# Architecture of ML Systems (AMLS)
## 09 Data Acquisition and Preparation

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Last update: Jun 10, 2023

# Announcements / Org

- **#1 Hybrid & Video Recording**
  - Hybrid lectures (in-person, zoom) with optional attendance https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09
  - Zoom **video recordings**, links from website https://mboehm7.github.io/**teaching**/ss23_amls/index.htm

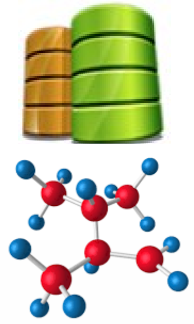
- **#2 Virtual Lectures June 22**
  - **Thu, June 22, 4pm-6pm** due to SIGMOD 2023 in Seattle (7am-9am PST)
  - **Thu, June 29, 6.30pm-8.30pm** due to BMBF visit at BIFOLD
  - **Virtual lecture and video recording**

# Recap: The Data Science Lifecycle (aka KDD Process, aka CRISP-DM)

Data extraction, schema alignment, entity resolution, data validation, data cleaning, outlier detection, missing value imputation, semantic type detection, data augmentation, feature selection, feature engineering, feature transformations

Data Scientist

**Key observation:** SotA data integration/cleaning based on ML



**Data Integration**
**Data Cleaning**
**Data Preparation**

**Model Selection**
**Training**
**Hyper-parameters**

**Validate & Debug**
**Deployment**
**Scoring & Feedback**

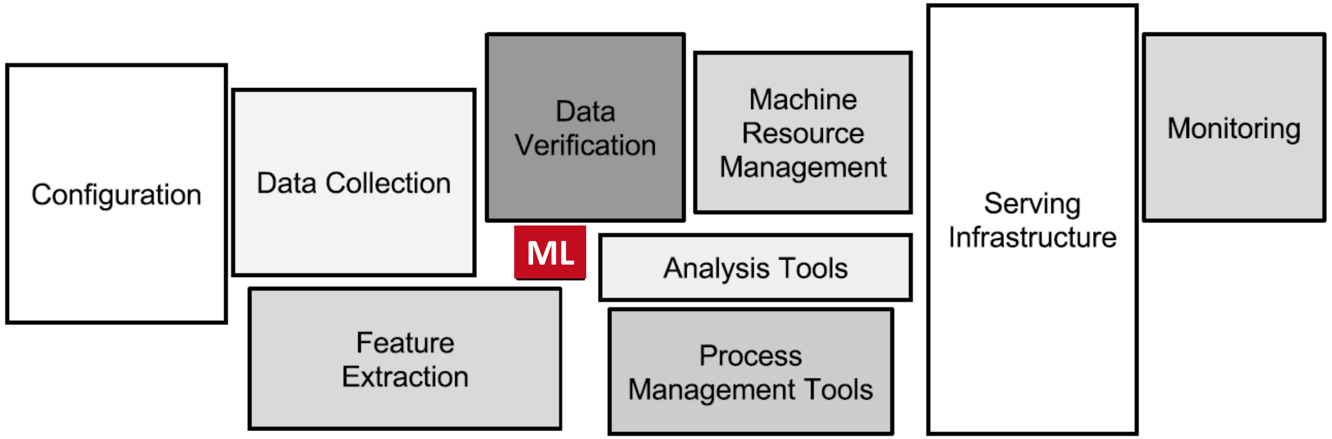
**Exploratory Process**
(experimentation, refinements, ML pipelines)

Data/SW Engineer

DevOps Engineer

# The 80% Argument

- **Data Sourcing Effort**
  - Data scientists spend **80-90% time** on finding, integrating, cleaning datasets
- **Technical Debts in ML Systems**




  - Glue code, pipeline jungles, dead code paths
  - Plain-old-data types (arrays), multiple languages, prototypes
  - Abstraction and configuration debts
  - Data testing, reproducibility, process management, and cultural debts

