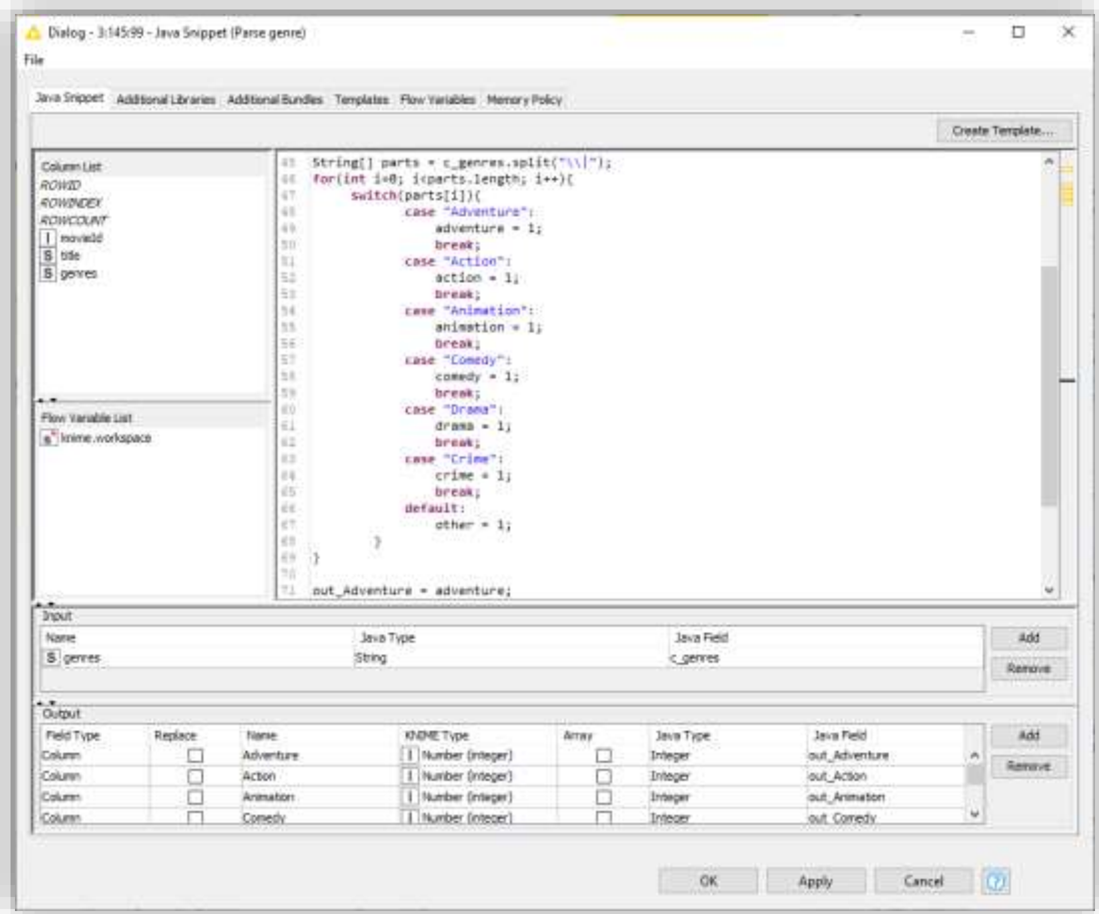


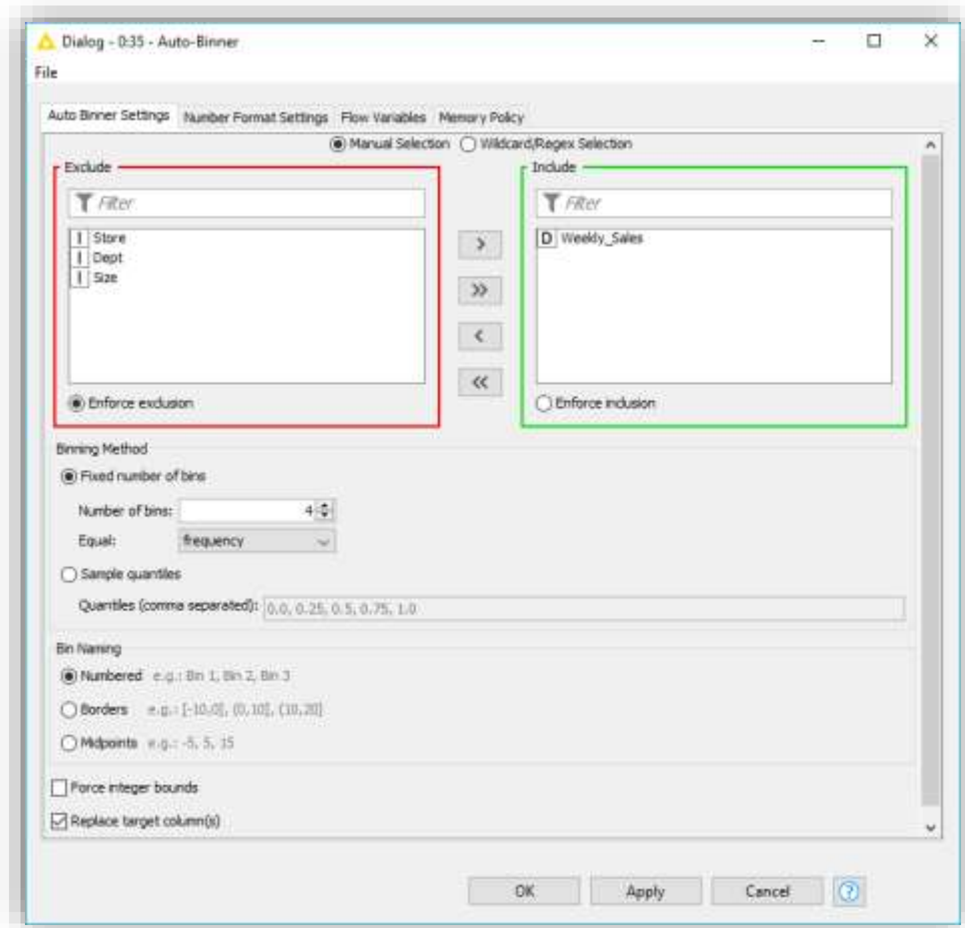


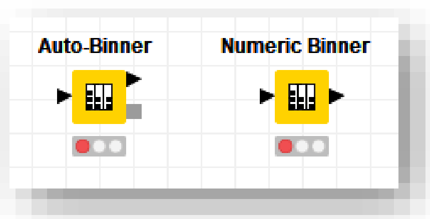
Binning

6. Binning, i.e., group numeric data into intervals - called bins:

   Rationale:

   Make the model more robust and prevent overfitting. However, it penalizes the model's performance since every time you bin something, you sacrifice information.





