



Open for Innovation

KNIME

What's new in KNIME

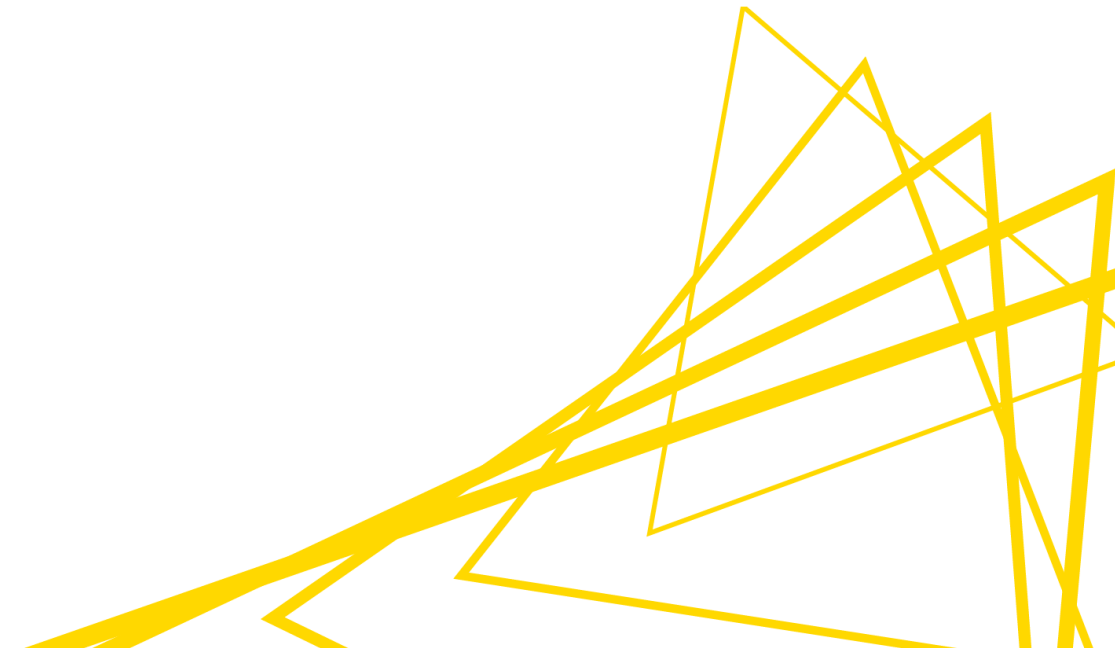
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KNIME.com AG

Agenda

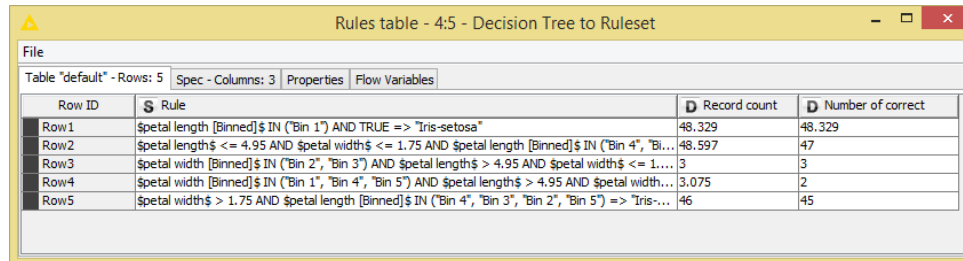
- New in 2.12/4.1
 - Analytics
 - Tool integration
 - Misc
 - KNIME Server and Automation
- Cooking for 3.0
 - Internal & API changes
 - New Look&Feel

