



Mit Metadatenmanagement hinzu
reproduzierbaren und flexiblen
Data-Science-Workflows auf Kubernetes

Sebastian Jäger, Kevin Exel

Ludwigshafen, 23. Oktober 2019



Sebastian Jäger

Working student

Data Science Platform, Data Science Student



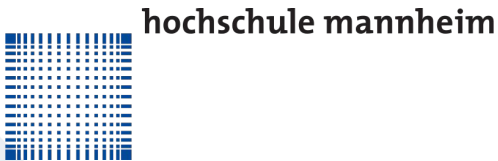
Kevin Exel

Working student

Data Science Platform, Computer Science Student

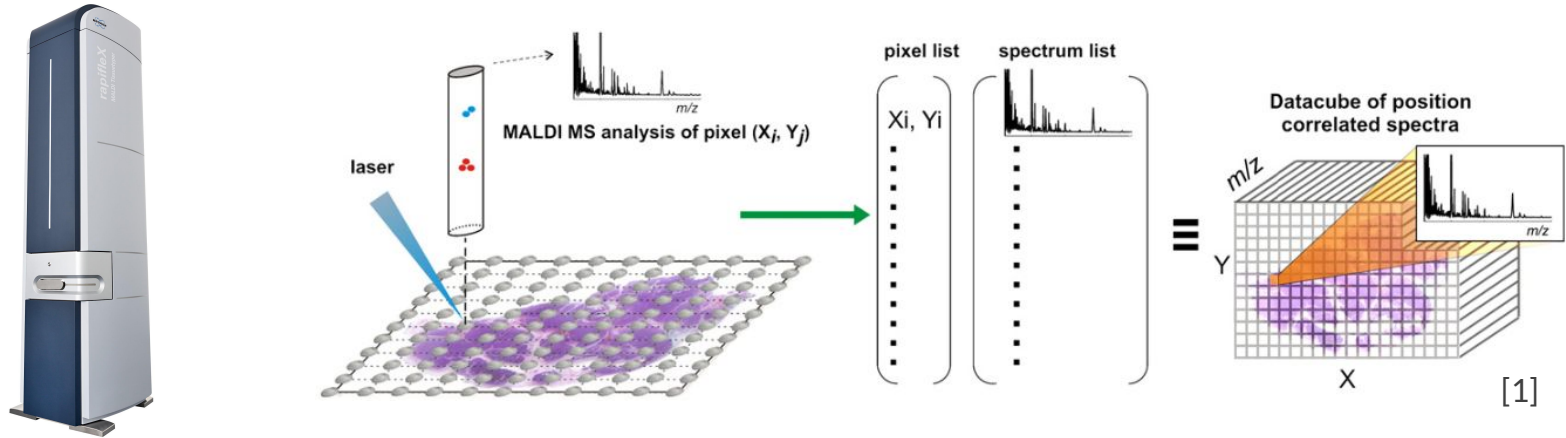
Use Case: EMQ

- › Expert system for quality evaluation and analysis of 3-dimensional mass spectrometry data
- › Duration: 01.11.2017 - 31.10.2019



3-Dimensional Mass Spectrometry

Matrix-Assisted Laser Desorption/Ionisation-Mass Spectrometry Imaging (MALDI-MSI)



[1] Jones, E., Deininger, S., Hogendoorn, P., Deelder, A. and McDonnell, L. (2012). Imaging mass spectrometry statistical analysis. *Journal of Proteomics*, 75(16), pp.4962-4989.