Binning

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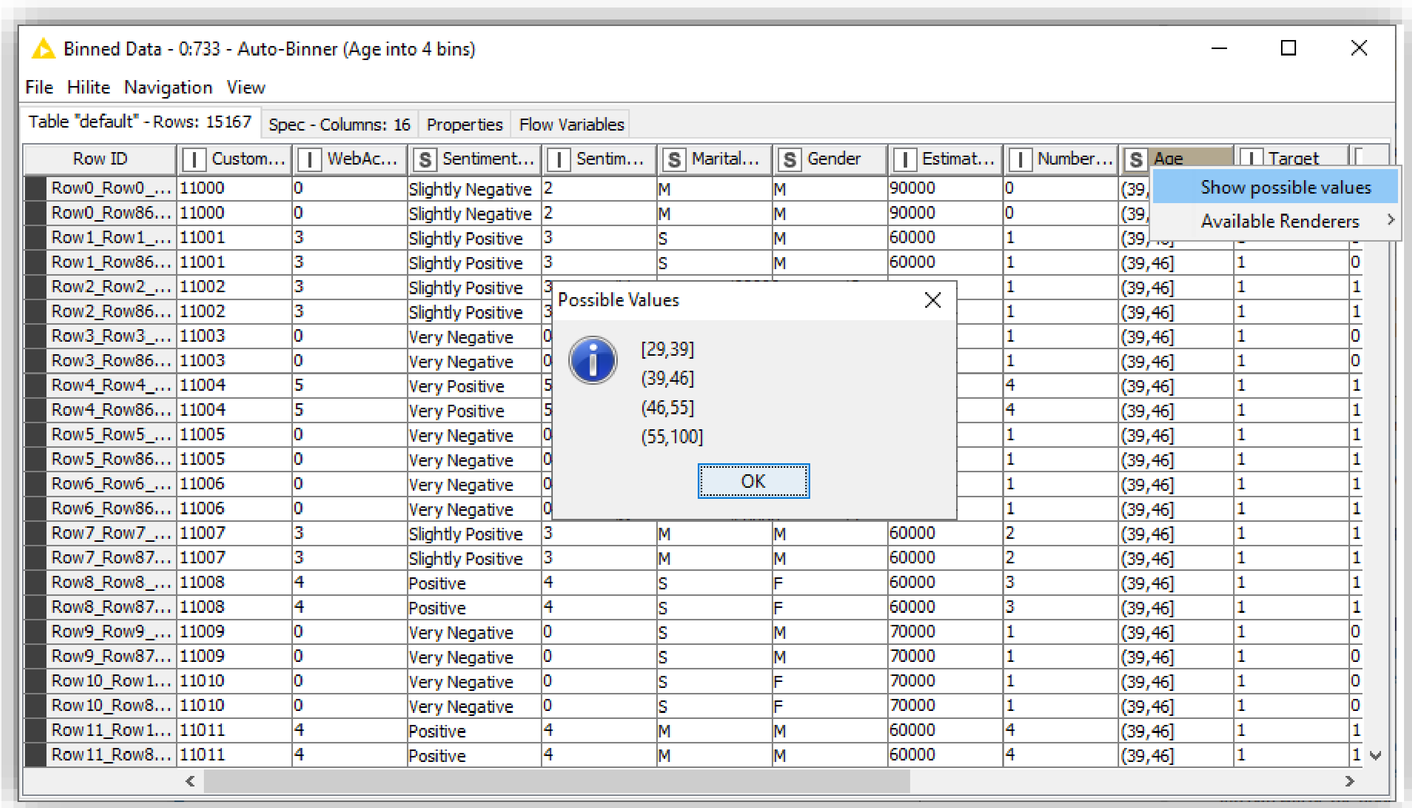

Feature Engineering

7. Feature Engineering:

   Rationale:

   The process of creating new features! The goal is to improve the performance of ML models.

   Example: from the creation date of an observation what can we extract?

   2020-10-29 16h30

Feature Engineering

7. Feature Engineering:

Rationale:

The process of creating new features! The goal is to improve the performance of ML models.

Example: from the creation date of an observation what can we extract?

2020-10-29 16h30

We may extract new features such as:

- Year, month and day
- Hour and minutes
- Day of week (Thursday)
- Is Weekend? (No)
- Is Holiday? (No)
- …

Feature Engineering

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   Rationale:

   The process of creating new features! The goal is to improve the performance of ML models.

   Example: from the geographic coordinates of a road

   (41.561859, -8.397455)

Feature Engineering

7. Feature Engineering:

Rationale:

The process of creating new features! The goal is to improve the performance of ML models.