New in 2.12/4.1



Analytics I

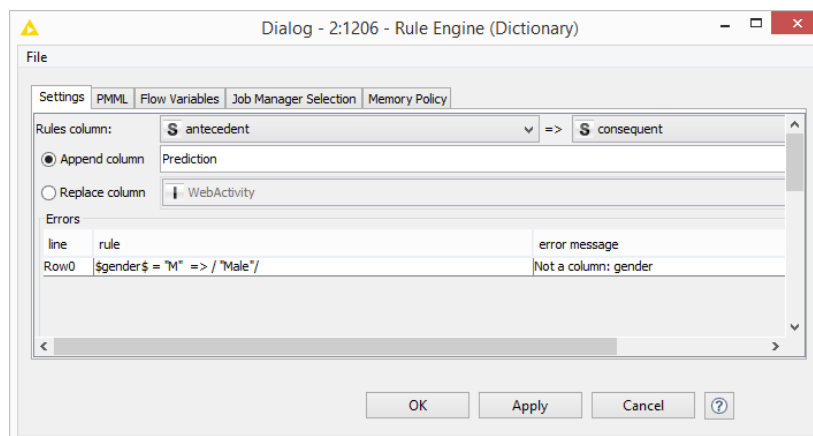
- Decision Tree to Ruleset node



Rules table - 4:5 - Decision Tree to Ruleset

Row ID	S Rule	D Record count	D Number of correct
Row1	spetal length [Binned]\$ IN ("Bin 1") AND TRUE => "Iris-setosa"	48.329	48.329
Row2	spetal length\$ <= 4.95 AND spetal width\$ <= 1.75 AND spetal length [Binned]\$ IN ("Bin 4", "Bi...	48.597	47
Row3	spetal width [Binned]\$ IN ("Bin 2", "Bin 3") AND spetal length\$ > 4.95 AND spetal width\$ <= 1....	3	3
Row4	spetal width [Binned]\$ IN ("Bin 1", "Bin 4", "Bin 5") AND spetal length\$ > 4.95 AND spetal width...	3.075	2
Row5	spetal width\$ > 1.75 AND spetal length [Binned]\$ IN ("Bin 4", "Bin 3", "Bin 2", "Bin 5") => "Iris-...	46	45

- Rule Engine (Dictionary)



Dialog - 2:1206 - Rule Engine (Dictionary)

Settings | PMML | Flow Variables | Job Manager Selection | Memory Policy

Rules column: S antecedent => S consequent

Append column Prediction

Replace column WebActivity

Errors

line	rule	error message
Row0	\$gender\$ = "M" => / "Male"/	Not a column: gender

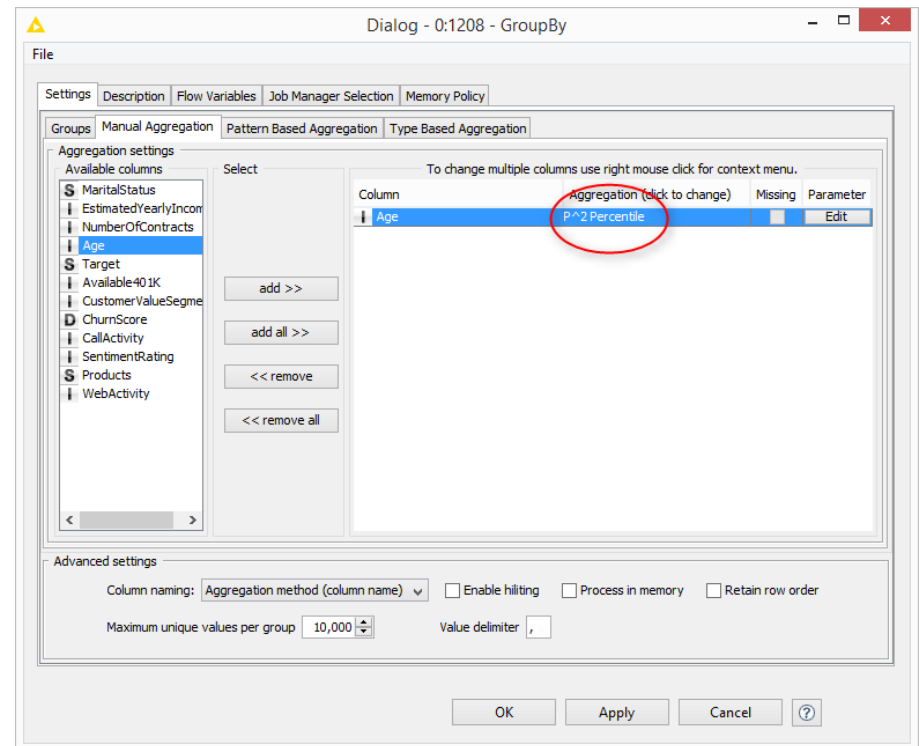
OK Apply Cancel ?

