Visual Workflows for Pushing Data Literacy

Dr. Stefan Helfrich (KNIME GmbH)

January 27, 2021

KNIME in a Nutshell

- KNIME, the Company
  - Offices in Europe and USA
  - Close ties to Universities and Research
  - Global Partners Network
  - Long-term funding

- KNIME Software
  - Used by 96% of EUROSTOXX 50 and DOW JONES Indu companies

- KNIME Analytics Platform
  - Gather, Wrangle, Model, Visualize
  - Open source and free

- KNIME Server
  - Deploy, Manage, Consume, Optimize
  - Commercial complement

KNIME Software – One Ecosystem

Create

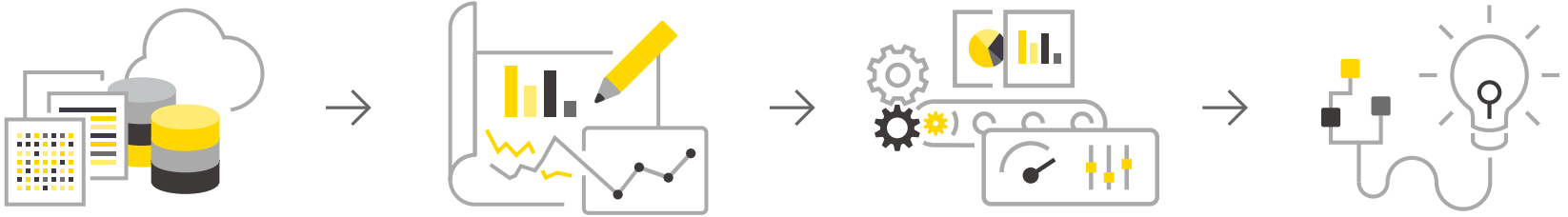
Productionize

Blend & Transform

Model & Visualize

Deploy & Manage

Consume & Interact



KNIME Analytics Platform

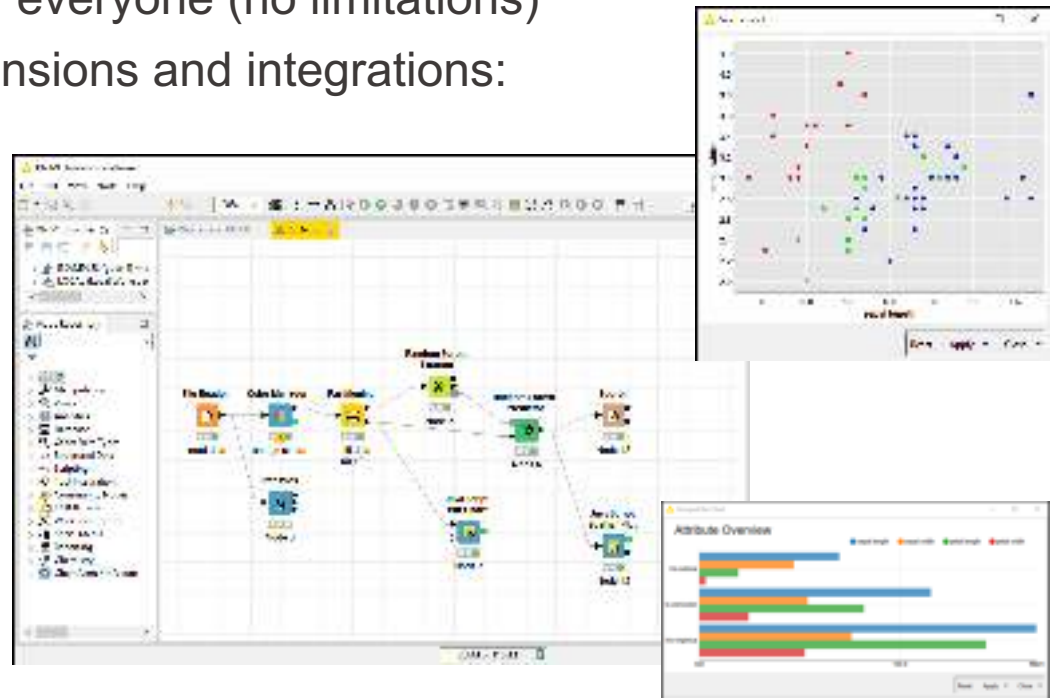
- KNIME Extensions
- KNIME Integrations
- Community Extensions
- Partner Extensions

KNIME Server

- Team Collaboration
- End User Applications
- API Services
- Managed Execution

What is KNIME Analytics Platform?

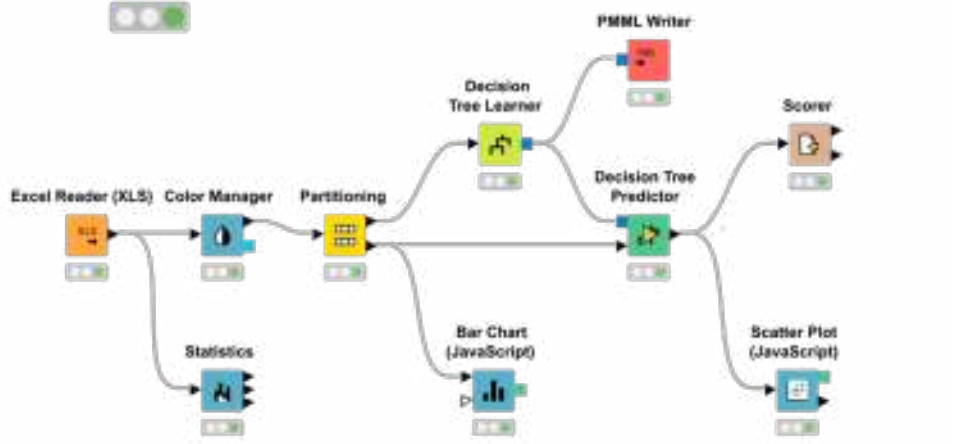
- A platform for data analysis/mining, manipulation, visualization, ML and AI
- Build around **visual workflows** (what you see is what you run)
- Open source and free to use for everyone (no limitations)
- Provides a diverse array of extensions and integrations:
  - Text Mining
  - Network Mining
  - Cheminformatics
  - Image Mining
  - Other Tools: Weka, Keras, H2O, …
  - Other Languages: R, Python,



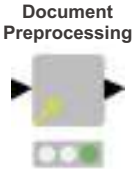
Visual KNIME Workflows

Nodes
perform tasks on data

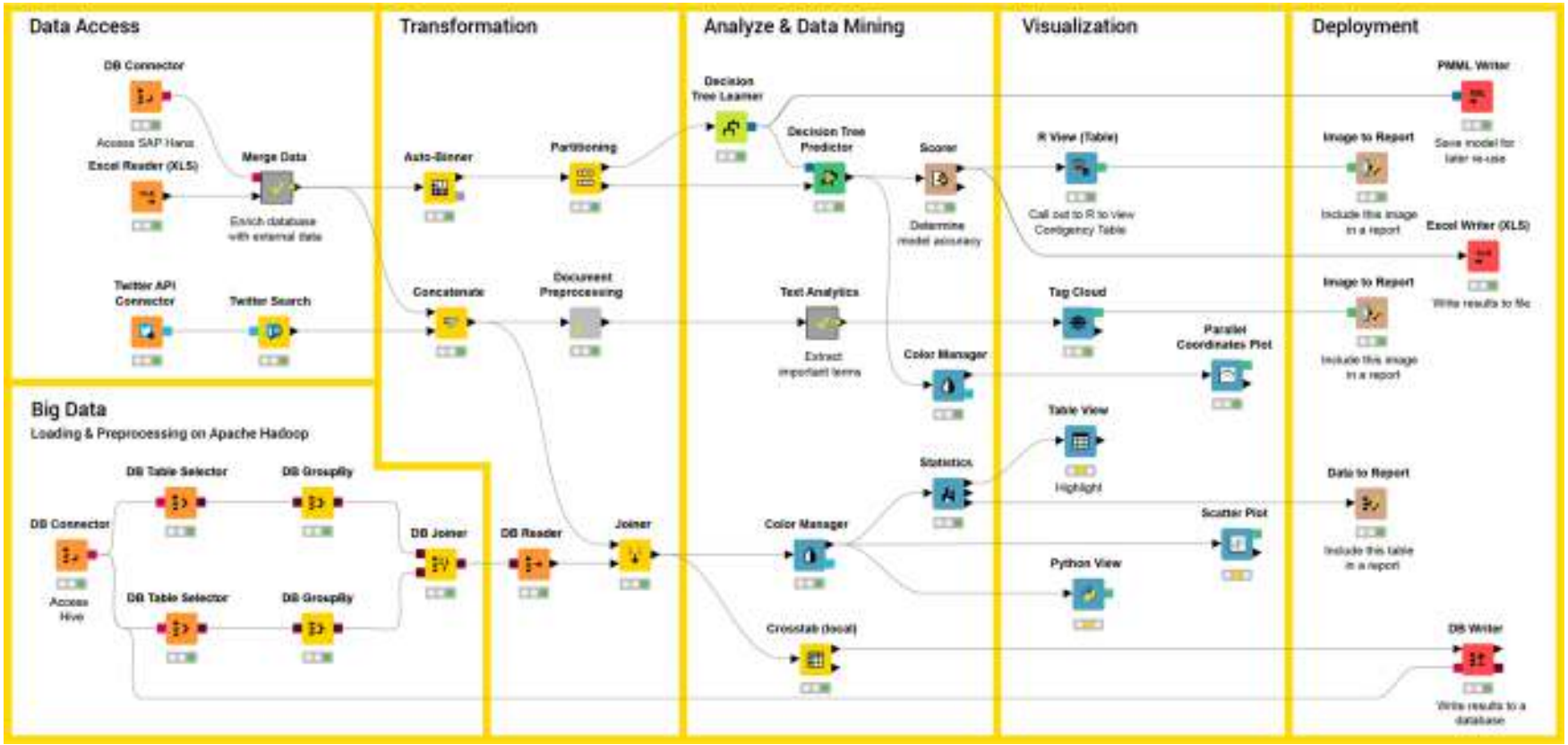
Workflows
combine nodes to model data flow



Components
encapsulate complexity & expertise



Covering all Stages of the Data Science Life Cycle



Open for Innovation KNIME

KNIME in Research

A **KNIME** Workflow for Automated Structure Verification

JA Lumley, G Sharman, T Wilkin... - ..., the Science of Drug ..., 2020 - journals.sagepub.com

Adequate characterization of chemical entities made for biological screening in the drug discovery context is critical. Incorrectly characterized structures lead to mistakes in the interpretation of structure–activity relationships and confuse an already multidimensional ...

☆ 99 Cited by 4 Related articles All 3 versions

[HTML] Integration of the ImageJ Ecosystem in **KNIME** Analytics Platform

C Dietz, CT Rueden, S Helfrich, ETA Dobson... - Frontiers in Computer ..., 2020 - frontiersin.org

Open-source software tools are often used for analysis of scientific image data due to their flexibility and transparency in dealing with rapidly evolving imaging technologies. The complex nature of image analysis problems frequently requires many tools to be used in ...

☆ 99 Cited by 3 Related articles All 2 versions ≫

[PDF] Data Analytics and Visualization Techniques of Corona Impact

A Pankh, S Shah, V Bhatt - researchgate.net

... We have taken around 1.5 million points to plot the graphs over the data analytic tools based on python and **Knime**. Keywords - Data Analytic, Python, **Knime**, Coronavirus visualization, descriptive analytic, machine learning prediction, Linear regression 1. Introduction ...

☆ 99 All 3 versions ≫

[PDF] Speech Signal Analysis and Classification of Dominant Parameter for Pathological Voices

W Christina Subiksha, A Nandhini, KP Bharath... - researchgate.net

... The secondary objective is the classification of the voice signal into normal and abnormal voice samples using the machine learning software Konstanz Information Miner (**KNIME**) ... For classification of voice signal to be normal or abnormal, the **Knime** software is used ...

☆ 99 ≫

Five years of the **KNIME** vernalis cheminformatics community contribution

SD Roughley - Current medicinal chemistry, 2020 - ingentaconnect.com

Since the official release as a **KNIME** Community Contribution in June 2013, the Vernalis **KNIME** nodes have increased from a single node (the 'PDB Connector'node) to around 126 nodes (November 2017; Version 1.12. 0); furthermore, a number of nodes have been ...

☆ 99 Cited by 6 Related articles All 3 versions

Data Analysis and Application of Retail Enterprises Based on **Knime**

X Pu, N Qi, J Huang - MS&E, 2020 - iopscience.iop.org

With the rapid development of information technology, the application of cross-discipline has shown explosive growth. Data mining, big data and other technologies are rapidly entering all walks of life. Research on data mining technology and its application in data analysis of ...

☆ 99 Related articles All 2 versions

[PDF] Hitachi Materials Informatics Analytics Platform Assisting Rapid Development.

Y Osakabe, A Asahara, H Morita - AAAI Spring Symposium: Combining ..., 2020 - ceur-ws.org

... Second, upload them to the MIAP database. MIAP automatically converts files with different formats into a predetermined format using **KNIME**, the open source Figure 2: Screen capture of checking learning results software (**KNIME** 2019) ...