[Michael Stonebraker, Ihab F. Ilyas: Data Integration: The Current Status and the Way Forward. **IEEE Data Eng. Bull. 41(2) (2018)**]

[D. Sculley et al.: Hidden Technical Debt in Machine Learning Systems. **NeurIPS 2015**]

# Agenda

- **Data Acquisition, Integration, and Validation**
- **Feature Transformations and Engineering**
- **Data Preparation and Cleaning**
- **Data Augmentation** (next week)

**"least enjoyable tasks in data science lifecycle"**

**Data Integration and Large-Scale Analysis (DIA)**
(WiSe, bachelor/master)

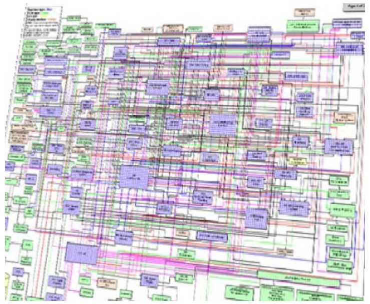
# Data Acquisition, Integration, and Data Validation

## Data Integration for ML and ML for Data Integration

# Data Sources and Heterogeneity

- **Terminology**
  - **Integration** (Latin integer = whole): consolidation of data objects / sources
  - **Homogeneity** (Greek homo/homoios = same): similarity
  - **Heterogeneity**: dissimilarity, different representation / meaning
- **Heterogeneous IT Infrastructure**
  - Common enterprise IT infrastructure contains >100s of **heterogeneous and distributed systems and applications**
  - E.g., health care data management: 20 - 120 systems

[**Credit:** Albert Maier]



- **Multi-Modal Data (example health care)**
  - **Structured patient data**, patient records incl. prescribed drugs
  - **Knowledge base** drug APIs (active pharmaceutical ingredients) + interactions
  - **Doctor notes** (text), diagnostic codes, outcomes
  - **Radiology images** (e.g., MRI scans), **patient videos**
  - **Time series** (e.g., EEG, ECoG, heart rate, blood pressure)

# Types of Data Formats

- **General-Purpose Formats**
  - CSV (comma separated values), JSON (javascript object notation), XML, Protobuf
  - CLI/API access to DBs, KV-stores, doc-stores, time series DBs, etc
- **Sparse Matrix Formats**
  - Matrix market: text IJV (row, col, value)
  - Libsvm: text compressed sparse rows
  - Scientific formats: NetCDF, HDF5
- **Large-Scale Data Formats**
  - Parquet (columnar file format)
  - Arrow (cross-platform columnar in-memory data)
- **Domain-Specific Formats**
  - Health care: DICOM images, HL7 messages (health-level seven, XML)
  - Automotive: MDF (measurements), CDF (calibrations), ADF (auto-lead XML)
  - Smart production: OPC (open platform communications)

```
%%MatrixMarket matrix coordinate real general
% ----------------------------------------------
% 0 or more comment lines
% ----------------------------------------------
5  5  8
1 1 1.000e+00
2 2 1.050e+01
3 3 1.500e-02
1 4 6.000e+00
4 2 2.505e+02
4 4 -2.800e+02
4 5 3.332e+01
5 5 1.200e+01
```

# Types of Heterogeneity

[J. Hammer, M. Stonebraker, and O. Topsakal: THALIA: Test Harness for the Assessment of Legacy Information Integration Approaches. U Florida, TR05-001, **2005**]

**Heterogeneity**

- **Semantic Heterogeneity**
  - **Attribute Heterogeneity**
    1. **Synonyms/homonyms**
    2. **Simple mapping** (mathematical)
    3. **Different data types**
    4. Complex mappings
    5. **Language expressions**
  - **Missing Data**
    6. **Nulls** (Missing Values)
    7. **Virtual columns**
    8. Semantic incompatibility
- **Structural Heterogeneity**
  9. **Same attribute in different structure**
  10. **Handling Sets**
  11. **Attribute name w/o semantics**
  12. **Attribute composition**