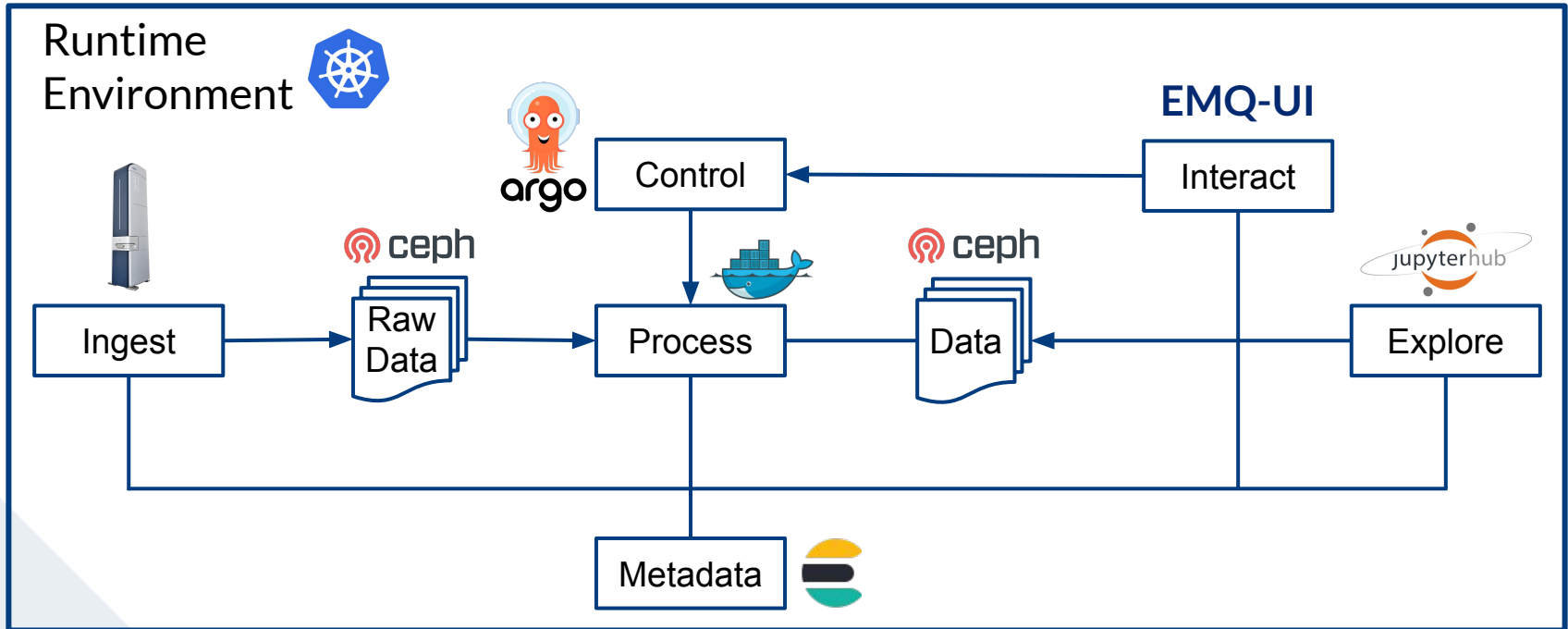
EMQ: Personas

- › **Biologists**
 - › upload data sets
 - › run algorithms (quality evaluation & analysis)
- › **Data Scientists**
 - › interactive exploration
 - › optimize and develop algorithms