Analytics II

- Statistical measures in Group By node

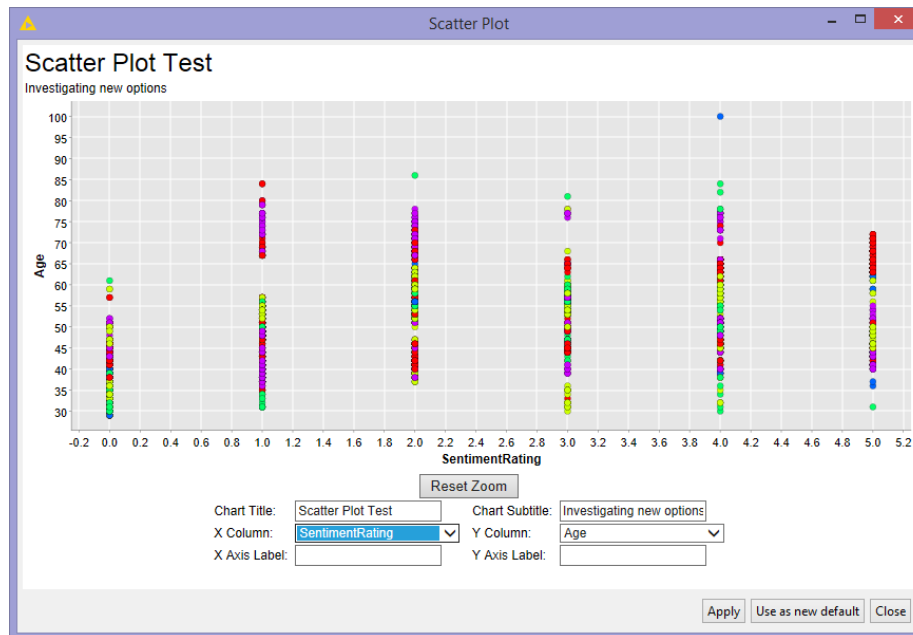
- More statistic nodes

- Statistics
 - Cronbach Alpha
 - Standardized Cronbach Alpha
 - Rank Correlation
 - Odds and Risk Ratios
 - Kruskal-Wallis Test
 - Wilcoxon Mann Whitney Test
 - Wilcoxon Signed-Rank
 - Linear Discriminant Analysis



Tool integration I

- JavaScript integration

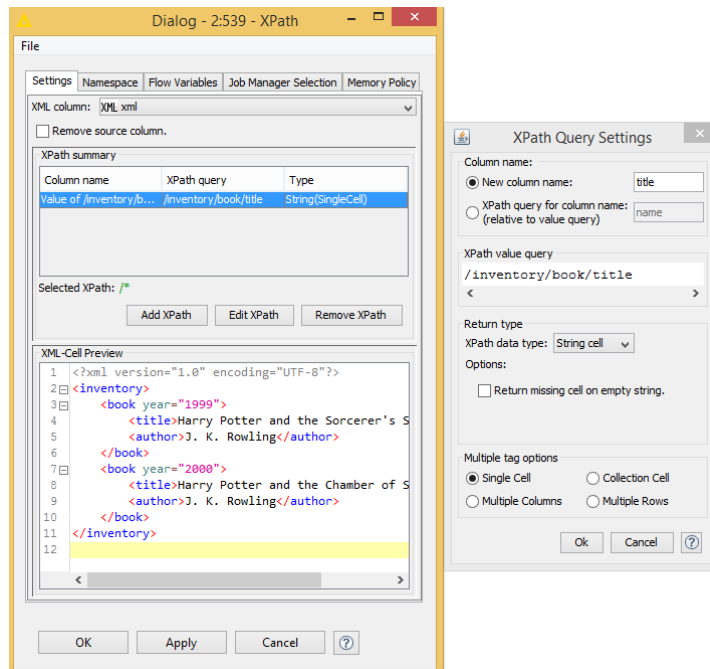


- MongoDB integration

- MongoDB
 - MongoDB Reader
 - MongoDB Remove
 - MongoDB Save
 - MongoDB Update
 - MongoDB Writer

