Workflow Mining:

Identification of frequent patterns in a large collection of KNIME workflows

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Overview

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- Motivation
  - History & current status
  - Why “Workflow Mining”?
- “Static Workflow Mining”
  - Extraction of workflow graphs
  - Frequent sub-graph mining
  - Results
- “Dynamic Workflow Mining”
  - KNIME Profiler Plugin
  - Analysis of profiling logs
- Conclusions and Outlook

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History

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- 2009
  - First look at KNIME, decision to perform in-depth evaluation
  - Identification of critical functional gaps
  - Inhouse developer training
  - Start of collaboration with KNIME.com
- 2010
  - Implementation of missing nodes, integration of various external chemistry tools
  - Licensing of additional node collections from commercial vendors
  - Migration of deployed workflows (e.g. QSAR-models for ADME parameters)
- 2011
  - Migration of end-users from computational chemistry
  - Inhouse end-user trainings
  - Extension of user base to other groups (e.g. computational biology, IS, HTS)

Development of KNIME usage

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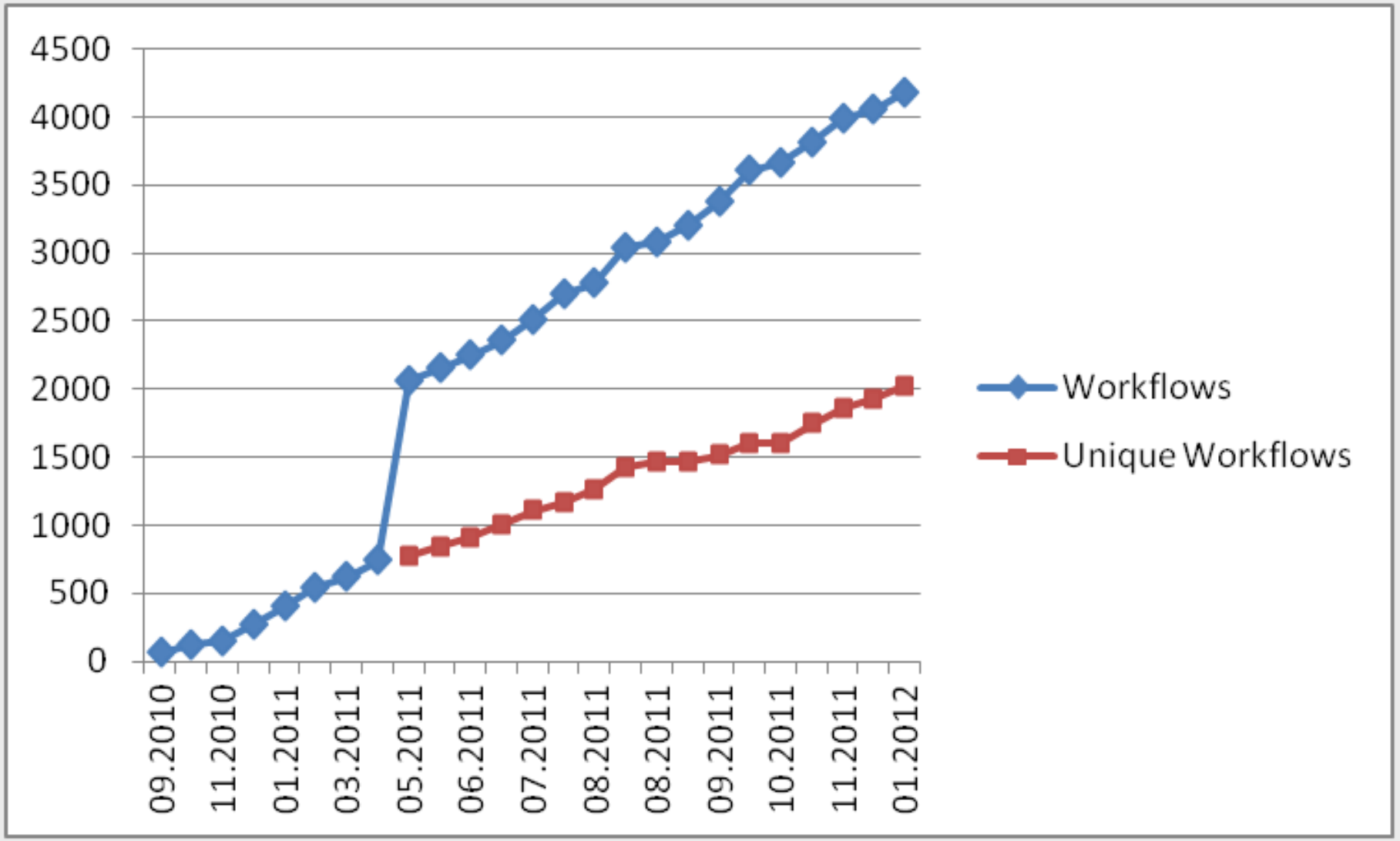