Example: from the geographic coordinates of a road

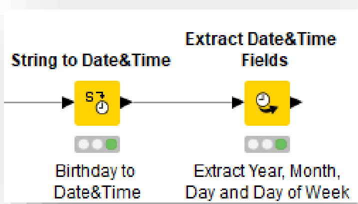
(41.561859, -8.397455)

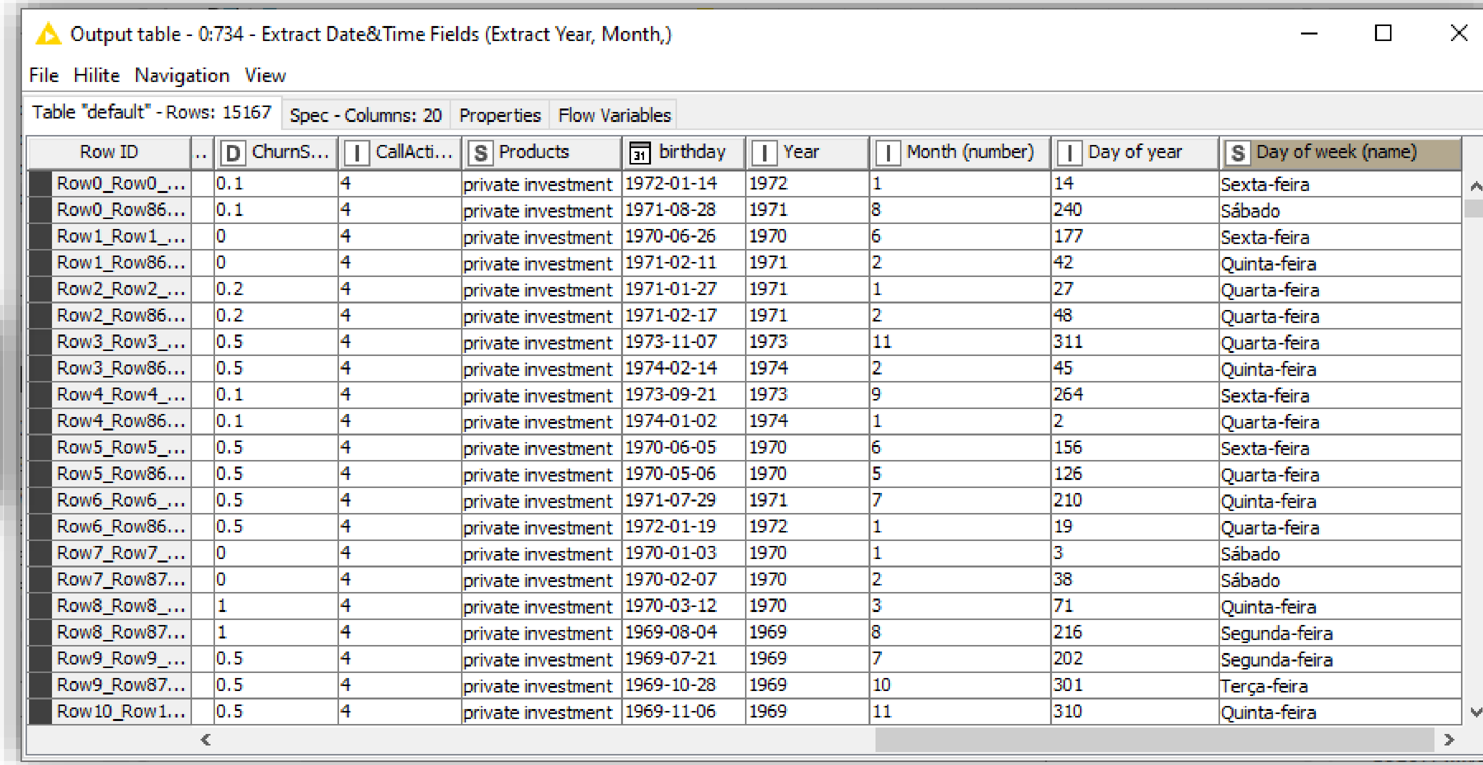
We may extract new features such as:

- Number of roads in the vicinity
- Are there schools nearby?
- …

Feature Engineering

7. Feature Engineering:





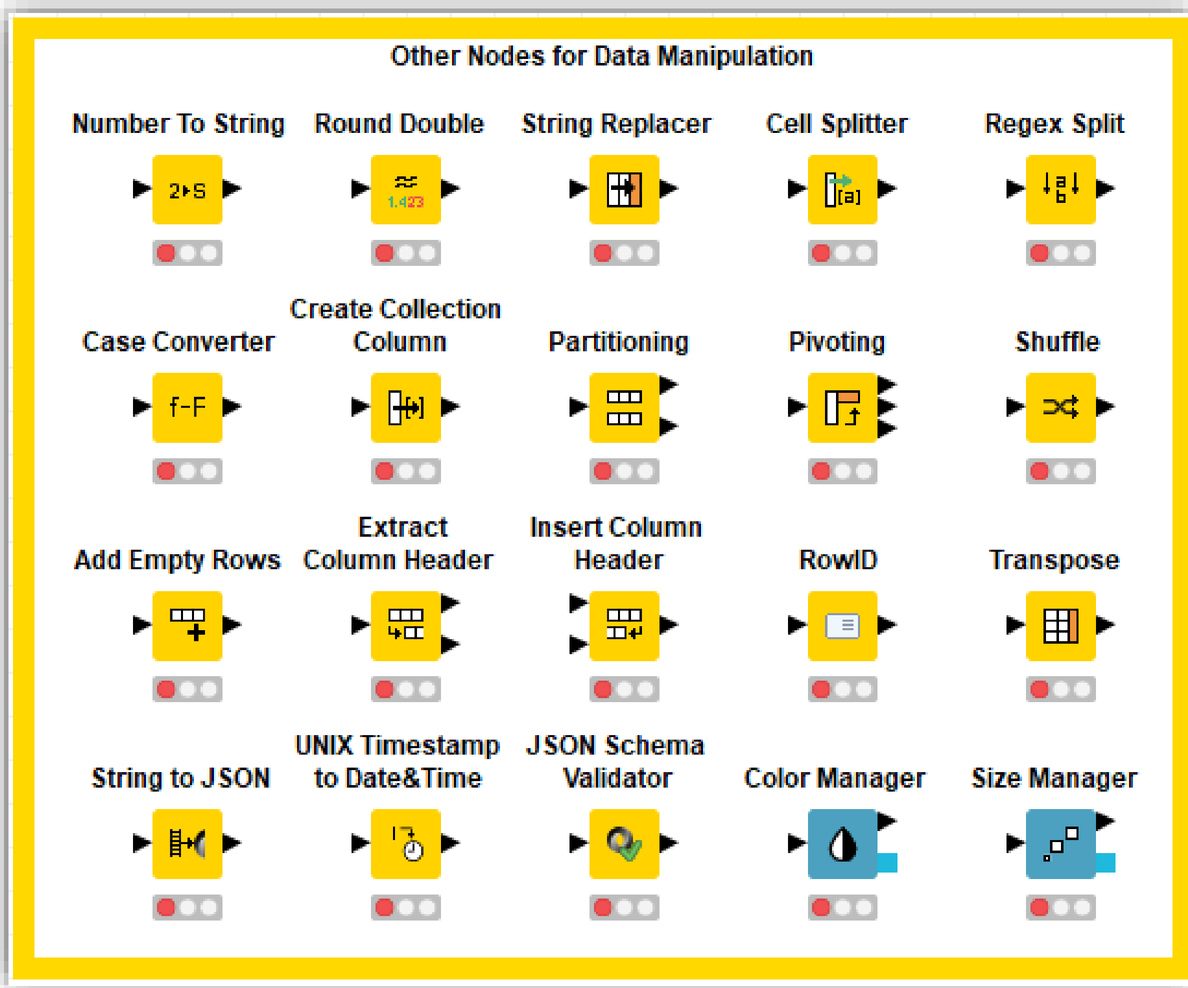
Output table - 0:734 - Extract Date&Time Fields (Extract Year, Month,)