Tool integration II













- More JSON nodes
- Extended XPath node



- JSON
- JSON Input
- JSON Output
- JSON Reader
- JSON Writer
- String to JSON
- Table to JSON
- JSON to Table
- Columns to JSON
- XML To JSON
- JSON To XML
- JSON Path
- JSON Path (Dictionary)
- JSON Column Combiner
- JSON Row Combiner
- JSON Row Combiner and Writer
- JSON Transformer
- JSON Schema Validator
- JSON Diff

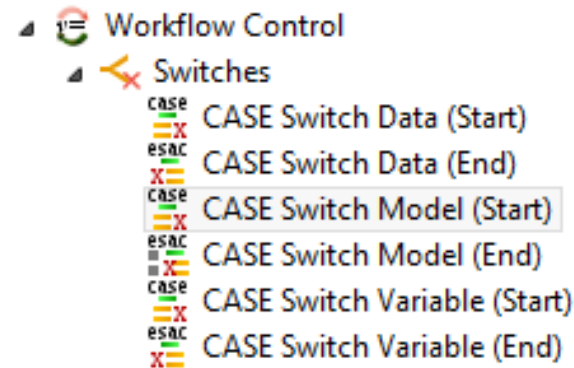
Tool integration III

- More Python nodes

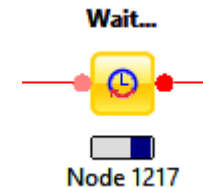
- ▾  Python
 -  Python Edit Variable
 -  Python Source
 -  Python Script
 -  Python Script (2:1)
 -  Python View
 -  Python Object Reader
 -  Python Object Writer
 -  Python Learner
 -  Python Predictor
 -  Python Script (DB)
 -  Python Script (Hive)

Misc

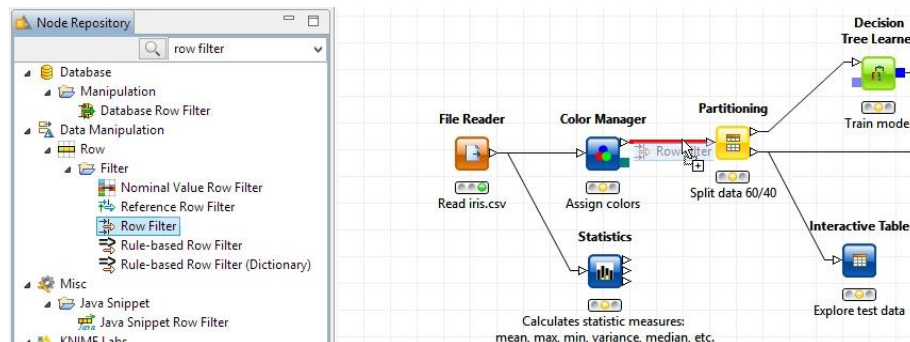
- New CASE Switch nodes



- New Sleep/Pause/Timer nodes
 - Shamelessly stolen from Vernalis



- Replacing and inserting nodes via drag&drop



KNIME Server and Automation I

- Basic REST interface
 - Repository browsing
 - Job execution

```
thor@crest ~ $ curl -X POST -u 'knime:knime' -i http://localhost:8080/com.knime.enterprise.server/rest/v4/jobs/1afee03d-1b13-41a7-a18a-a2c7b181b963?asyn
{
  "@controls" : {
    "knime:execute-job" : {
      "href" : "http://localhost:8080/com.knime.enterprise.server/rest/v4/jobs/1afee03d-1b13-41a7-a18a-a2c7b181b963{?async}",
      "isHrefTemplate" : true,
      "template" : {
        "json-input-1" : {
          "col0" : "A12",
          "col18" : "A191",
          "col19" : "A201",
          "target" : "2"
        }
      }
    },
    "type" : "application/json",
    "method" : "POST"
  }
},
  "id" : "1afee03d-1b13-41a7-a18a-a2c7b181b963",
  "isOutdated" : false,
  "hasReportRun" : false,
  "inputParameters" : {
    "json-input-1" : {
      "col0" : "A12",
      "col18" : "A191",
      "col19" : "A201",
      "target" : "2"
    }
  }
},
  "hasReport" : false,
  "state" : "IDLE",
  "name" : "/UGM 2015/REST Demo/Predictor Flow job 1afee03d-1b13-41a7-a18a-a2c7b181b963",
```