Current status

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- A significant group of end-users is applying KNIME on a regular / daily basis
  - Consistently more than 100 new, unique workflows are created per month
  - Significant exchange and sharing of workflows among users

- A lot of feedback from end-users
  - Bug reports
  - Feature requests
  - How do I …
  - …

- Collecting feedback is simple, but …
  - … how to prioritize feature requests ?
  - … what are best practices / common pitfalls / bottlenecks ?

Use data mining to support decisions!

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- Difficult to assess significance of requests in a growing and diverse user community
  - Many different application scenarios
  - How are our users actually using KNIME?
  - Different people solve the same problem in a different way!
  - Which nodes are really important?

- Identify key users to cover diversity in user community
  - Still, a lot of gut feeling involved

- Analyze existing workflow collection to get reliable usage statistics

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Extraction of useful descriptors from KNIME workflows

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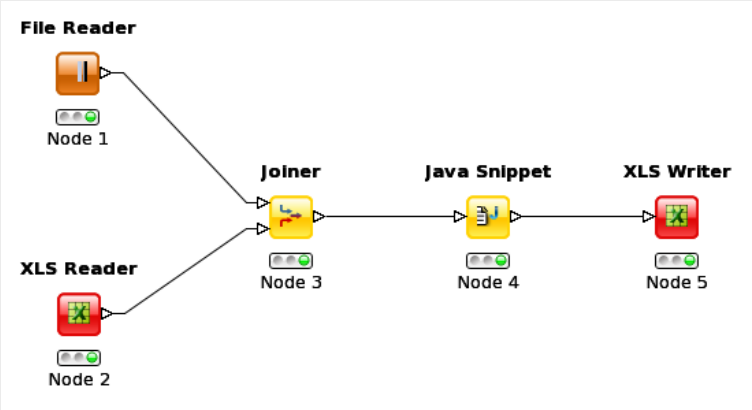

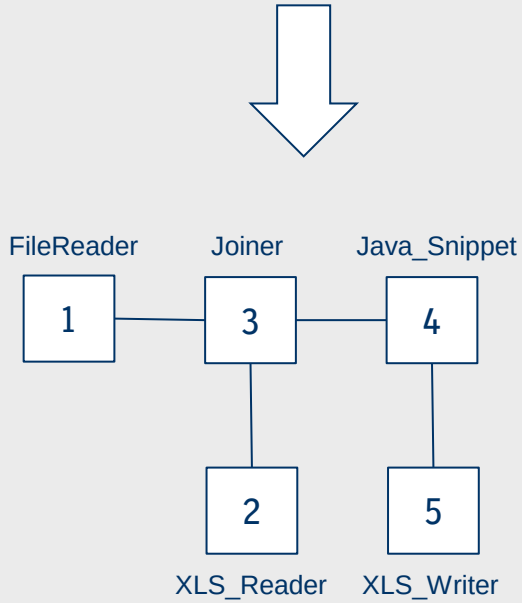

- KNIME workflows are stored in a generic XML format
- A simple parser extracts the **workflow graph**:
  - Nodes
  - Connections
- The analysis discards:
  - Node configuration / labels
  - Connection type / direction
  - Workflow layout
  - Workflow annotations
  - Personal information
  - …