# Identification of Data Sources

- **Data Catalogs**
  - Data curation in repositories for finding datasets in **data lakes**
  - **Metadata and provenance**
  - Augment data with open and linked data sources
- **Examples**

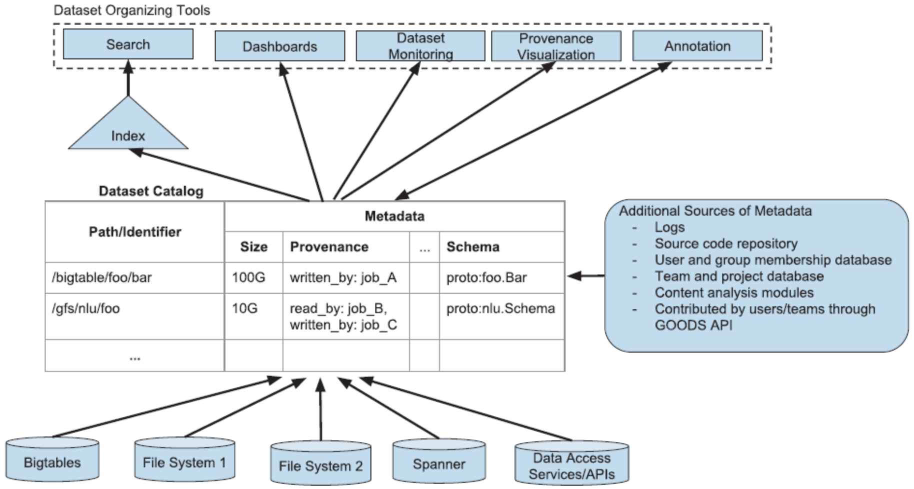
[Alon Y. Halevy et al: Goods: Organizing Google's Datasets. **SIGMOD 2016**]

[Dan Brickley, Matthew Burgess, Natasha F. Noy: Google Dataset Search: Building a search engine for datasets in an open Web ecosystem. **WWW 2019**]

**SAP Data Hub**


[SAP Sapphire Now 2019]

**Google Dataset Search**



# Schema Detection and Integration

- **Syntactic Schema Detection**
  - Sample of the input dataset
  - Extract basic data types via rules, and regular expressions

```
./data/players.csv:
pid,name,pos,jnum,ncid,tid
5435,Miroslav Klose,FW,11,789,144
6909,Manuel Neuer,GK,1,163,308
```

```
Dataset<Row> ds = sc.read()
  .format("csv")
  .option("header", true)
  .option("inferSchema", true)
  .option("samplingRatio", 0.001)
  .load("./data/players.csv");
```

```
StructType(
  StructField(pid,IntegerType,true),
  StructField(name,StringType,true),
  StructField(pos,StringType,true),
  StructField(jnum,IntegerType,true),
  StructField(ncid,IntegerType,true),
  StructField(tid,IntegerType,true))
```

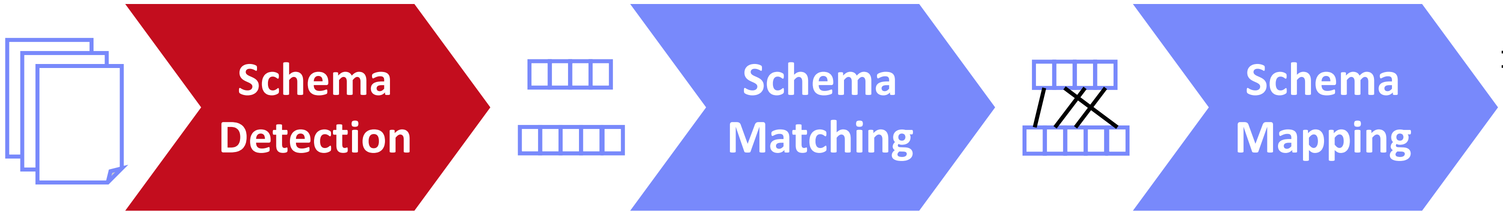
- **Feature Type Detection**
  - Numerical vs Categorical vs Ordinal
  - Rules and trained ML model
- **Semantic Type Detection**
  - Extract common feature types (e.g., location, date, rank, name)