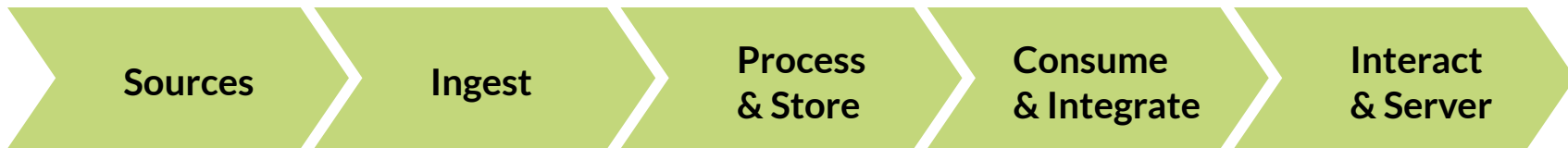
EMQ-UI

 Jupyter

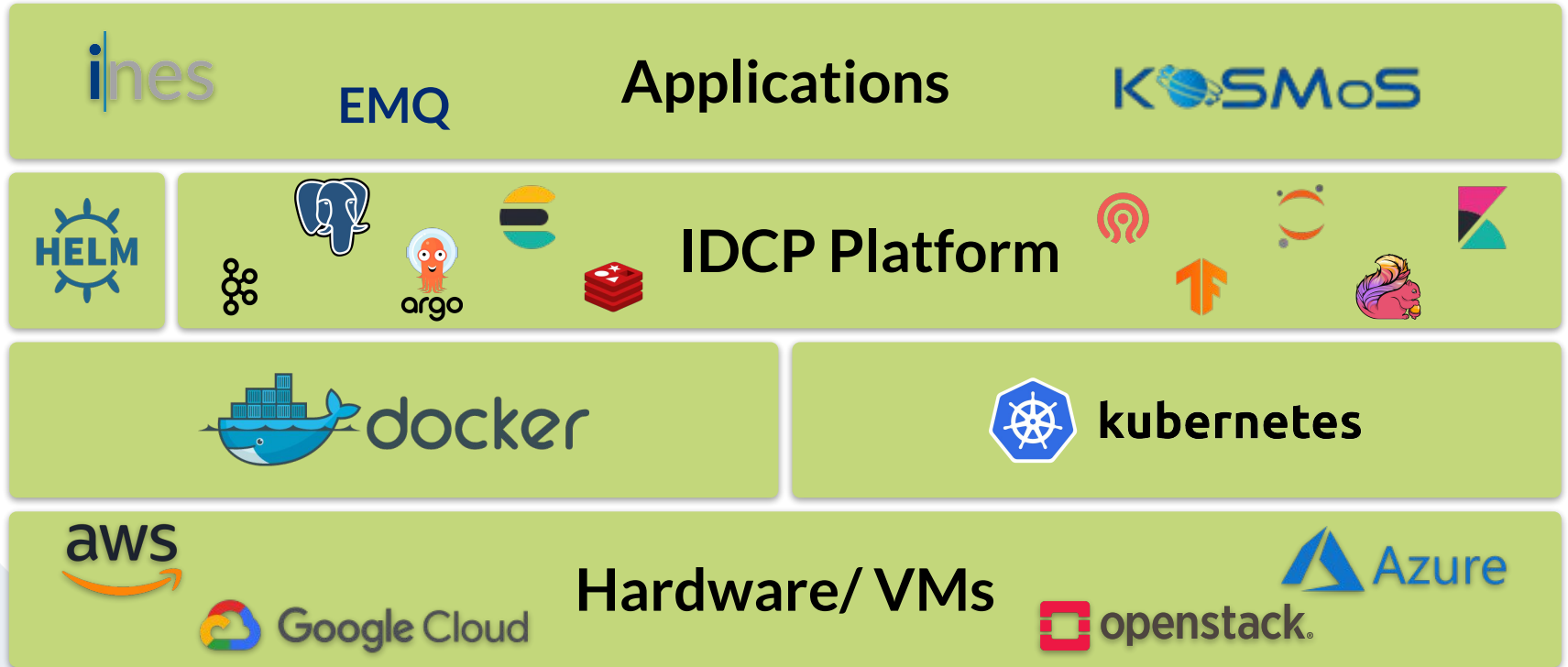
EMQ Architecture



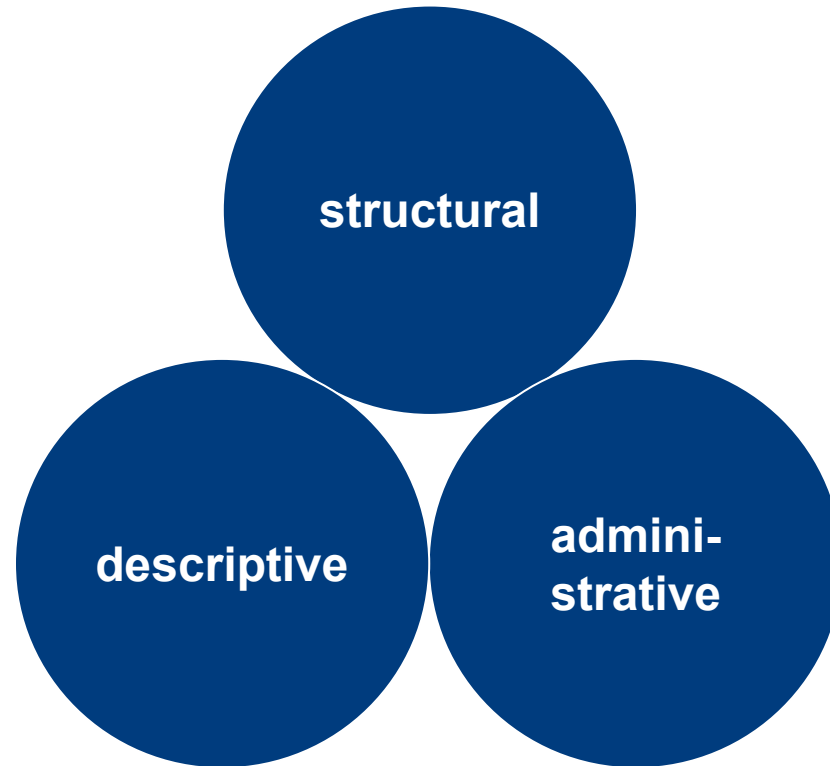
The Base: **I**novex **D**ata **C**loud **P**latform



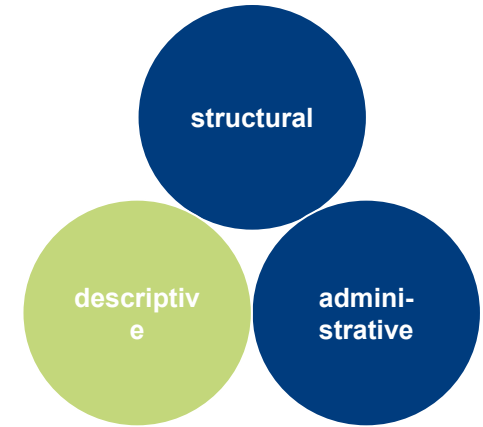
IDCP Architecture



Metadata



Metadata



Dataset 20160429_Imatinib_Sampling rate comparison.mis

Metadata

Dataset ID	MSI-Rapiflex-20160429-144500	Operator	Kevin
Acquisition Date	01.08.2019 00:00	Ionization Source	MALDI
Analyzer	TOF	Equipment	autoflex
Acquisition Type	imaging	Acquisition Mode	positive
Matrix Sprayer	MS	Matrix Type	DHB
Number Regions	2	Timestamp	2019-10-20_15:52:23