☆ 99 Related articles ≫

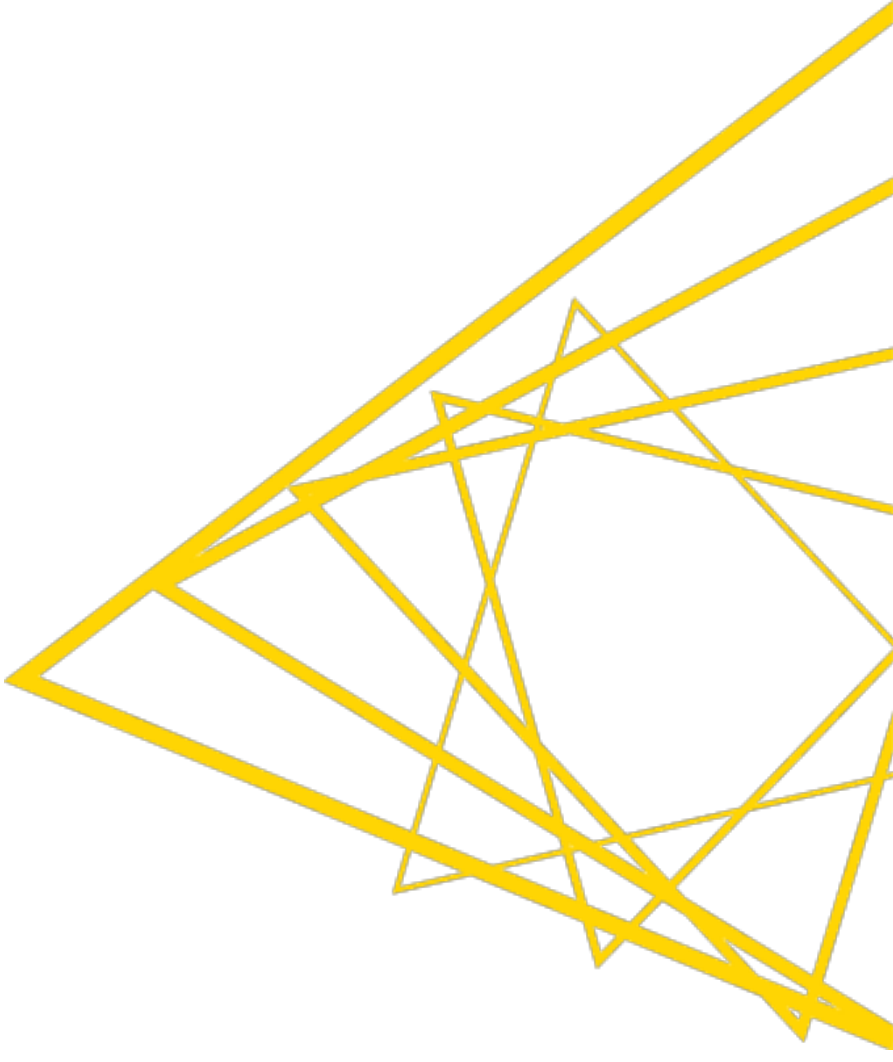
[PDF] AI supported Topic Modeling using **KNIME**-Workflows.

J Al Qundus, S Peikert, A Paschke - Qurator, 2020 - pdfs.semanticscholar.org

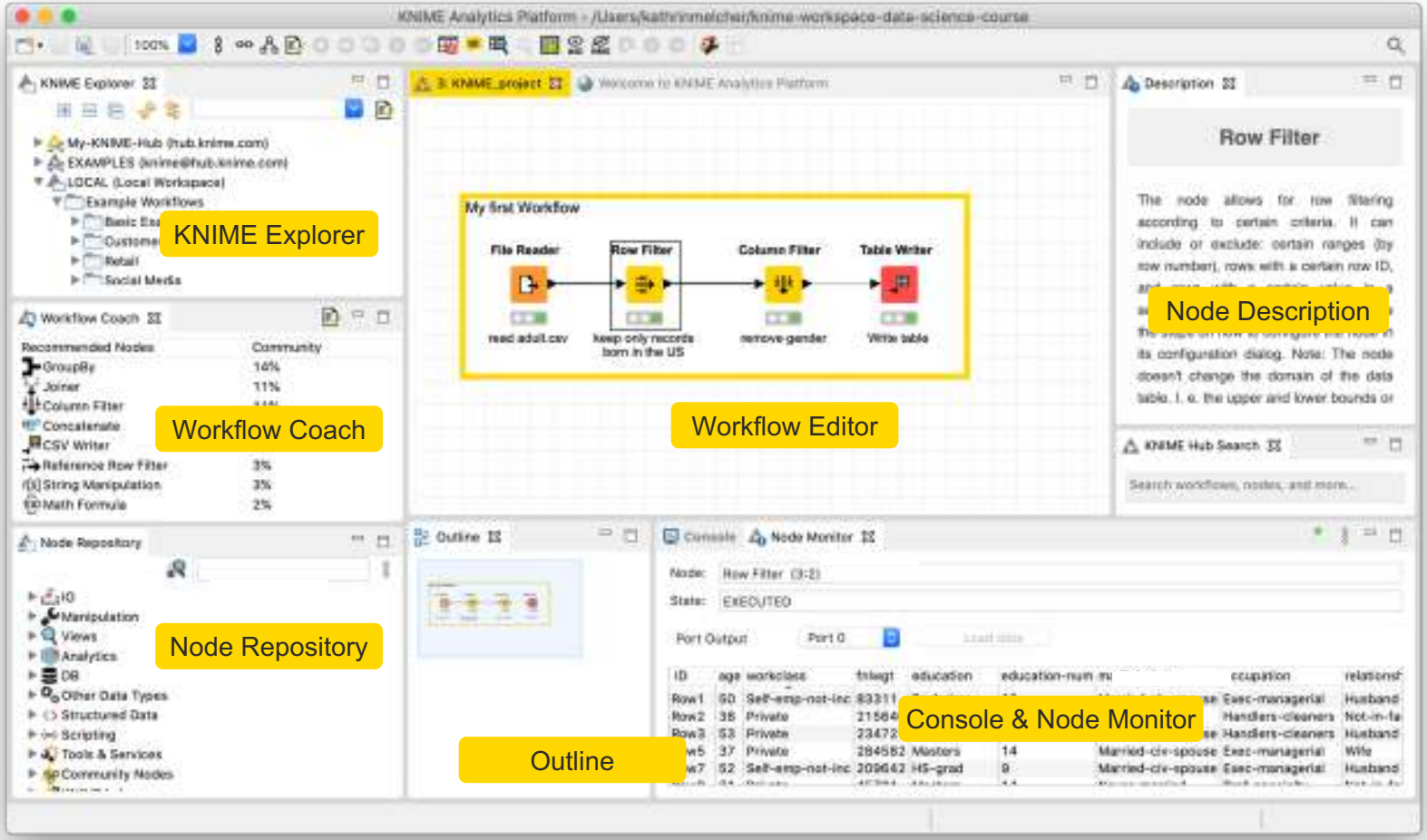
Topic modeling algorithms traditionally model topics as list of weighted terms. These topic models can be used effectively to classify texts or to support text mining tasks such as text summarization or fact extraction. The general procedure relies on statistical analysis of term ...

☆ 99 Cited by 1 Related articles All 4 versions ≫

Let’s Take a Look at KNIME (Demo)



The KNIME Analytics Platform Workbench

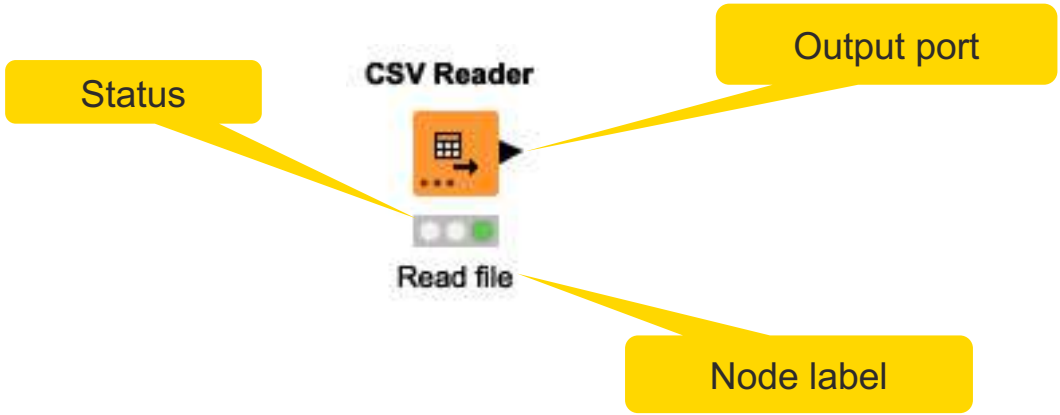


Importing Data and File Handling

Data Source Nodes

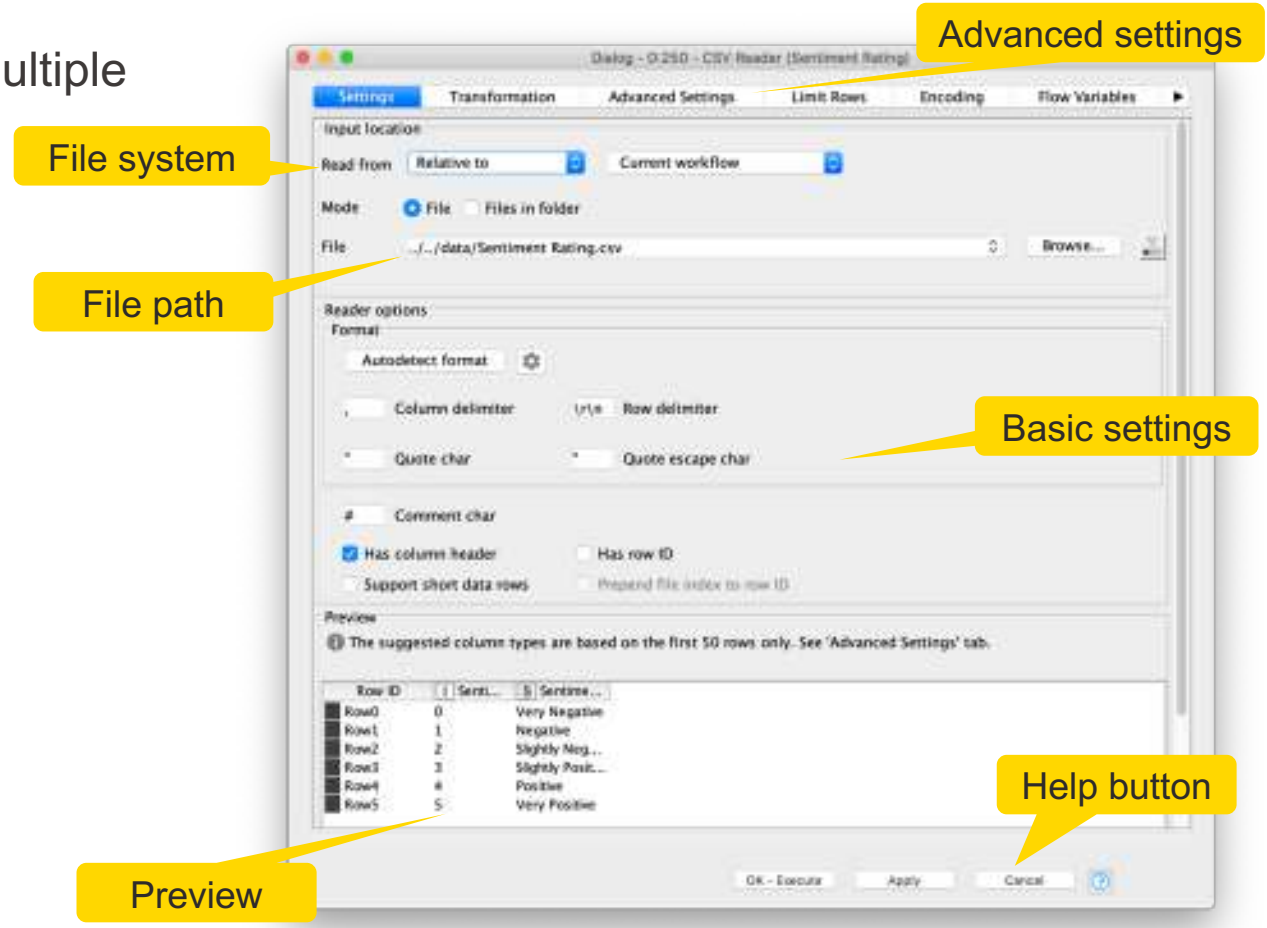
Typically characterized by:

- Orange color
- By default no input ports, 1-2 output ports
- Consistent UX across all nodes and files systems (ongoing work)
- Able to manage various file systems within the same workflow



CSV Reader

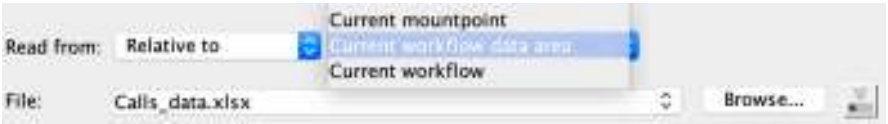
- Reads either one or multiple .csv and .txt files
- Further tabs to
  - limit the rows
  - select encoding



Default File Systems

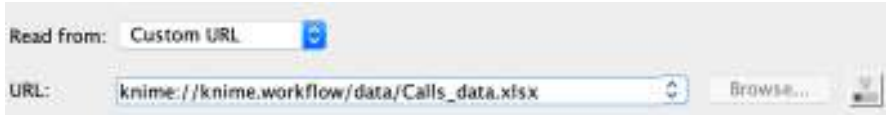
- **Local File System**

- **Relative to …**



- **Mountpoint**

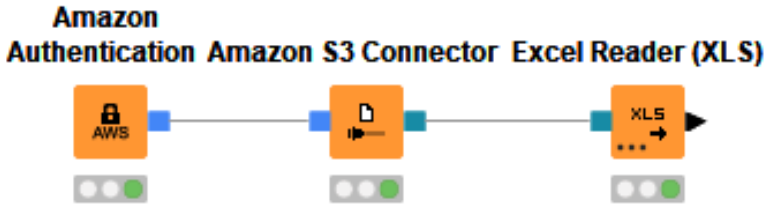
- **Custom URL**

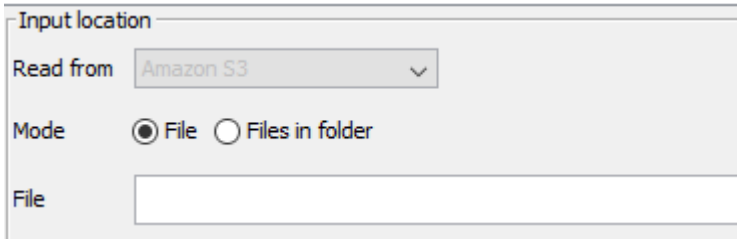


Connecting to other File Systems

- Add file system connection port to connect to another file system
  - Click on the three dots on the lower left to add or remove a dynamic port.