Frequent sub-graph mining

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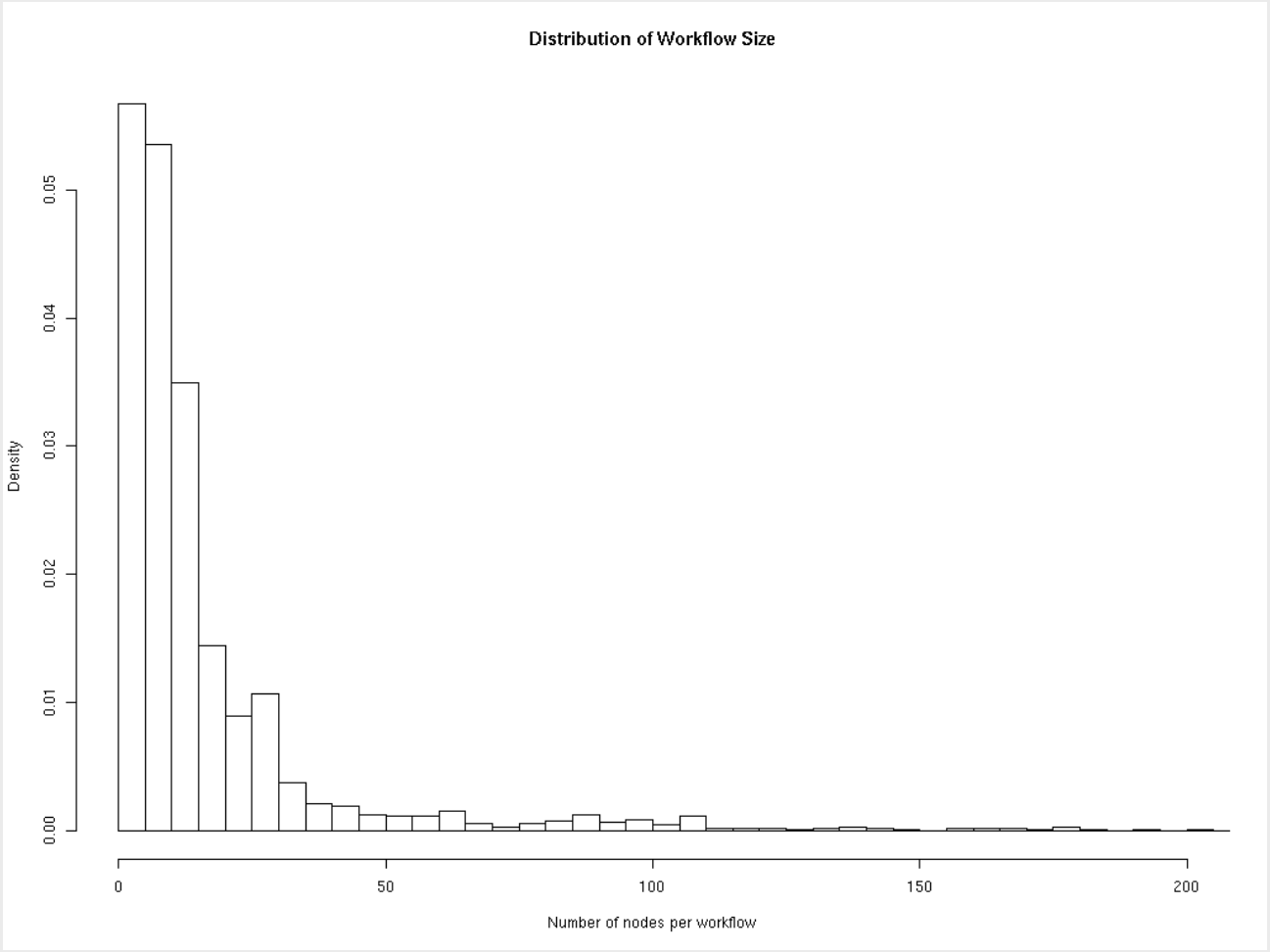
- What is frequent sub-graph mining?
  - Problem: Given a database of (labeled) graphs **G** = $\{G_1, ..., G_n\}$ return all (connected) sub-graphs **S** = $\{S_1, ..., S_k\}$ occurring at least **x** times in **G**.
  - Related to frequent item set mining & association rule mining
  - Many applications in the life-sciences
    - Chemical structures
    - Biological networks
    - …
  - Different algorithms and implementations available
    - MoSS node in KNIME for chemical data
    - …