KNIME Server and Automation II

- WebPortal templates

COSMOS KNIME WEBPORTAL
Integrated *In Silico* Models for the Prediction of Human Repeated Dose Toxicity of COSmetics to Optimise Safety

Welcome to the COSMOS KNIME WebPortal

COSMOS is a unique collaboration addressing the safety assessment needs of the cosmetics industry, without the use of animals. The main aim of COSMOS is to develop freely available tools and workflows to predict the safety to humans following the use of cosmetic ingredients.

The models developed within COSMOS have been implemented into KNIME workflows. The KNIME Analytics Platform integrates access to chemical databases, data processing and analysis, modelling approaches, profiling of structures and calculation of properties in a flexible way.

The COSMOS KNIME WebPortal versions of these workflows allow users, not experienced with the software, to execute the workflows in a web browser, without local software installation required. The results are downloadable as pdf reports and other formats e.g. Excel sheets.

The models are documented and user guidance is available through [COSMOS Space](#). A list of all workflows available can be found [here](#).

Login

Username

Password

How to get your login

Registration is free. To get your login details from the COSMOS Space follow the following steps:

1. Visit <http://cosmospace.cosmostox.eu>
2. Click on Login
3. Click on register
4. Fill in your email address and choose a password.

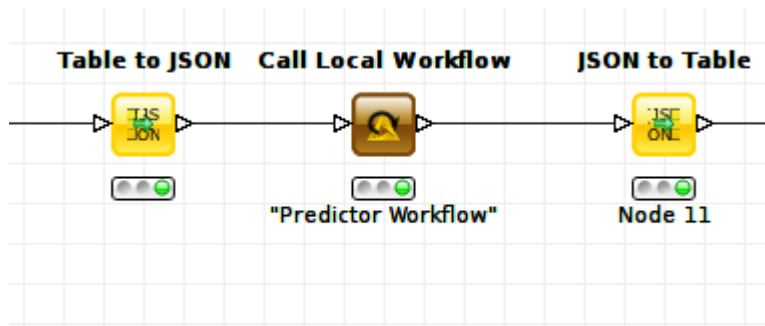
Running on KNIME Server version 4.1.0

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KNIME

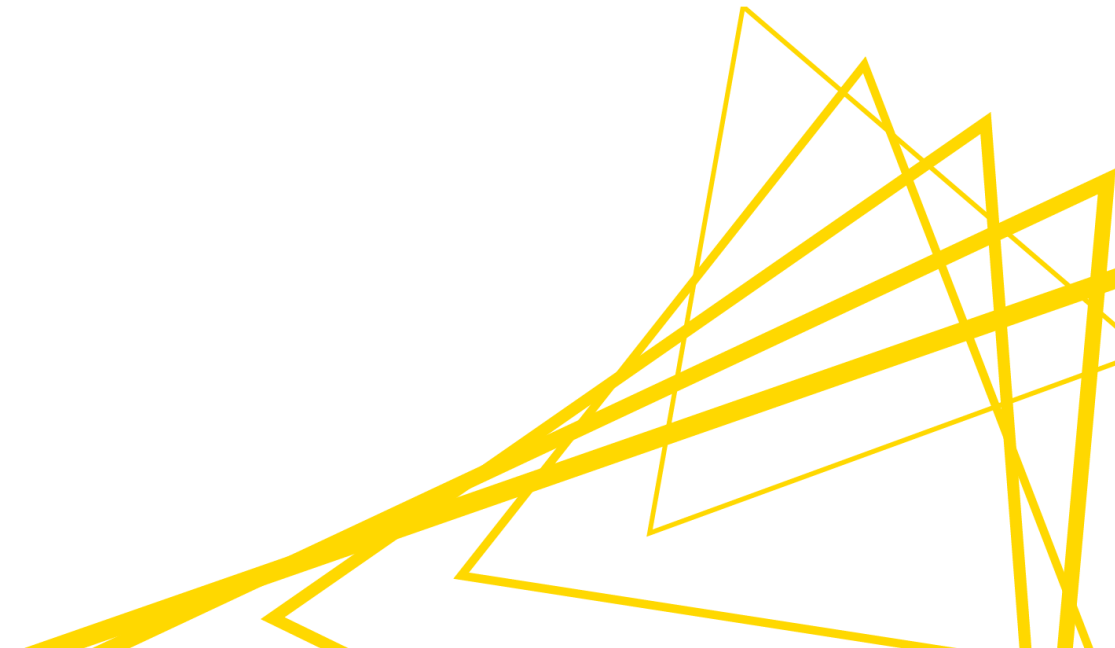
European Union
Horizon Europe
SEURAT-1

KNIME Server and Automation III

- Call Workflow nodes
 - Remote on server via REST interface
 - Locally



Cooking for 3.0



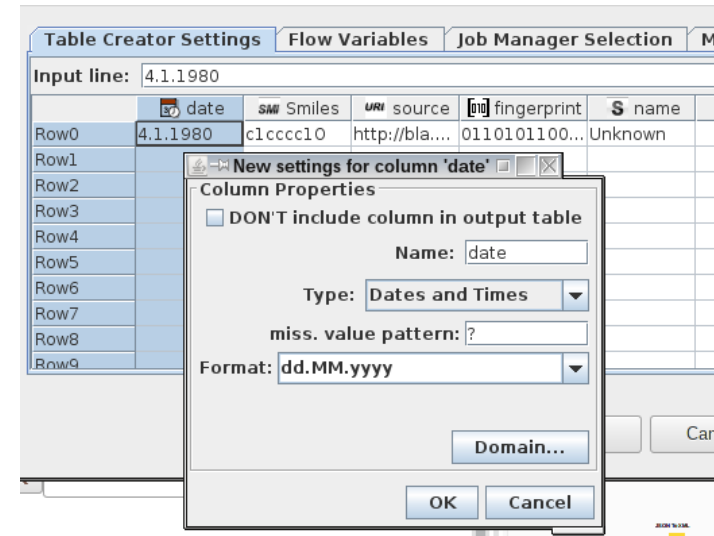
Internal changes I

- Update to Java 8
- Update to Eclipse 4.5
- Support for more than 2 billion rows
 - Nodes must be adapted to new API
- Deprecated flag for nodes in extension point