- Supported file systems
  - Microsoft Azure
  - Google
  - Amazon
  - Databricks
  - BigData file systems (hdfs, httpFS, …)
  - On-premise (e.g. ssh, ftp, …)

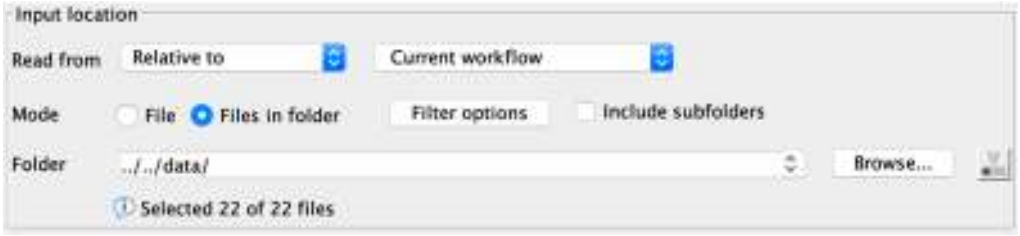




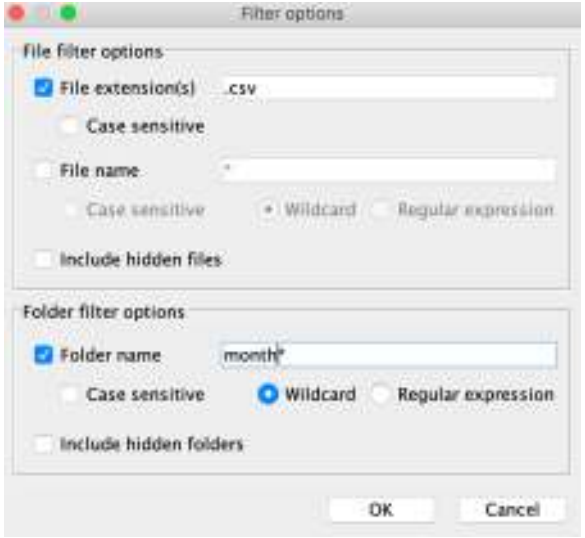
Read Single or Multiple Files

- Single file

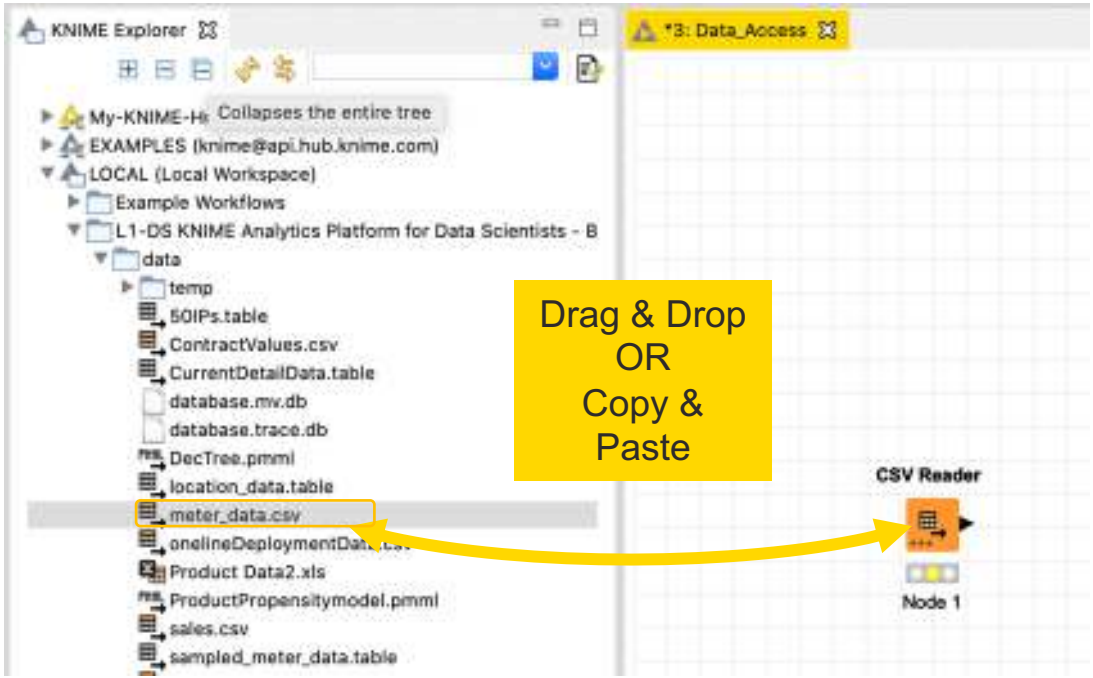
- Files in a folder



  - Option to include subfolder
  - Option to define filter criterions

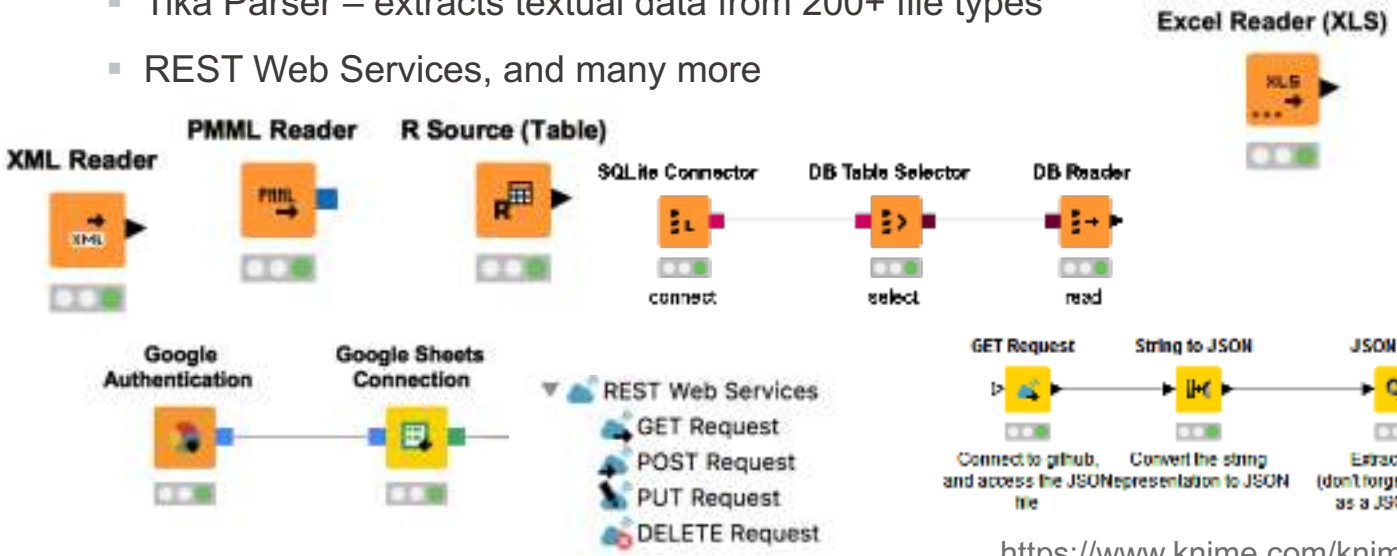


Alternative Faster Way …



Other Useful Data Sources

- KNIME Analytics Platform provides many more options to access data:
  - PMML Reader – reads standard predictive models
  - XML Reader with XPATH support
  - Python/R Source nodes
  - Tika Parser – extracts textual data from 200+ file types
  - REST Web Services, and many more

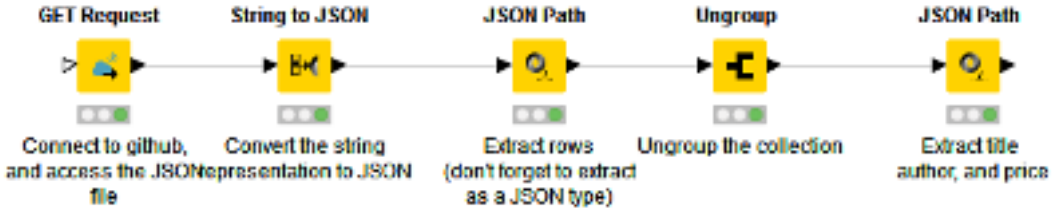


https://www.knime.com/knimepress/download-will-they-blend

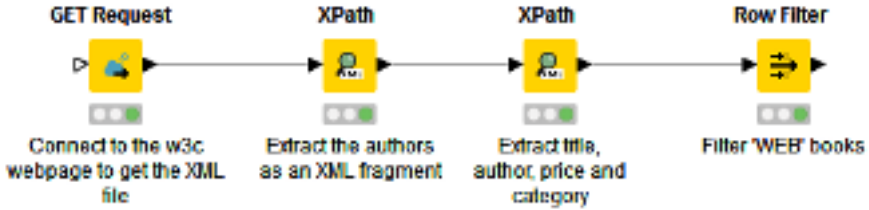
RESTful Web Services

- Use KNIME nodes to interact with RESTful web services
- Send requests using standard HTTP methods

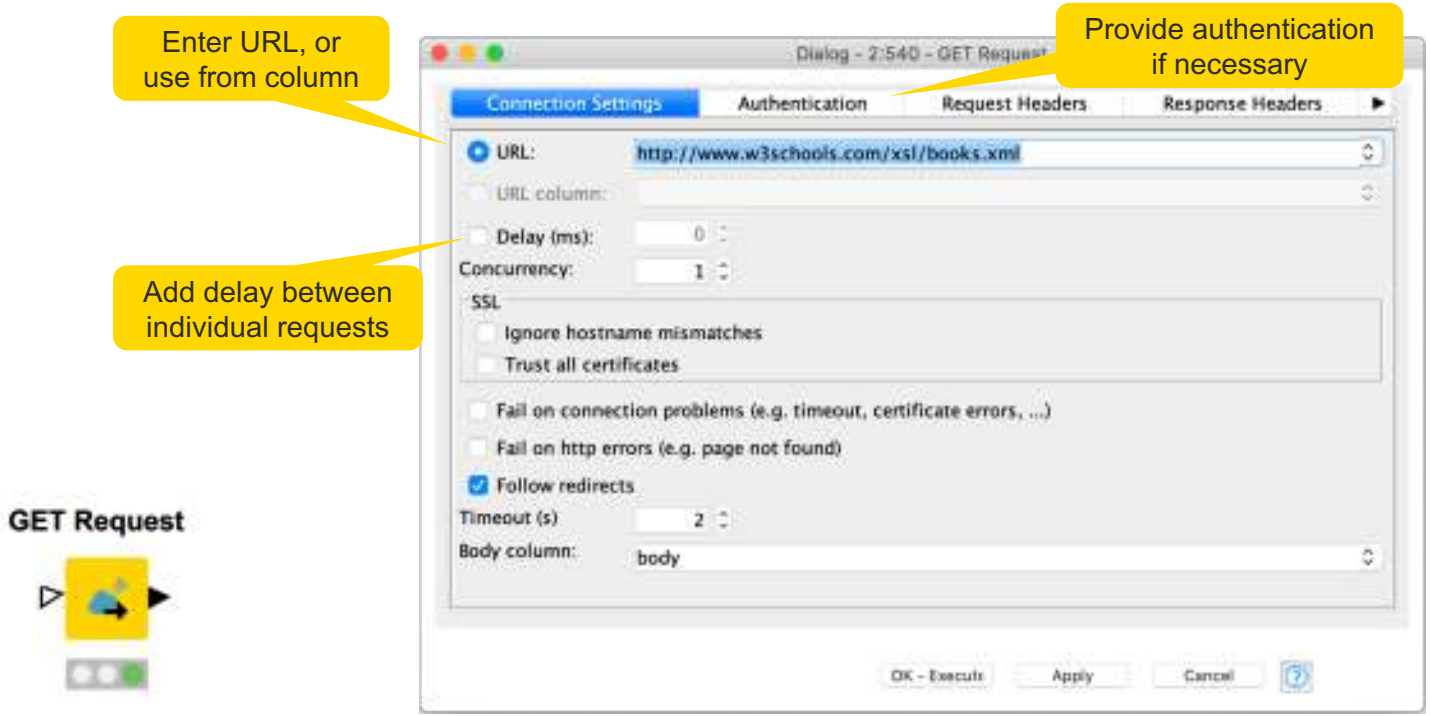
JSON Response:



XML Response:



RESTful Web Services

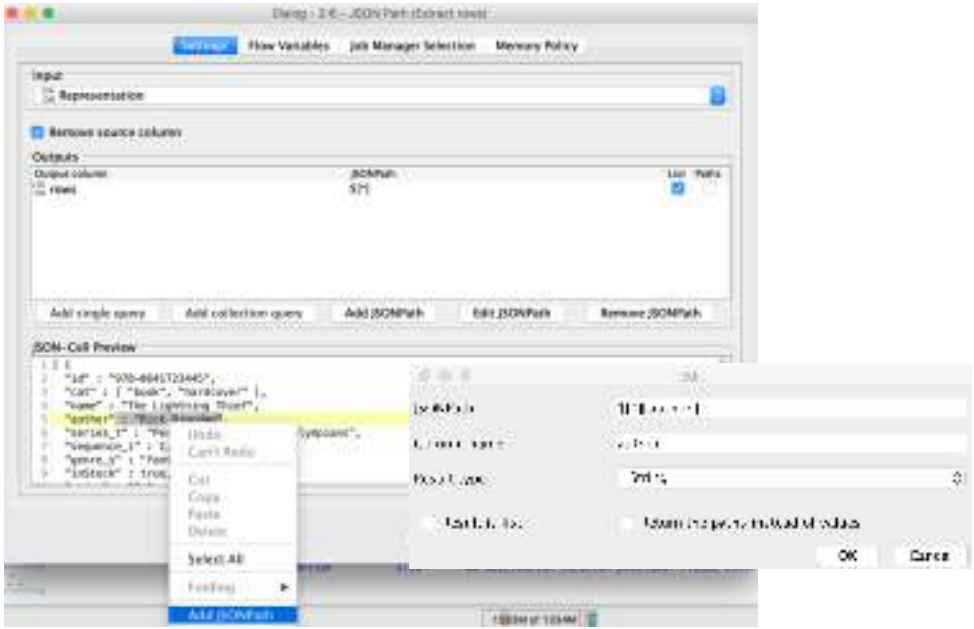


https://www.knime.com/blog/a-restful-way-to-find-and-retrieve-data

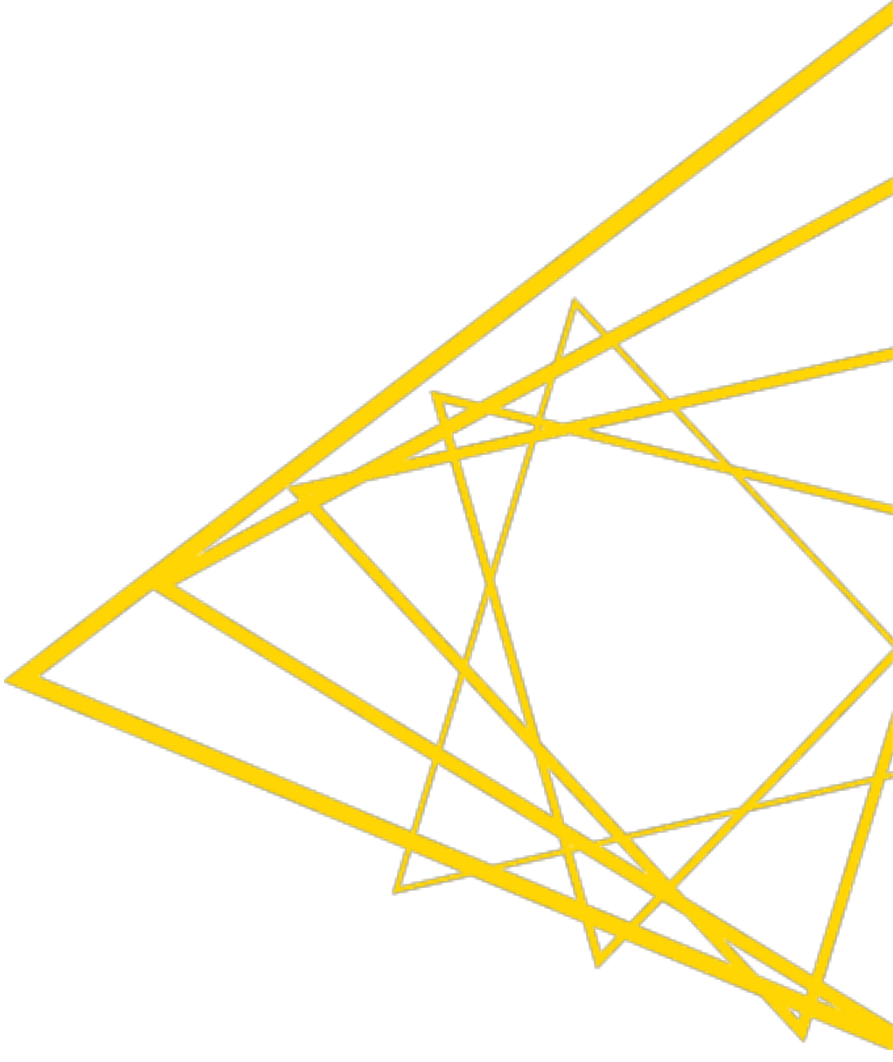
https://www.knime.com/blog/OSM-meets-CSV-file-and-Google-API

JSON Reader and JSON Path nodes

- Use the JSON Reader (or GET Request) node to get a JSON cell
- Use the JSON Path node to query the JSON file and extract parameters
- Editor window simplifies construction of JSON queries by auto-generating them (click on properties)

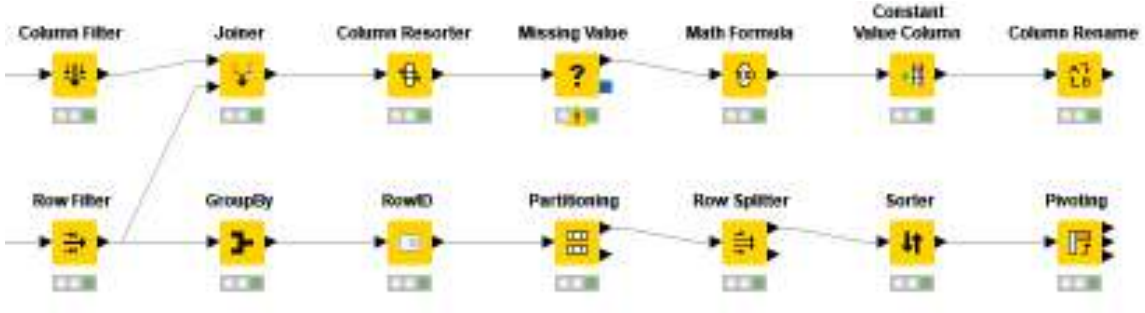


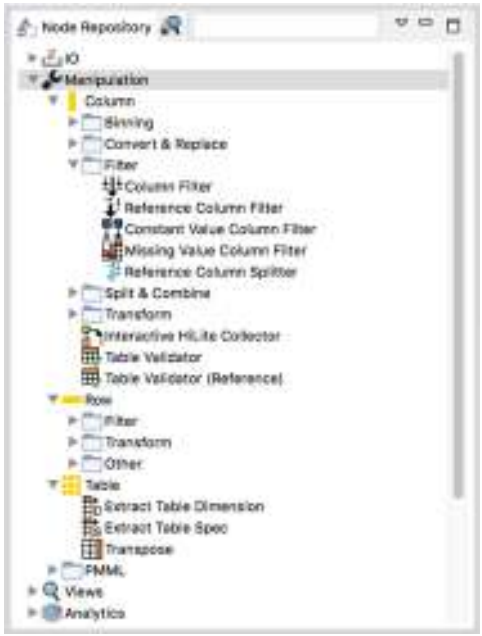
Data Transformation



Data Transformation Nodes

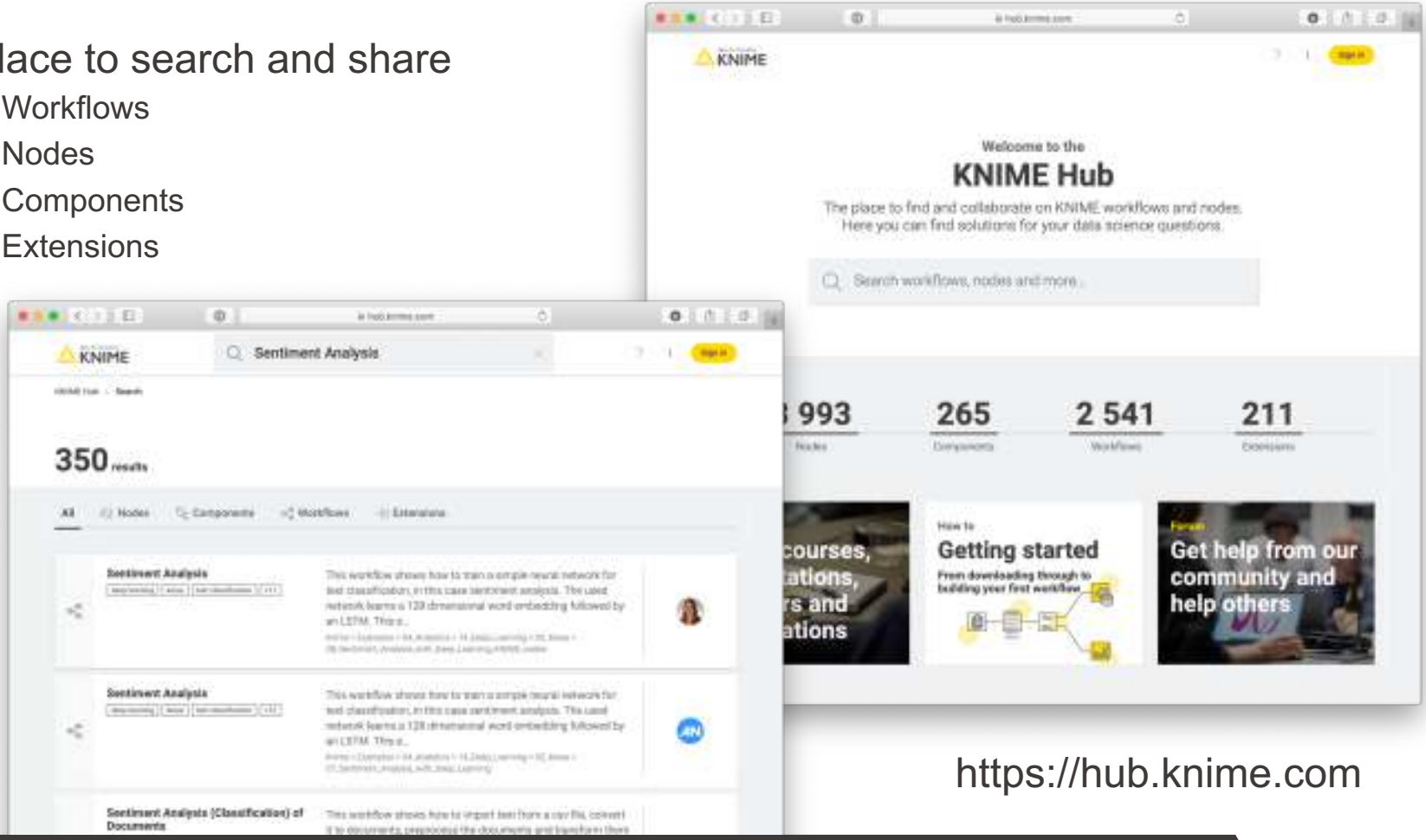
- Yellow color with a variety of input and output ports
- Apply a transformation to input data
- Many, many nodes!