Dataset

- Using all workflows from central installation (~4.000 as of 2012-01-10)
- 3.899 workflows were parseable and non-empty
- 64.357 nodes
- 62.841 connections



Results – Top 10 nodes

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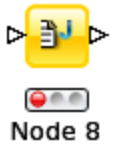
Java Snippet



9907

GroupBy

5275

Joiner

4534

Rename

4290

Row Filter

4144

Column Filter

3326

File Reader

1720

DB Open v1

1707

Sorter

1628

Java Edit Variable

1570

Results – Top 11-20 nodes

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Table Reader  Node 4	1567
Concatenate  Node 9	1267
Table Writer  Node 5	1212
Metanode  Node 5	1136
DB PreparedQuery v1  Node 2	1051
Reference Row Filter  Node 1	893
Double To Int  Node 17	882
DB MethodsView v1  Node 8	790
JPython Script 1:1  Node 3	683
DB Query v1  Node 6	660

Results – Workflow patterns with 10% support (selection)

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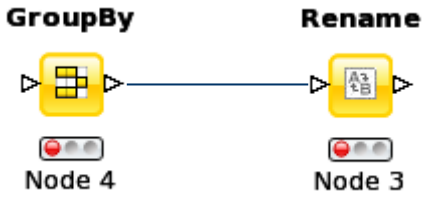
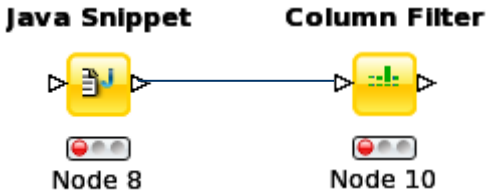
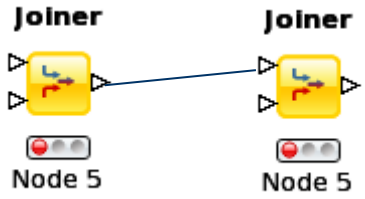
- Allow addition of multiple columns in Java Snippet ?
- Collaboration with KNIME.com



- Allow for more flexibility in column naming / typing ?



- Make users aware of “Replace columns” option



- Allow joining multiple input tables? (e.g. “Joiner (optional in)”)

Results – Workflow patterns with 7.5% support (selection)

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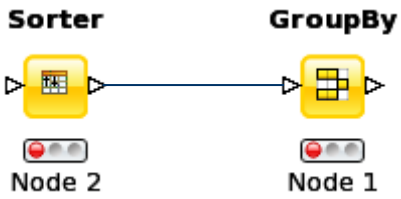

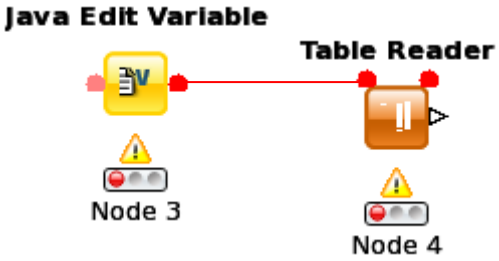

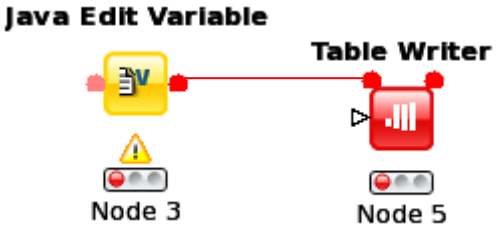

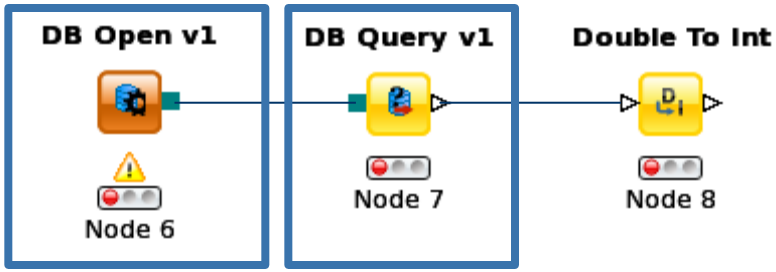

- Issues with sorting stability until v2.3.4 (Bug 2682)
- Develop a concept for simple and efficient data transfer among related workflows?
- Improve column typing in inhouse database integration