 - No need to remove deprecated node from extension point any more

Internal changes II

- Extension point for data types
 - Serializers registered via extension point
 - New data cell factories for use in input nodes

- Extension point for port objects
 - Serializers registered via extension point



Internal changes III

- Molecule readers now create adapter cells
 - SmilesAdapterCell, SdfAdapterCell, ...
 - Should have any noticeable effects
 - Molecule converters should simply add their representation to the existing adapter
 - Original format always visible

New Look&Feel

The screenshot displays the KNIME software interface with a workflow titled '*0: Community Contributions Usage'. The workflow consists of several nodes: RowID, Row Filter, Table Creator, Cell Replacer, Row Filter, RowID, Row Filter, Row Filter, Cell Replacer, Pivoting, and RowID. The workflow is connected to a 'Data to Report' node and a 'Line Plot' node. The 'Data to Report' node shows a table with columns for 'month=>row id' and 'total downloads'. The 'Line Plot' node shows a line graph with 'total downloads' on the y-axis and 'month=>row id' on the x-axis. The 'Row Filter' nodes have various filters applied, such as 'remove scripting core', 'remove experimental stuff', and 'feature id => feature name'. The 'Cell Replacer' node has a filter 'feature id => feature name'. The 'Pivoting' node has a filter 'by month & feature name'. The 'RowID' nodes have filters 'month=>row id' and 'month => row id'. The 'Table Creator' node has a filter 'feature id => feature name'. The 'Row Filter' node (Node 36) has a warning icon and the text 'No row filter specified'. The 'Node Description' panel on the right is empty. The 'Node Repository' panel on the left shows a search for 'row fi' and a list of nodes under 'Database', 'Data Manipulation', and 'Misc'. The 'Console' panel at the bottom shows the warning message: 'WARN Row Filter 0:36 No row filter specified'. The status bar at the bottom right shows '383 of 1134M'.