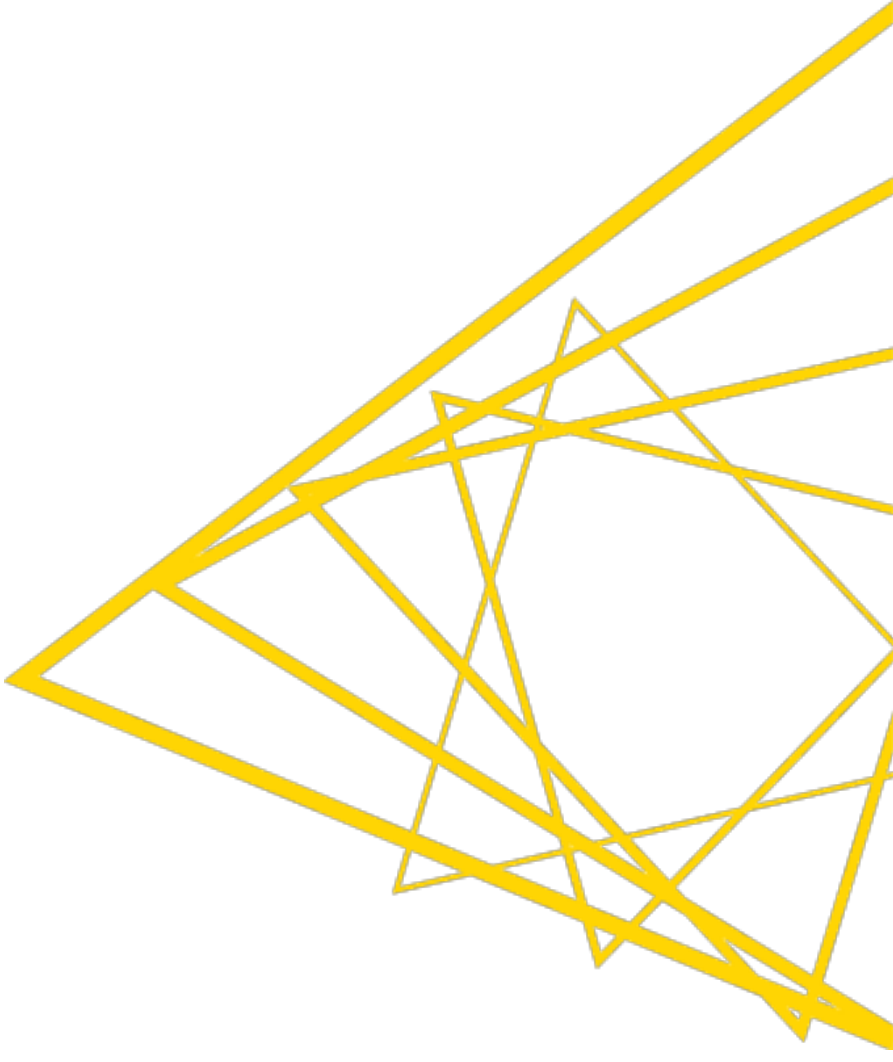
Finding Your Way: KNIME Hub

- Place to search and share
  - Workflows
  - Nodes
  - Components
  - Extensions



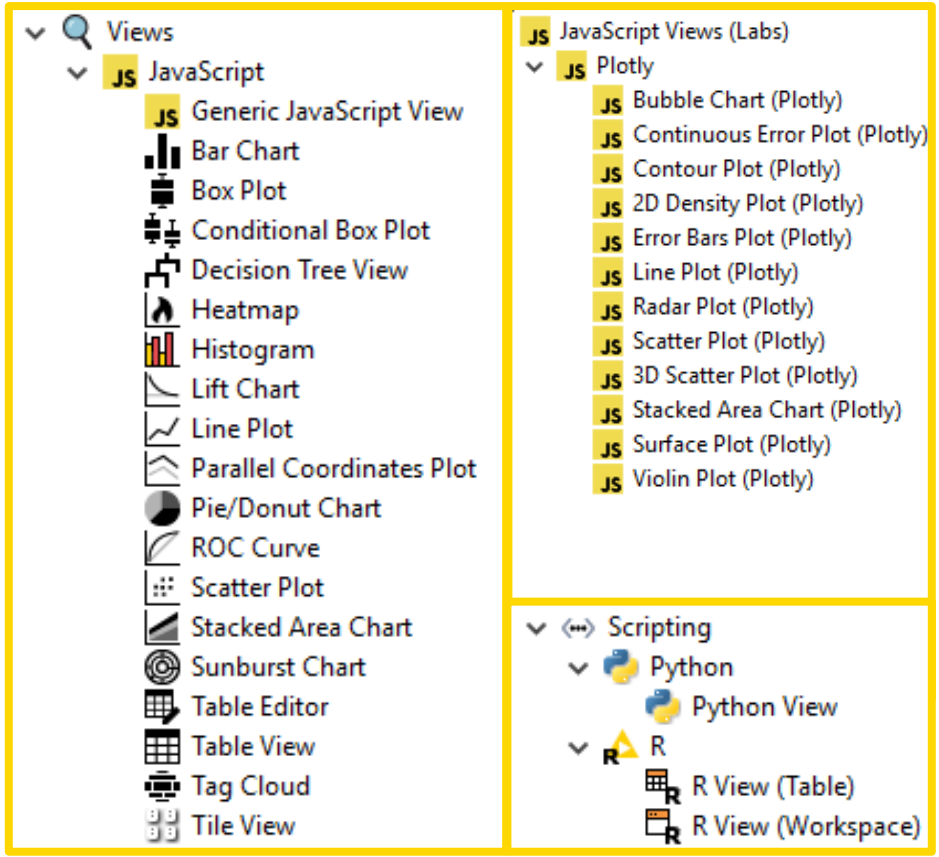
https://hub.knime.com

Data Visualization



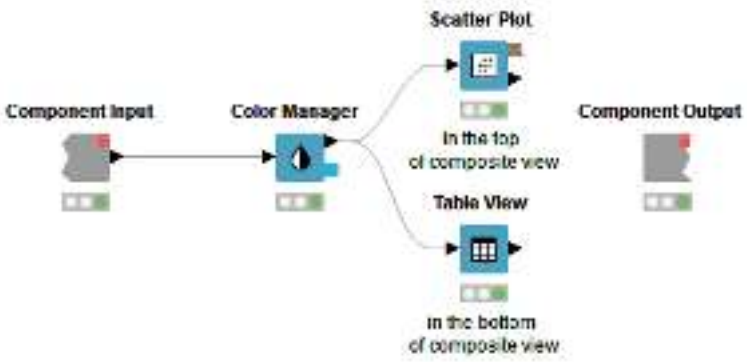
Data Visualization

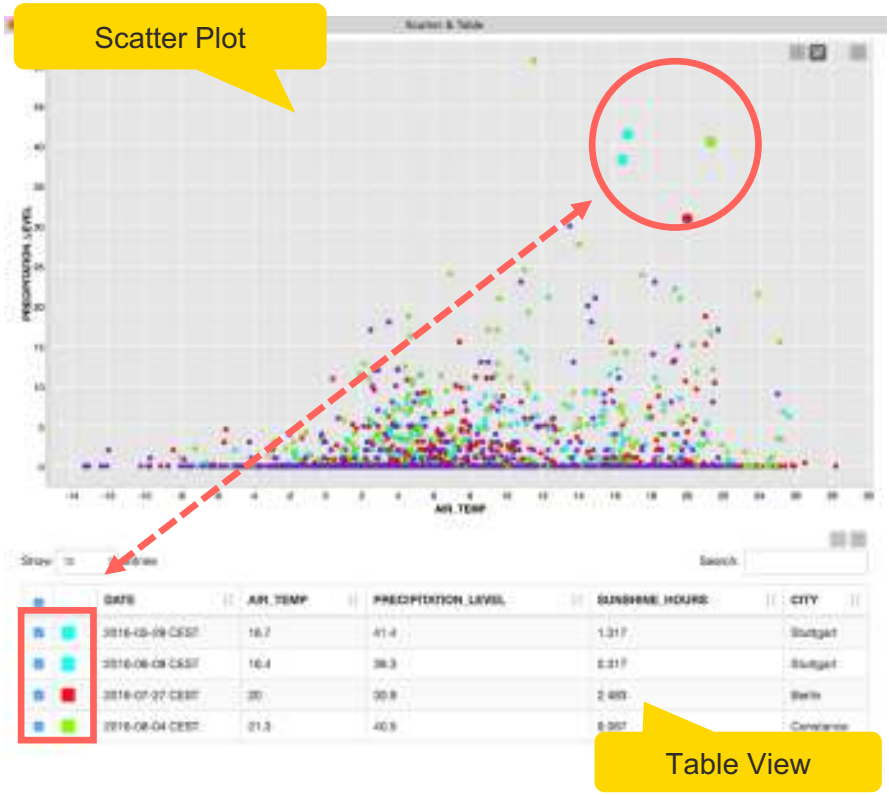
- Large selection of easy to use visualization nodes
  - Web-based and interactive
  - Dedicated nodes,
  - no scripting required
- Plotly nodes
  - Similar but integrated from an external library
- R and Python View nodes for highly customizable graphics
  - Require scripting



Components – Combined Views

- Multiple JavaScript View nodes can be combined in Components
- Selections are transmitted to all other views
- Also for use on the KNIME

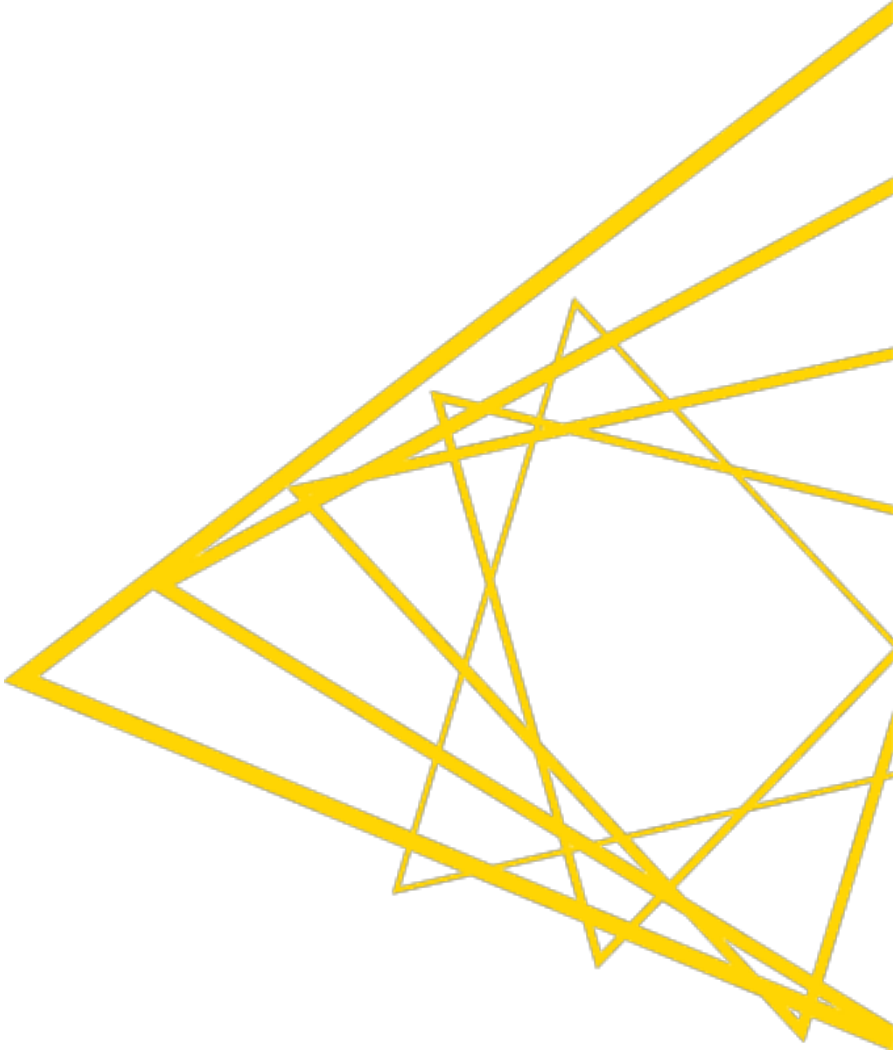




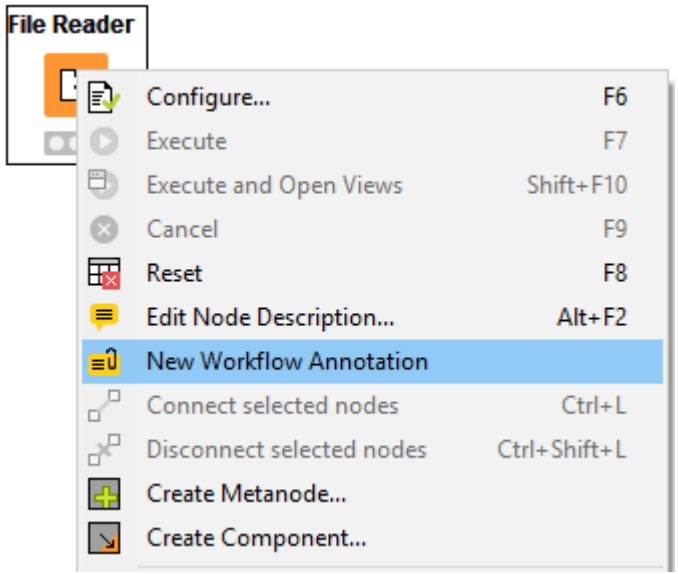
Interactivity across Charts: Selection and Filter Events