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Static vs. dynamic workflow analysis

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- Collection consists mainly of ad hoc-workflows
  - On average, only few executions per workflow
  - Non-interactive batch processes responsible for most workflow executions (20.000.000+ property predictions over the last 12 months)
  - Static analysis of all stored workflows might yield biased results

- No insights into bottlenecks and performance issues
  - Influence of different implementations for the same node
  - Improvements of the KNIME framework

- Limited ability to capture influence of “control flow” constructs
  - Include or exclude inactive branches in analysis?
  - How to handle loops?

KNIME Execution Profiler Plugin
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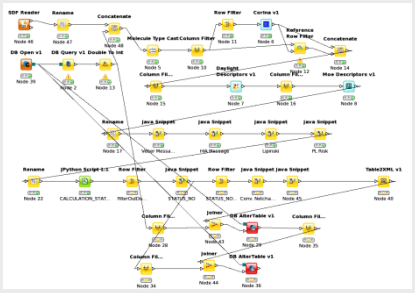

Timestamp	Workflow Path	Node Name	Node Index	Custom Name	State
2011-11-12;06:45:54.662		<Metanode>	0	Node 0	EXECUTED
2011-11-12;06:45:54.670		<Metanode>	0	Node 0	CONFIGURED
2011-11-12;06:45:55.237	PROP4	DB Open v1	39	Node 39	IDLE
2011-11-12;06:45:55.240	PROP4	DB Open v1	39	Node 39	CONFIGURED
2011-11-12;06:45:55.262	PROP4	SDF Reader (deprecated)	46	Node 46	IDLE
2011-11-12;06:45:55.317	PROP4	SDF Reader (deprecated)	46	Node 46	CONFIGURED
2011-11-12;06:45:55.372	PROP4	DB Query v1	2	Node 2	IDLE
2011-11-12;06:45:55.706	PROP4	DB Query v1	2	Node 2	CONFIGURED
2011-11-12;06:45:55.751	PROP4	Rename	47	Node 47	IDLE
2011-11-12;06:45:55.757	PROP4	Rename	47	Node 47	CONFIGURED
2011-11-12;06:45:55.761	PROP4	Double To Int	13	Node 13	IDLE
2011-11-12;06:45:55.764	PROP4	Double To Int	13	Node 13	CONFIGURED
2011-11-12;06:45:55.769	PROP4	Concatenate	48	Node 48	IDLE
2011-11-12;06:45:55.774	PROP4	Concatenate	48	Node 48	CONFIGURED
2011-11-12;06:45:55.778	PROP4	Column Filter	28	Node 28	IDLE
2011-11-12;06:45:55.779	PROP4	Column Filter	28	Node 28	CONFIGURED
2011-11-12;06:45:55.790	PROP4	Molecule Type Cast	5	Node 5	IDLE
2011-11-12;06:45:55.793	PROP4	Molecule Type Cast	5	Node 5	CONFIGURED
2011-11-12;06:45:55.797	PROP4	Column Filter	10	Node 10	IDLE
2011-11-12;06:45:55.798	PROP4	Column Filter	10	Node 10	CONFIGURED
2011-11-12;06:45:55.807	PROP4	Row Filter	11	Node 11	IDLE
2011-11-12;06:45:55.807	PROP4	Row Filter	11	Node 11	CONFIGURED
2011-11-12;06:45:55.868	PROP4	Corina v1	6	Node 6	IDLE
2011-11-12;06:45:55.876	PROP4	Corina v1	6	Node 6	CONFIGURED