Metadata

- ▼ **Data2Day**

- ▼ **Vortrag**

- ▼ 20160429_Imatinib_Sampling

- rate comparison.mis

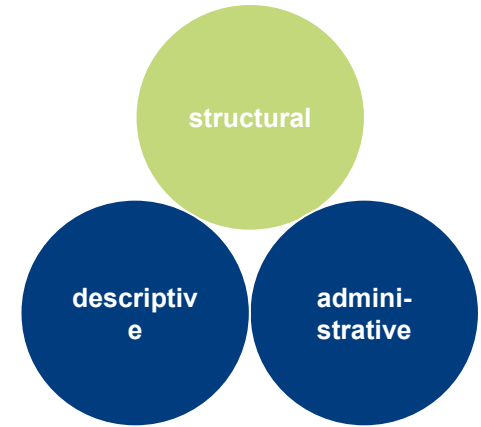
- Krank

- Gesund

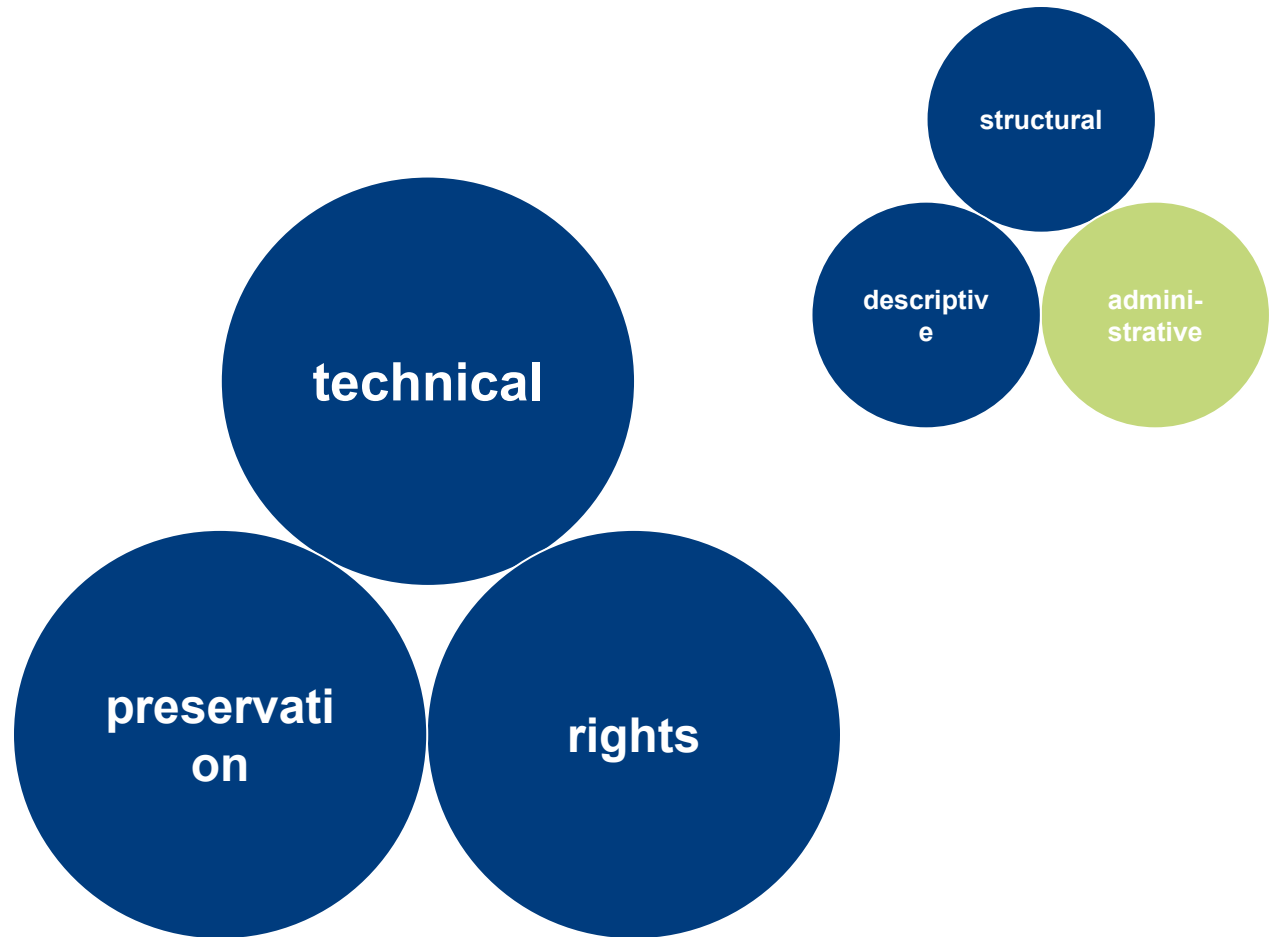
- ▼ **nyakas**