[Vraj Shah, Jonathan Lacanlale, Premanand Kumar, Kevin Yang, Arun Kumar: Towards Benchmarking Feature Type Inference for AutoML Platforms, **SIGMOD 2021**]

[Madelon Hulsebos et al: Sherlock: A Deep Learning Approach to Semantic Data Type Detection. **KDD 2019**]

GitTables (Uni Amsterdam) https://gittables.github.io/

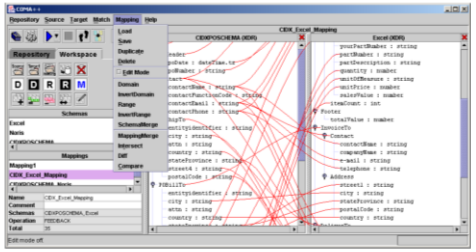
# Schema Detection and Integration, cont.




```
INSERT INTO Orders
  SELECT BELNR,
    SUMME, DATUM
  FROM Bestellungen
```

- **Schema Matching**
  - Semi-automatic mapping of schemas S1 to S2 → **output:** schema correspondences
  - Approaches: Schema- vs instance-based; element- vs structure-based; linguistic vs rules
  - One-to-one matching: stable marriage problem
  - Many-to-one matching: hospitals-residents / college-admission problems

[**Credit:** Erhard Rahm]



- **Schema Mapping**
  - Given two schemas and correspondences, generate transformation program → **output:** executable data transformation
  - Challenges: complex mappings (1:N cardinality), new values, PK-FK relations and nesting, creation of duplicates, different data types, sematic preserving

# Corrupted Data

- **Heterogeneity of Data Sources**
  - Update anomalies on denormalized data / eventual consistency
  - Changes of app/preprocessing over time (US vs us) → inconsistencies
- **Human Error**
  - Errors in semi-manual data collection, laziness (see default values), bias
  - Errors in data labeling (especially if large-scale: crowd workers / users)
- **Measurement/Processing Errors**
  - Unreliable HW/SW and measurement equipment (e.g., batteries)
  - Harsh environments (temperature, movement) → aging

**Uniqueness & duplicates** | **Contradictions & wrong values** | **Missing Values** | **Ref. Integrity**

[**Credit:** Felix Naumann]