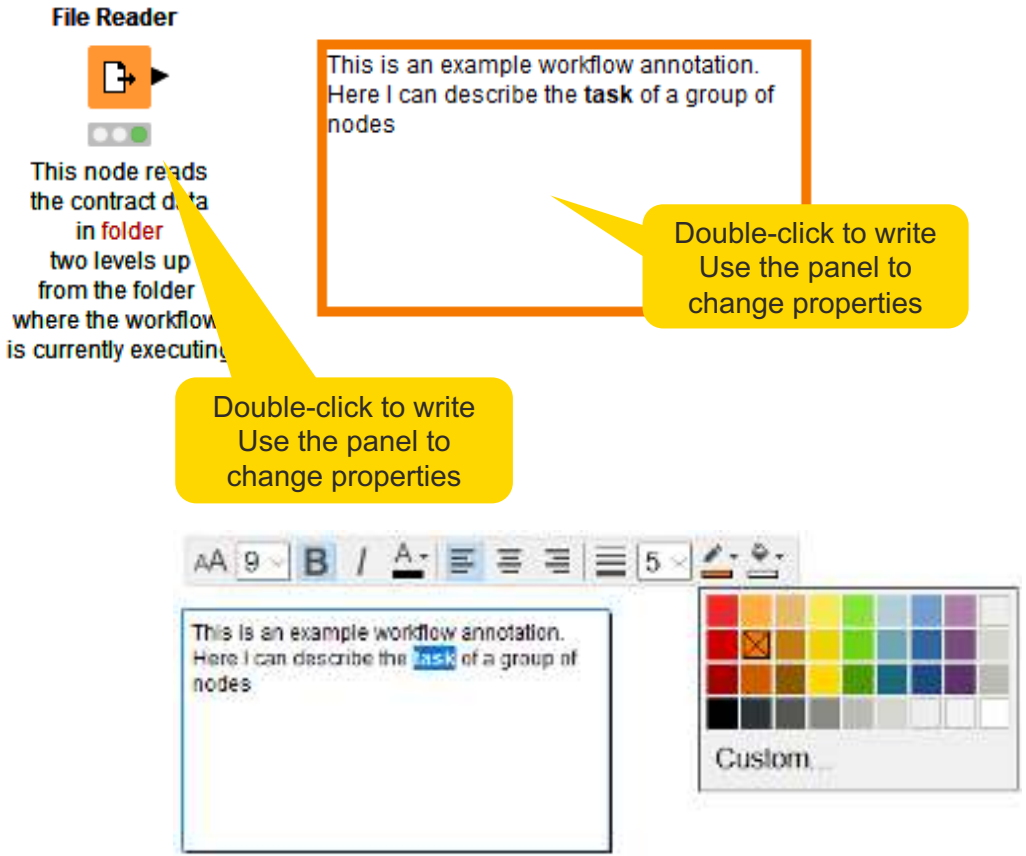
Interactivity across Charts: Selection and Filter Events

Workflow Organization and Documentation



Comments & Annotations



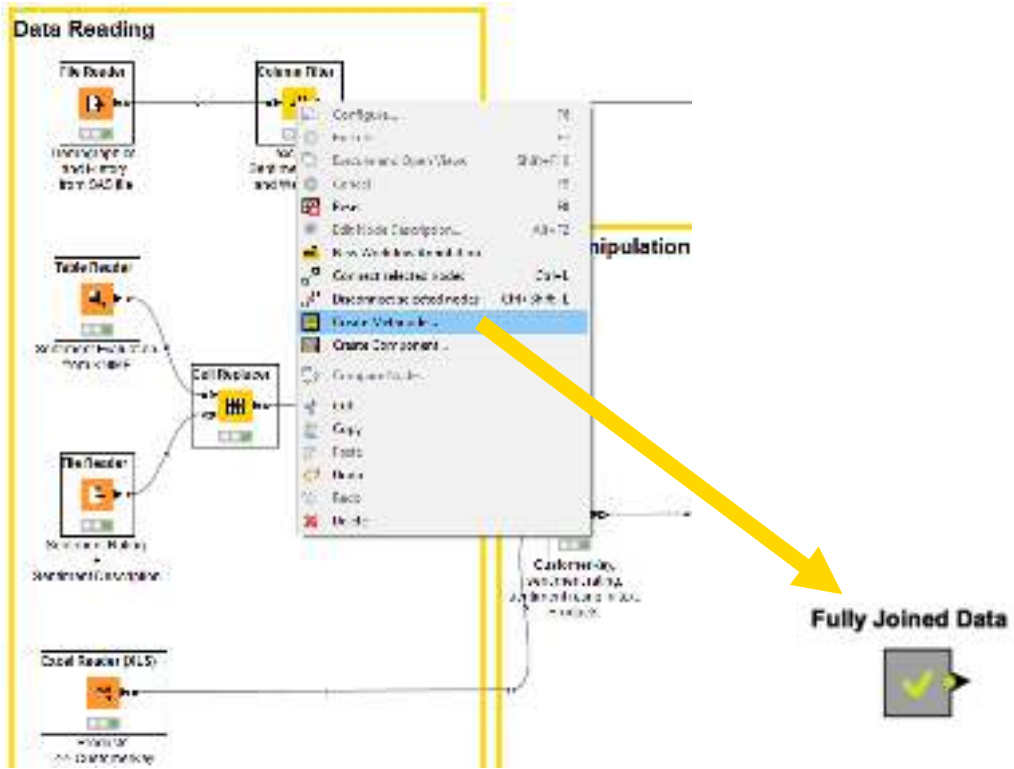


YouTube KNIME TV Channel:

https://youtu.be/AHURYB_O8sA

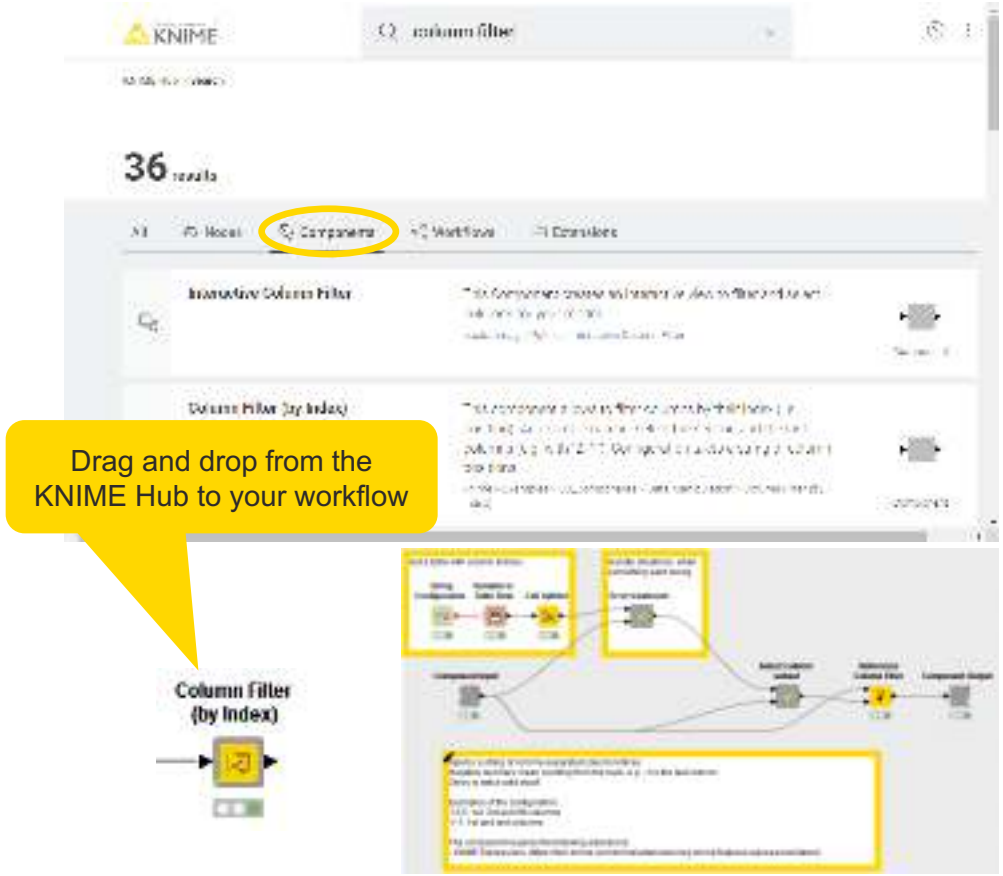
Workflow Organization – Good Practices

- Workflow annotations
- Node labels
- Metanodes
  - Right click -> Create Metanode...
  - Organize workflow by task
  - Hide complexity & improve readability



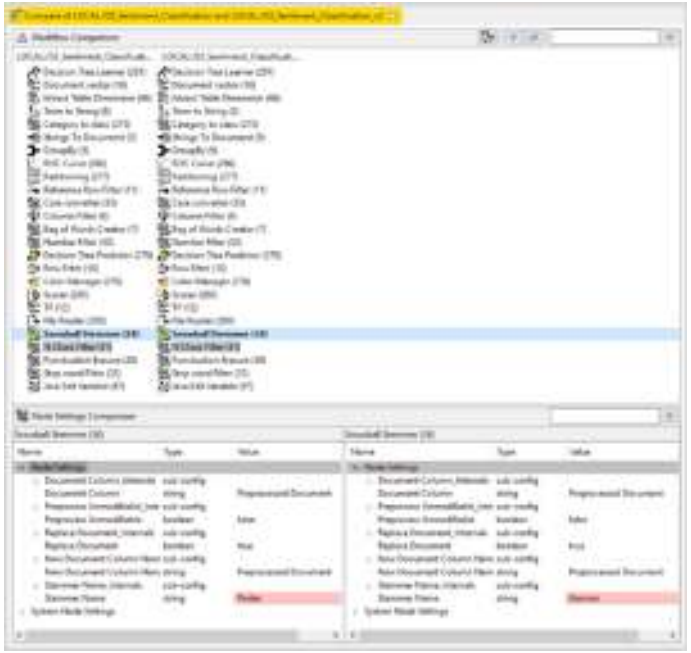
Workflow Organization – Components

- Component encapsulates a reusable functionality as a KNIME workflow
- Components can be configured as any KNIME nodes
- Access and share components on the KNIME Hub

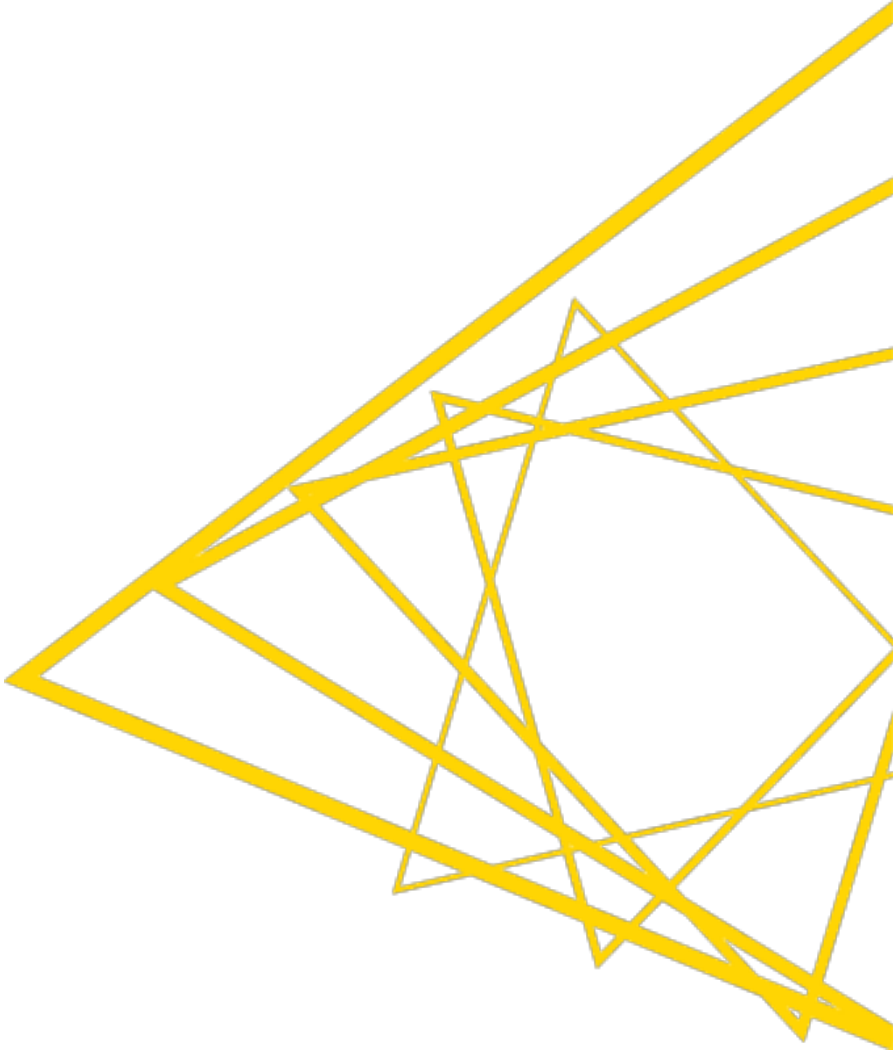


KNIME WorkflowDiff

- Automates identification and comparison of nodes in a workflow, metanodes, and two different workflows
- Identifies insertions, deletions, substitutions, and parameter changes