- ▼ **nyakas**

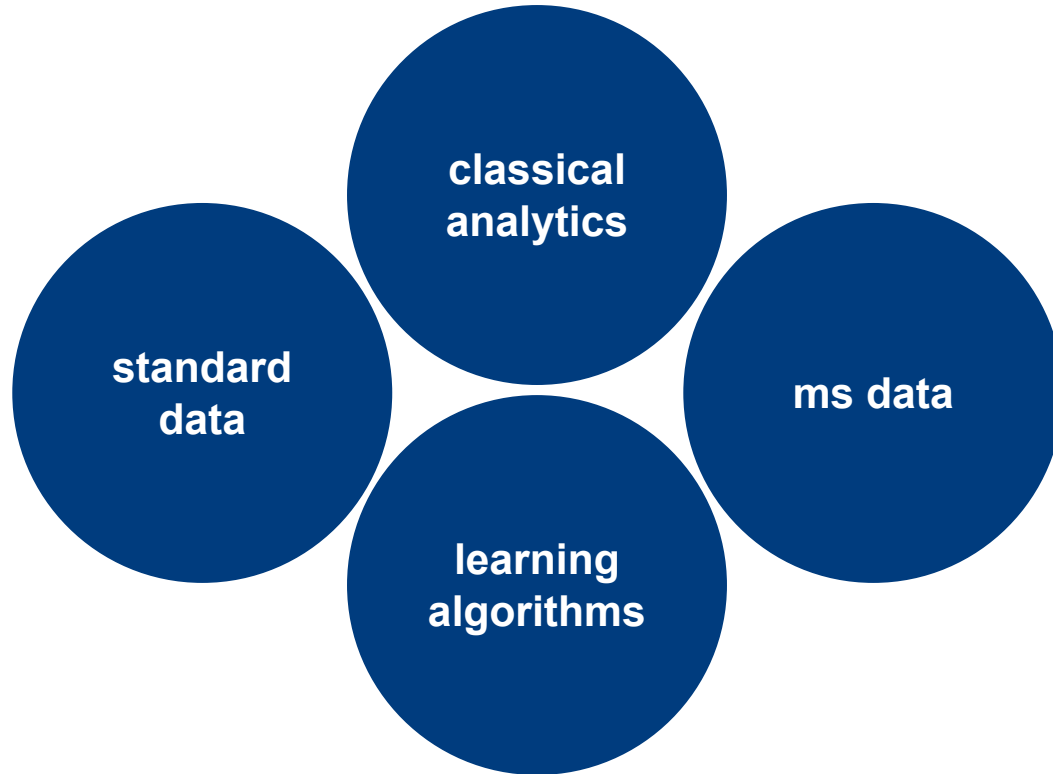
- nyakas2013



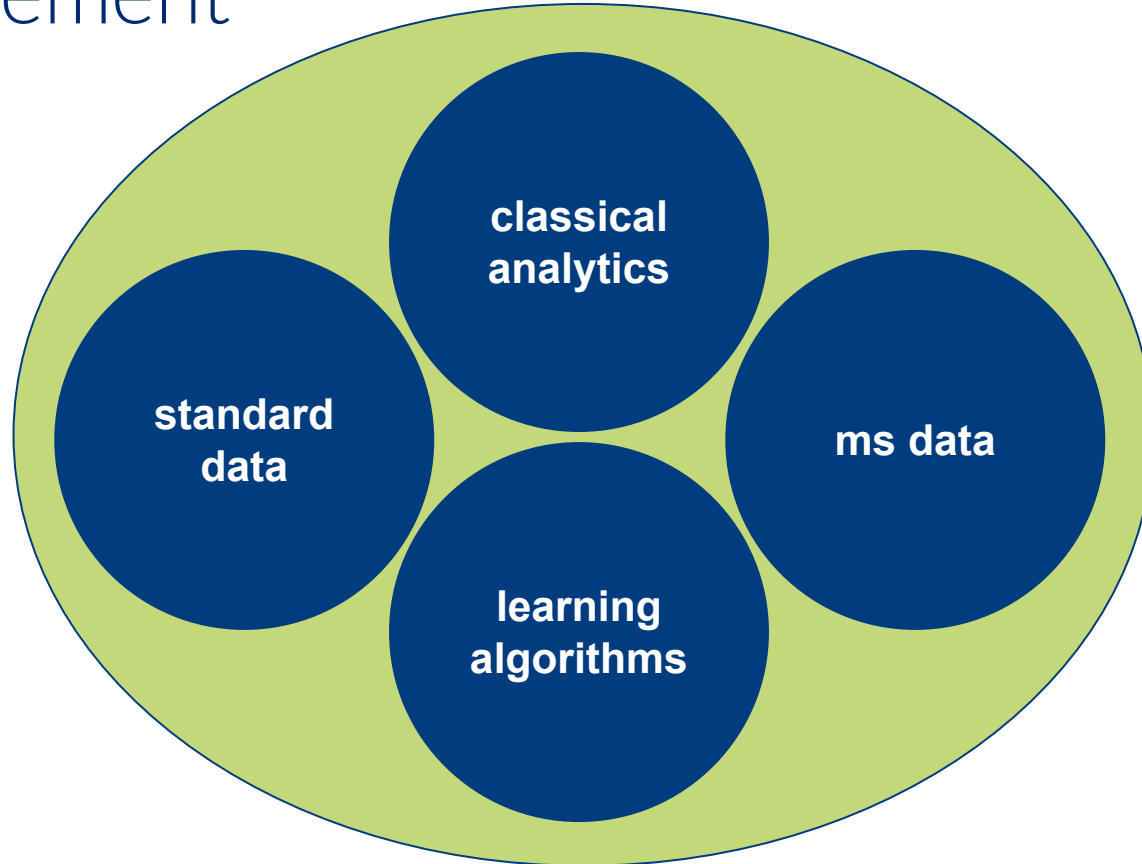
Metadata



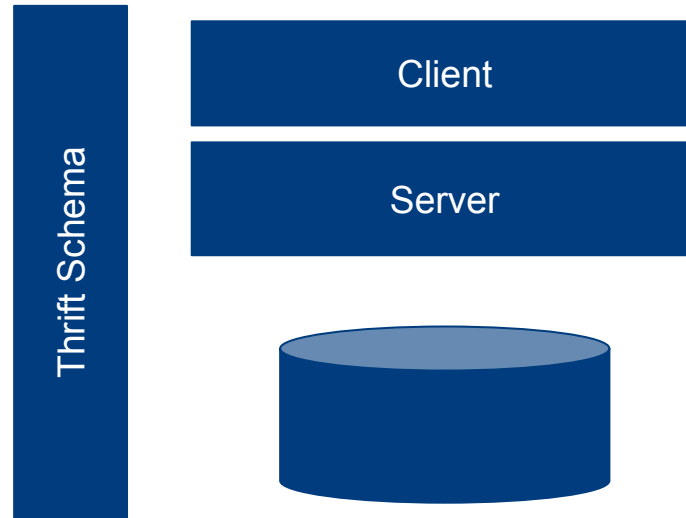
Management



Management



Metadata management



Demo

Reproduzierbar
Flexibel
Erweiterbar

Outlook

Vielen Dank

Sebastian Jäger

@se_jaeger

sebastian.jaeger@inovex.de

Kevin Exel

kevin.exel@inovex.de

inovex GmbH

Ludwig-Erhard-Allee 6

76131 Karlsruhe