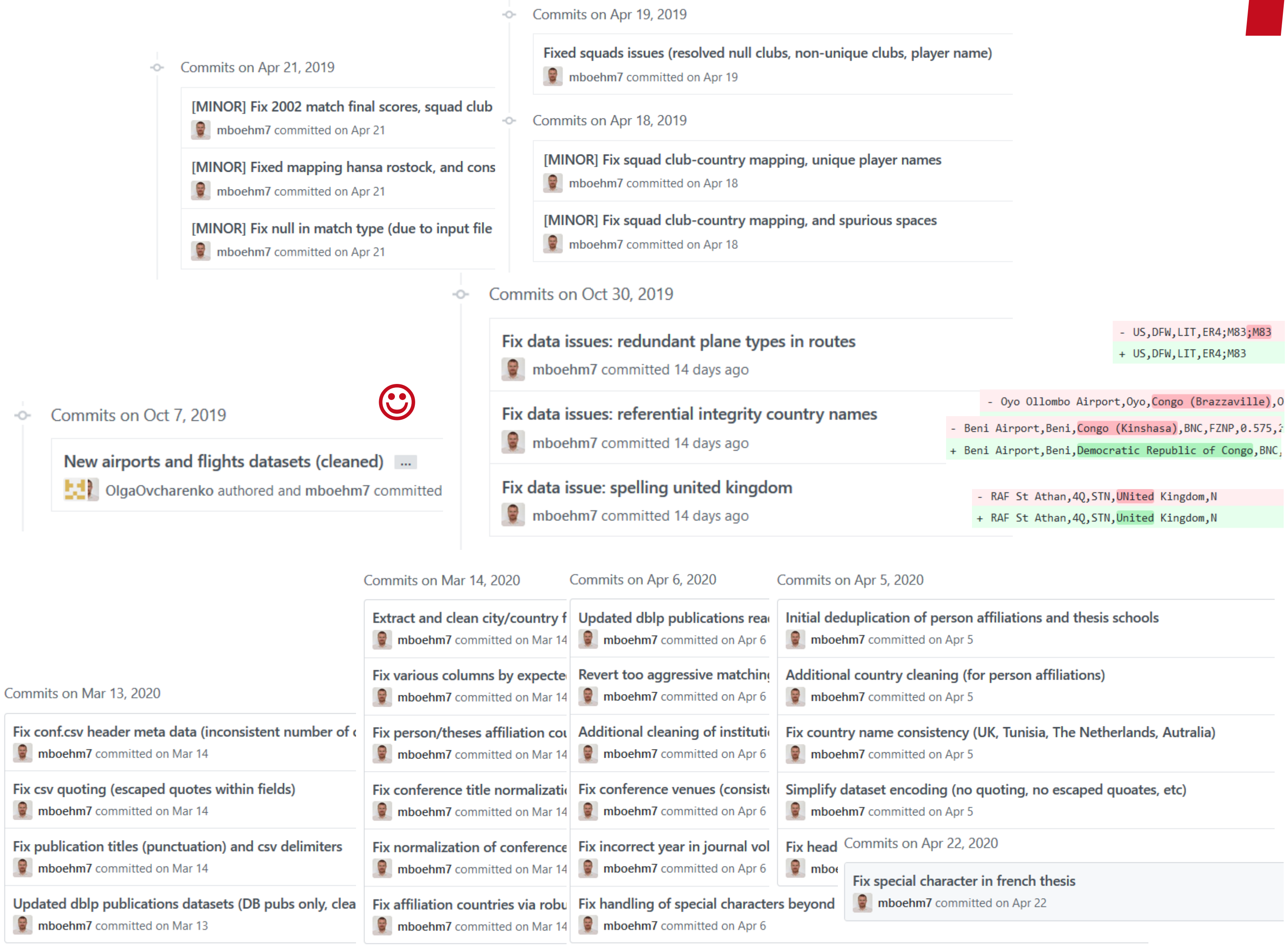
| ID | Name | BDay | Age | Sex | Phone | Zip |
|---|---|---|---|---|---|---|
| 3 | Smith, Jane | 05/06/1975 | 44 | F | 999-9999 | 98120 |
| 3 | John Smith | 38/12/1963 | 55 | M | 867-4511 | 11111 |
| 7 | Jane Smith | 05/06/1975 | 24 | F | 567-3211 | 98120 |

| Zip | City |
|---|---|
| 98120 | San Jose |
| 90001 | Lost Angeles |

**Typos**

# Examples (aka errors are everywhere)

- **DM SS'19** (Soccer World Cups)
- **DM WS'19/20** (Airports and Airlines)
- **DM SS'20** (DBLP Publications)



# Examples (aka errors are everywhere), cont.

- **DM SS'20, cont.**
  **(DBLP Publications)**
  → as a great, curated dataset

**2013**

[b1] Matei A. Zaharia:
**An Architecture for and Fast and General Data Processing on Large Clusters.** University of California, Berkeley, USA, 2013

Wrong meta data from UC Berkeley

> Home > Persons

[–] **Person information**

- *affiliation (PhD 2018):* Improving clinical decisions using correspondences within and across electronic health records

**2018**

[b1] Jen Jian Gong:
**Improving clinical decisions using correspondences within and across electronic health records.** Massachusetts Institute of Technology, Cambridge, USA, 2018

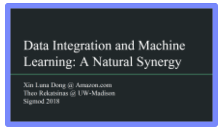
Misplaced data (wrong affiliation, MIT)