File Hilite Navigation View

Table "default" - Rows: 15167 | Spec - Columns: 20 | Properties | Flow Variables

Row ID	..	D ChurnS...	I CallActi...	S Products	birthday	I Year	I Month (number)	I Day of year	S Day of week (name)
Row0_Row0_...		0.1	4	private investment	1972-01-14	1972	1	14	Sexta-feira
Row0_Row86...		0.1	4	private investment	1971-08-28	1971	8	240	Sábado
Row1_Row1_...		0	4	private investment	1970-06-26	1970	6	177	Sexta-feira
Row1_Row86...		0	4	private investment	1971-02-11	1971	2	42	Quinta-feira
Row2_Row2_...		0.2	4	private investment	1971-01-27	1971	1	27	Quarta-feira
Row2_Row86...		0.2	4	private investment	1971-02-17	1971	2	48	Quarta-feira
Row3_Row3_...		0.5	4	private investment	1973-11-07	1973	11	311	Quarta-feira
Row3_Row86...		0.5	4	private investment	1974-02-14	1974	2	45	Quinta-feira
Row4_Row4_...		0.1	4	private investment	1973-09-21	1973	9	264	Sexta-feira
Row4_Row86...		0.1	4	private investment	1974-01-02	1974	1	2	Quarta-feira
Row5_Row5_...		0.5	4	private investment	1970-06-05	1970	6	156	Sexta-feira
Row5_Row86...		0.5	4	private investment	1970-05-06	1970	5	126	Quarta-feira
Row6_Row6_...		0.5	4	private investment	1971-07-29	1971	7	210	Quinta-feira
Row6_Row86...		0.5	4	private investment	1972-01-19	1972	1	19	Quarta-feira
Row7_Row7_...		0	4	private investment	1970-01-03	1970	1	3	Sábado
Row7_Row87...		0	4	private investment	1970-02-07	1970	2	38	Sábado
Row8_Row8_...		1	4	private investment	1970-03-12	1970	3	71	Quinta-feira
Row8_Row87...		1	4	private investment	1969-08-04	1969	8	216	Segunda-feira
Row9_Row9_...		0.5	4	private investment	1969-07-21	1969	7	202	Segunda-feira
Row9_Row87...		0.5	4	private investment	1969-10-28	1969	10	301	Terça-feira
Row10_Row1...		0.5	4	private investment	1969-11-06	1969	11	310	Quinta-feira

More Nodes


Other Nodes for Data Manipulation
Number To String
Round Double
String Replacer
Cell Splitter
Regex Split
Case Converter
Create Collection Column
Partitioning
Pivoting
Shuffle
Add Empty Rows
Extract Column Header
Insert Column Header
RowID
Transpose
String to JSON
UNIX Timestamp to Date&Time
JSON Schema Validator
Color Manager
Size Manager

Hands On


KNIME Analytics Platform
File Edit View Node Help
KNIME Explorer
My-KNIME-Hub (hub.knime.com)
EXAMPLES (knime@hub.knime.com)
LOCAL (Local Workspace)
Aulas Exemplos
Aulas Exercicios
Example Workflows
ML Projects
KNIME_Aula_Exercicio
Workflow Coach
Recommended Nodes
File Reader
CSV Reader
Excel Reader (XLS)
Table Creator
Database Reader (legacy)
Table Reader
List Files
Database Connection T...
Node Repository
IO
Manipulation
Views
Analytics
DB
Other Data Types
Structured Data
Scripting
Tools & Services
Workflow Control
Workflow Abstraction
Reporting
Description
KNIME Hub Search
Console
Outline
HANDS ON