- Collected execution profiles for 10.000+ non-interactive batch runs
- Not used in interactive sessions, no monitoring of end-user behavior

Visualization – Gantt chart

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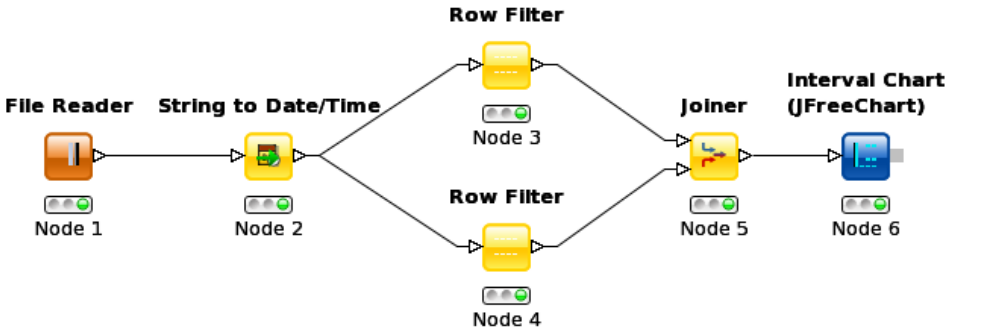

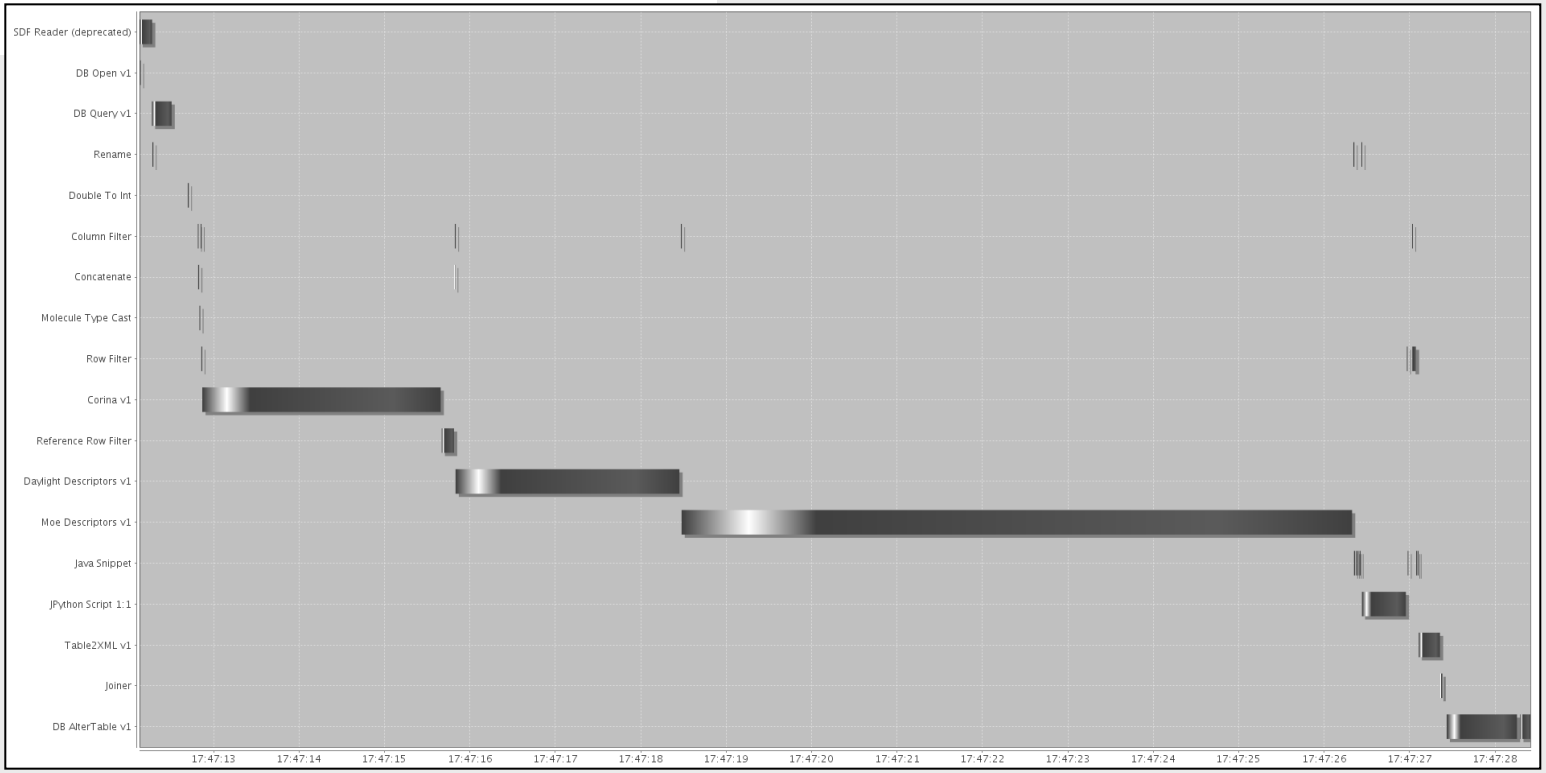

Results – Top 10 nodes (by number of executions)

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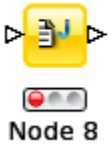
Java Snippet  Node 8	161.824	**Row Filter**  Node 11	37.590
Column Filter  Node 10	65.282	**GroupBy**  Node 4	25.774
Rename  Node 3	41.138	**Reference Row Filter**  Node 1	24.773
Joiner  Node 5	40.672	**Double To Int**  Node 8	21.351
JPython Script 1:1  Node 3	38.530	**Concatenate**  Node 9	19.952

Results – Top 10 nodes (by consolidated runtime)

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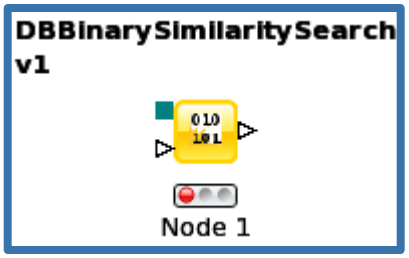

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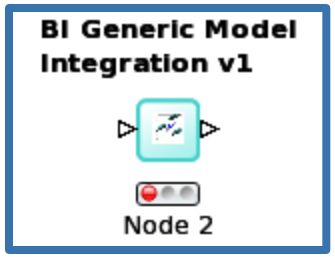

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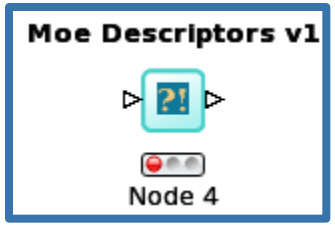

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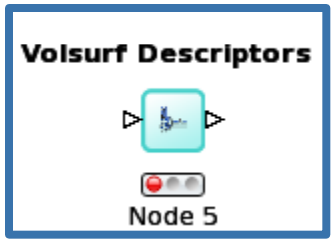

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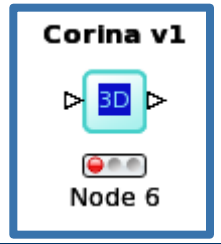

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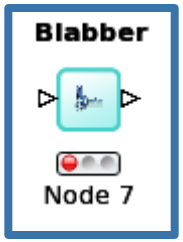

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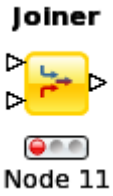

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Conclusions and Outlook

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- "Static Workflow Mining" serves as a tool to identify typical patterns in KNIME workflows
  - Supports prioritization of bug reports / feature requests
  - Identification of best practices and common pitfalls
  - Plans to provide useful Metanodes based on frequent patterns

- "Dynamic Workflow Mining" monitors workflow behavior under real-world conditions
  - Identification of bottlenecks and critical steps in workflows
  - Performance optimizations for batch-processes planned
  - Additional option to perform real-time monitoring of system health

- Large workflow collection an asset, but also a burden
  - Have to ensure compatibility of new node versions

Acknowledgements

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