Data Mining

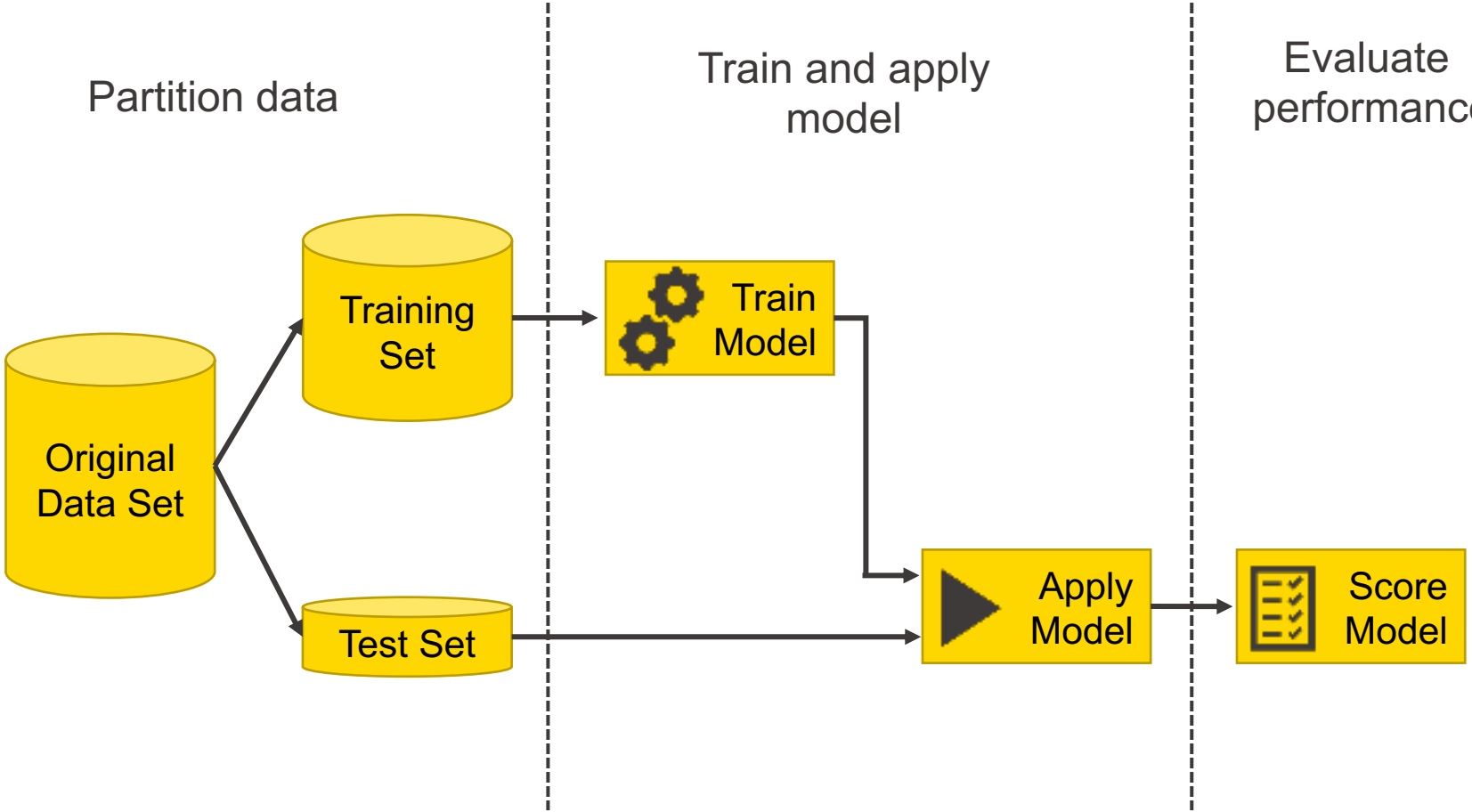


Data Mining Strategies

Example Applications:

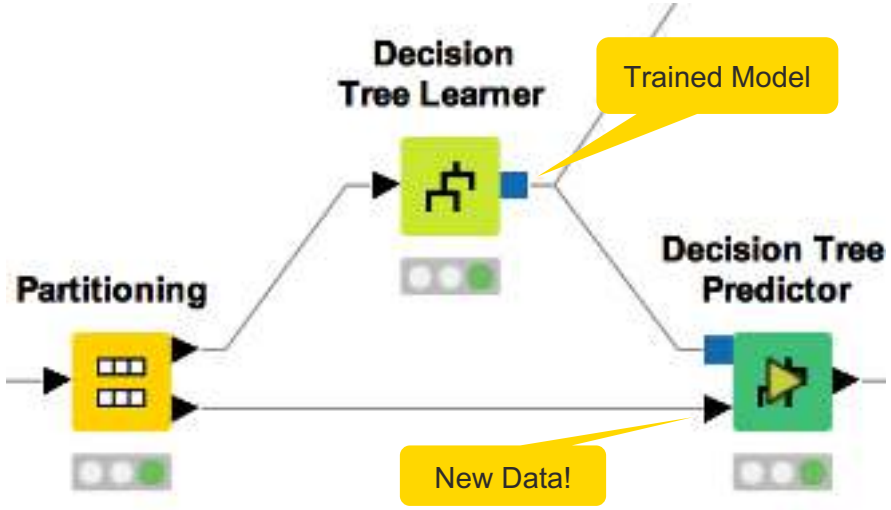
- Anomaly Detection (fraud, predictive maintenance)
- Association Rule Learning (market basket analysis)
- Clustering (customer / market segmentation)
- Classification (next best offer, churn preventions)
- Regression (trend estimation)

Data Mining: Process Overview

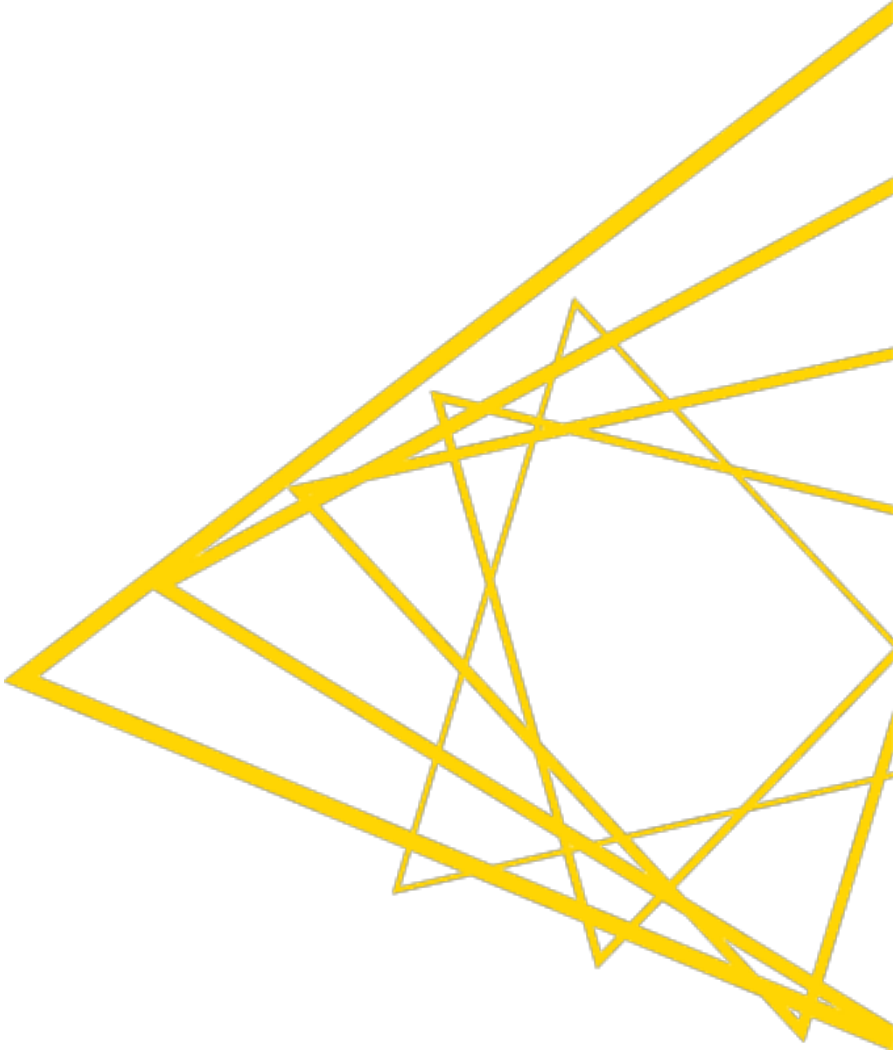


Learner-Predictor Motif

- Most data mining approaches in KNIME use a Learner-predictor motif.
- The Learner node trains the model with its input data.
- The Predictor node applies the model to a different subset of data.



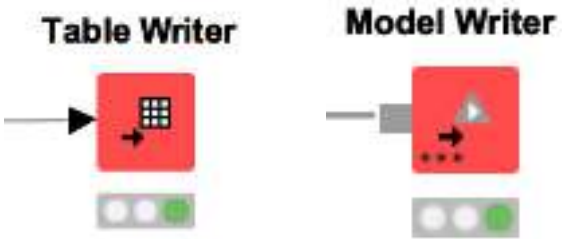
Deployment



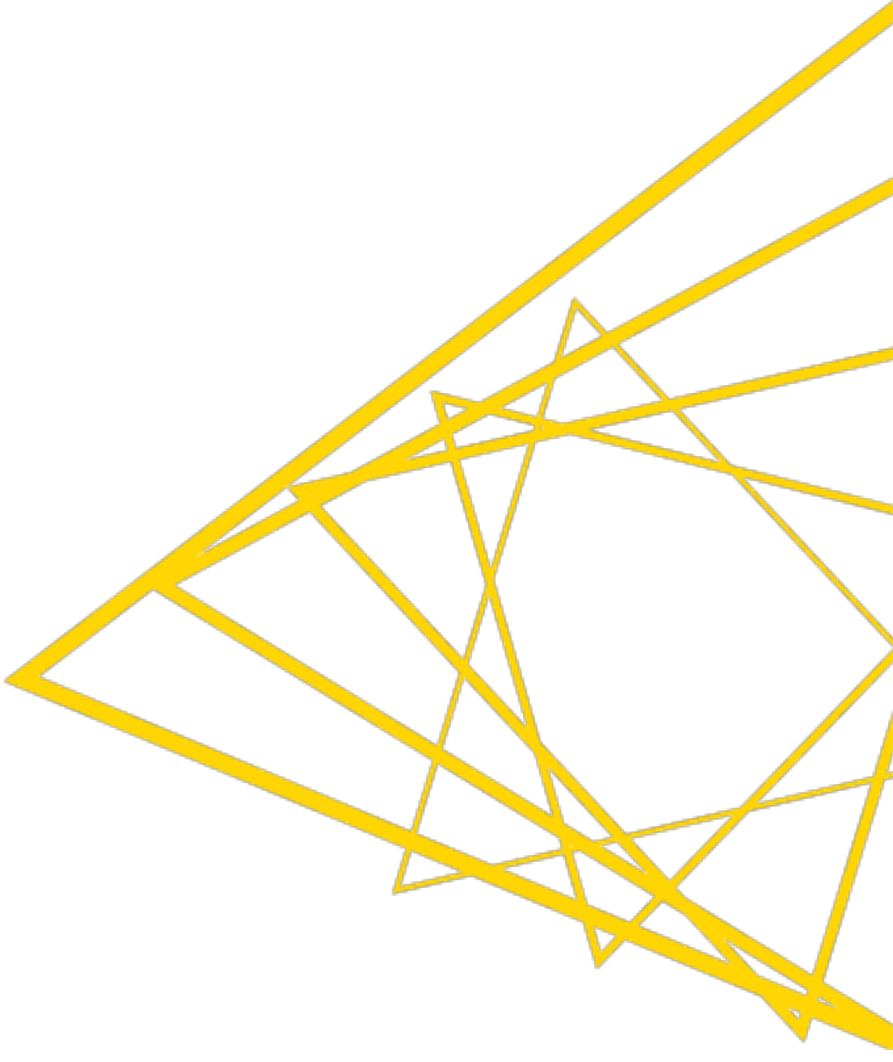
Data Export Nodes

Typically characterized by:

- Magenta color
- 1 input port, no output ports
- Create file on file system or write to database

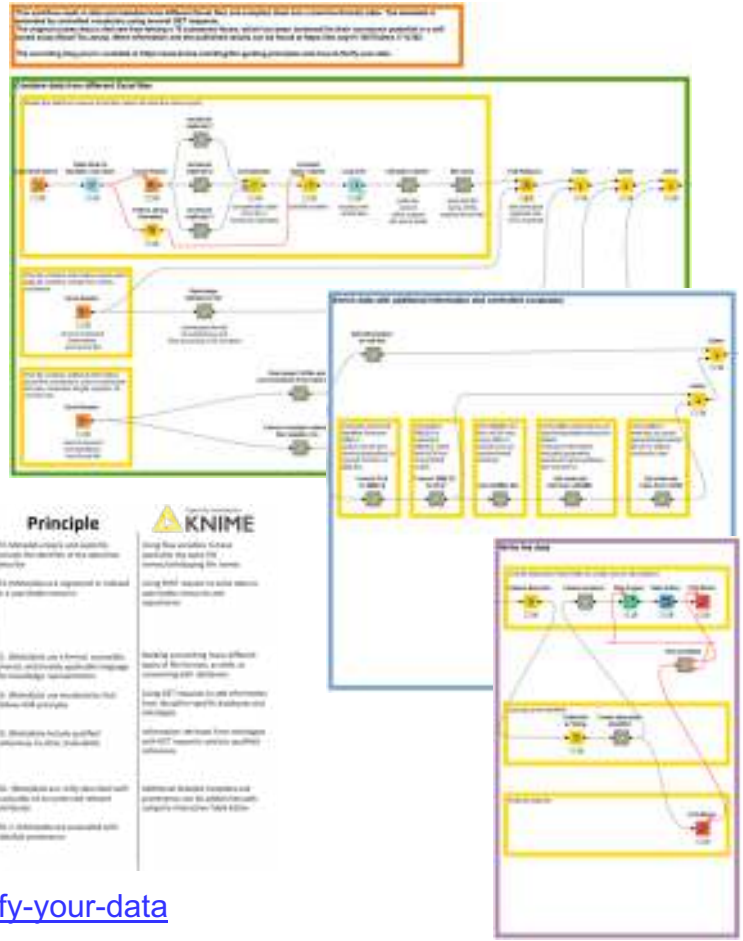


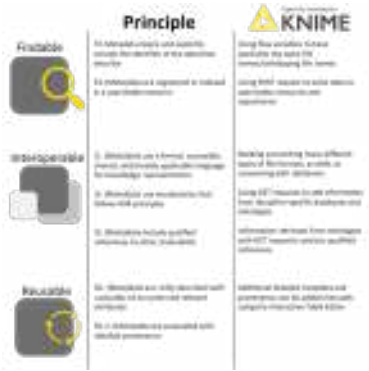
Some Use-Cases



How to use KNIME to make data FAIRer

- Restructure and combine previously generated bioassay data to comply with the FAIR principles
- Extend the metadata with domain-specific controlled vocabulary using GET requests
- Add user-defined information using the Interactive Table Editor

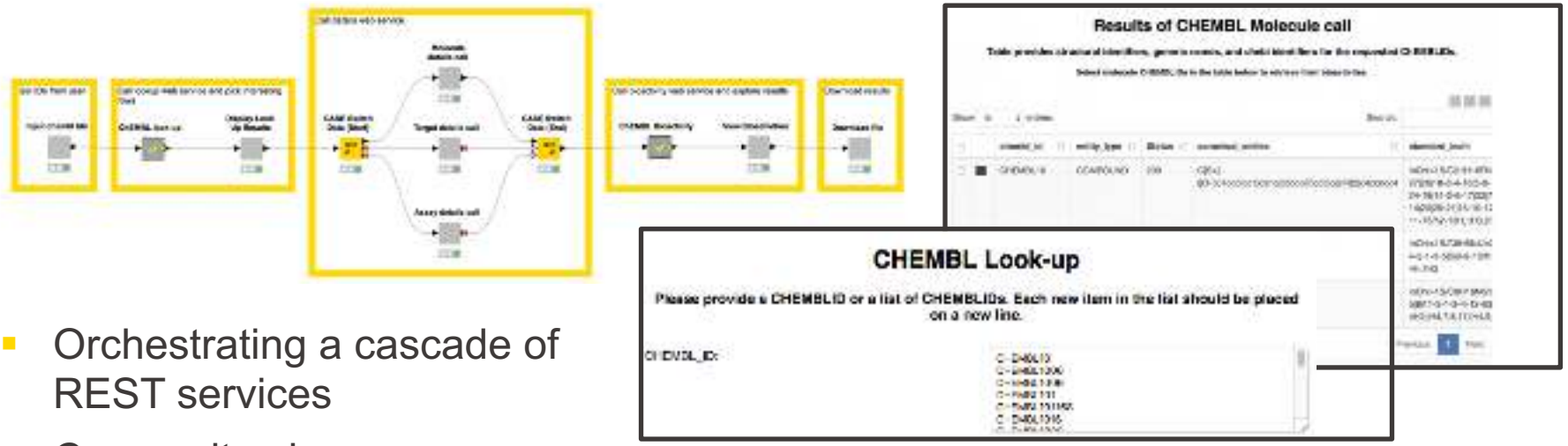




Workflow on the Hub: https://kni.me/w/Py9va0SQesbauPwS

Blog Post: https://www.knime.com/blog/fair-guiding-principles-and-how-to-fairify-your-data

Calling ChEMBL Web Services

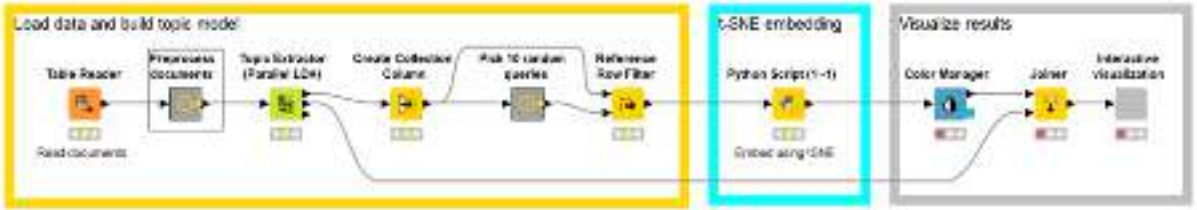


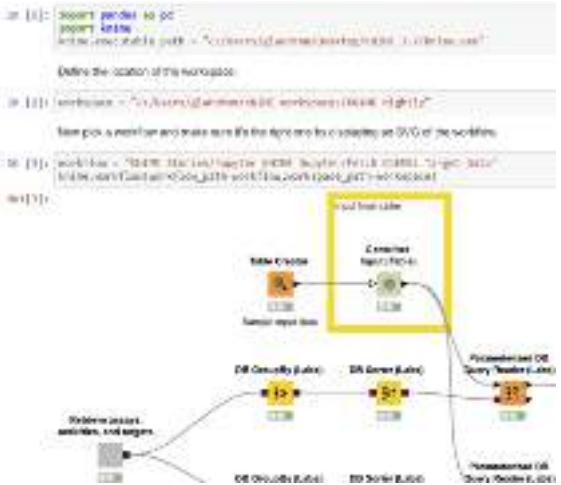
- Orchestrating a cascade of REST services
- Composite views
- WebPortal

Blog post: https://www.knime.com/blog/a-restful-way-to-find-and-retrieve-data
Workflows:
https://workflows.knime.com/knime/hub/workflows/50_Applications%3A30_RESTful_ChEMBL%3A01_ChEMBL_REST_Serviceshttps://workflows.knime.com/knime/hub/workflows/50_Applications%3A30_RESTful_ChEMBL%3A02_ChEMBL_Structure_Search
knime://EXAMPLES/50_Applications/30_RESTful_ChEMBL

Jupyter – KNIME - Jupyter

- Using Python code in Jupyter notebooks from KNIME
- Calling KNIME workflows from Jupyter notebooks





Workflows on KNIME EXAMPLES Server:

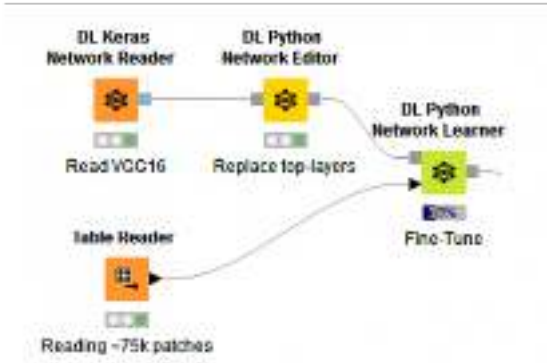
07_Scripting/03_Python/03_Fetch_ChEMBL_Target_Data

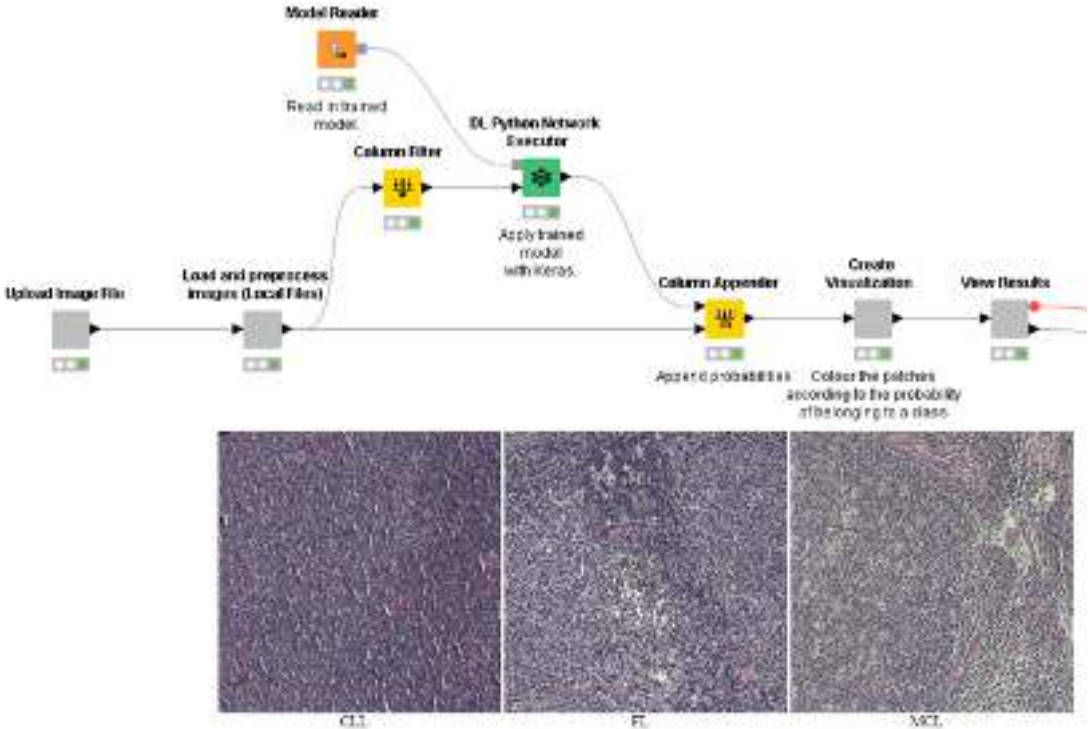
07_Scripting/03_Python/04_Using_Jupyter_from_ KNIME_to_embed_documents

Blog post: https://www.knime.com/blog/knime-and-jupyter

Deep Learning and Histopathology

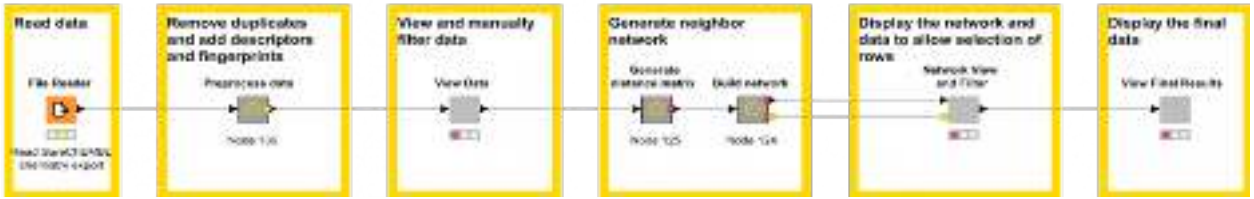
- Image analysis
- Deep learning
- Keras
- Custom visualization

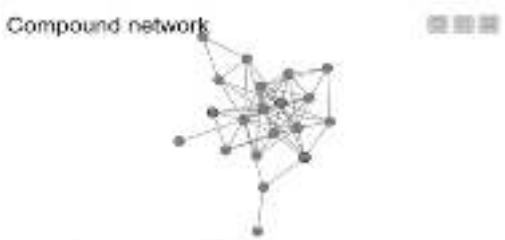




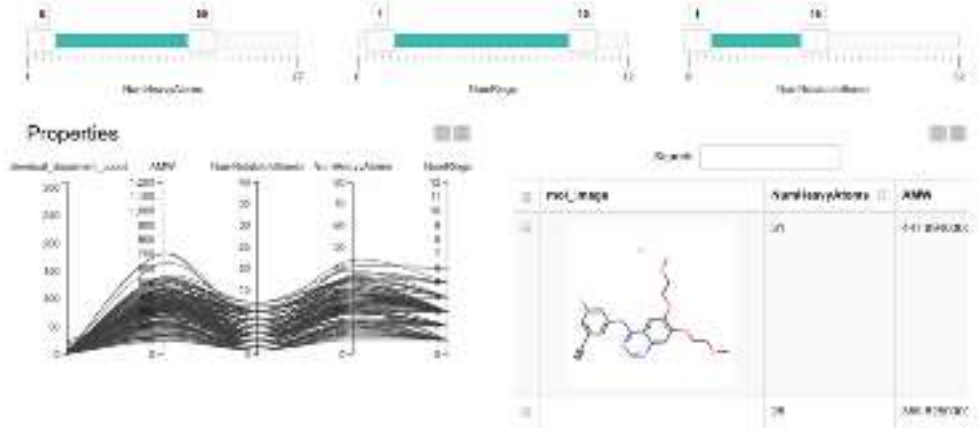
Workflow on KNIME EXAMPLES server: *50_Applications/31_Histopathology_Blog_Post*
Blog post: https://www.knime.com/blog/using-the-new-knime-deep-learning-keras-integration-to-predict-cancer-type-from-histopathology

Finding the key compound in a patent





- Interactive data analysis
- Cheminformatics
- Network analysis
- WebPortal



Video from ChemAxon UGM: https://www.youtube.com/watch?v=MQmmm7tzmB0
Workflow: https://workflows.knime.com/knime/hub/workflows/50_Applications%3A29_Patent_Network_Analysis%3A01_Tarceva_neighbor_network_from_SureChEMBL
knime://EXAMPLES/50_Applications/29_Patent_Network_Analysis

Some Final Remarks

- Visual workflows allow you build documented and reproducible analyses
- KNIME Analytics Platform is open-source and free to use (no limitations)
- KNIME covers the entire data (science) life cycle