- **DM WS'20/21 (Movies and Actors)**
- **DM SS'21 (Summer Olympics)**
- **DM WS'21/22 (AT Elections)**
- **DM SS'22 (Graz Districts)**

1) Best-effort automated cleaning
2) Reference impl data ingestion into relational schema + expected results of query processing
3) Decentralized validation (~600 students)

# Data Integration for ML and ML for DI

[Xin Luna Dong, Theodoros Rekatsinas: Data Integration and Machine Learning: A Natural Synergy. **SIGMOD 2018**]




- **#1 Data Extraction**
  - Extracting structured data from un/semi-structured data
  - Rule- and ML-based extractors, combination w/ CNN
- **#2 Schema Alignment**
  - Schema matching for consolidating data from heterogeneous systems
  - Spatial and Temporal alignment via provenance and query processing (e.g., sensor readings for object along a production pipeline)
- **#3 Entity Linking**
  - Linking records to entities (deduplication)
  - Blocking, pairwise matching, clustering, ML, Deep ML (via entity embedding)
- **#4 Data Fusion**
  - Resolve conflicts, necessary in presence of erroneous data
  - Rule- and ML-based, probabilistic GM, Deep ML (RBMs, graph embeddings)

# Data Validation

**Validity checks on expected shape**
**before training first model**

[Neoklis Polyzotis, Sudip Roy, Steven Euijong Whang, Martin Zinkevich: Data Management Challenges in Production Machine Learning. Tutorial, **SIGMOD 2017**]


Google
Data Management Challenges in Production Machine Learning
Neoklis Polyzotis, Sudip Roy, Steven Whang, Martin Zinkevich

(**Google Research**)

- **Check a feature's min, max, and most common value**
  - Ex: Latitude values must be within the range [-90, 90] or [-π/2, π/2]
- **The histograms of continuous or categorical values are as expected**
  - Ex: There are similar numbers of positive and negative labels
- **Whether a feature is present in enough examples**
  - Ex: Country code must be in at least 70% of the examples
- **Whether a feature has the right number of values (i.e., cardinality)**
  - Ex: There cannot be more than one age of a person

# Data Validation, cont.

- **Constraints and Metrics for quality check UDFs**

| constraint | arguments |
|---|---|
| dimension *completeness* | |
| isComplete | column |
| hasCompleteness | column, udf |
| dimension *consistency* | |
| isUnique | column |
| hasUniqueness | column, udf |
| hasDistinctness | column, udf |
| isInRange | column, value range |
| hasConsistentType | column |
| isNonNegative | column |
| isLessThan | column pair |
| satisfies | predicate |
| satisfiesIf | predicate pair |
| hasPredictability | column, column(s), udf |
| statistics (can be used to verify dimension *consistency* | |
| hasSize | udf |
| hasTypeConsistency | column, udf |
| hasCountDistinct | column |
| hasApproxCountDistinct | column, udf |
| hasMin | column, udf |
| hasMax | column, udf |
| hasMean | column, udf |
| hasStandardDeviation | column, udf |
| hasApproxQuantile | column, quantile, udf |
| hasEntropy | column, udf |
| hasMutualInformation | column pair, udf |
| hasHistogramValues | column, udf |
| hasCorrelation | column pair, udf |
| time | |
| hasNoAnomalies | metric, detector |

| metric |
|---|
| dimension *completeness* |
| Completeness |
| dimension *consistency* |
| Size |
| Compliance |
| Uniqueness |
| Distinctness |
| ValueRange |
| DataType |
| Predictability |
| statistics (can be used to |
| Minimum |
| Maximum |
| Mean |
| StandardDeviation |
| CountDistinct |
| ApproxCountDistinct |
| ApproxQuantile |
| Correlation |
| Entropy |
| Histogram |
| MutualInformation |

[Sebastian Schelter, Dustin Lange, Philipp Schmidt, Meltem Celikel, Felix Bießmann, Andreas Grafberger: Automating Large-Scale Data Quality Verification. **PVLDB 2018**]

(**Amazon Research**)

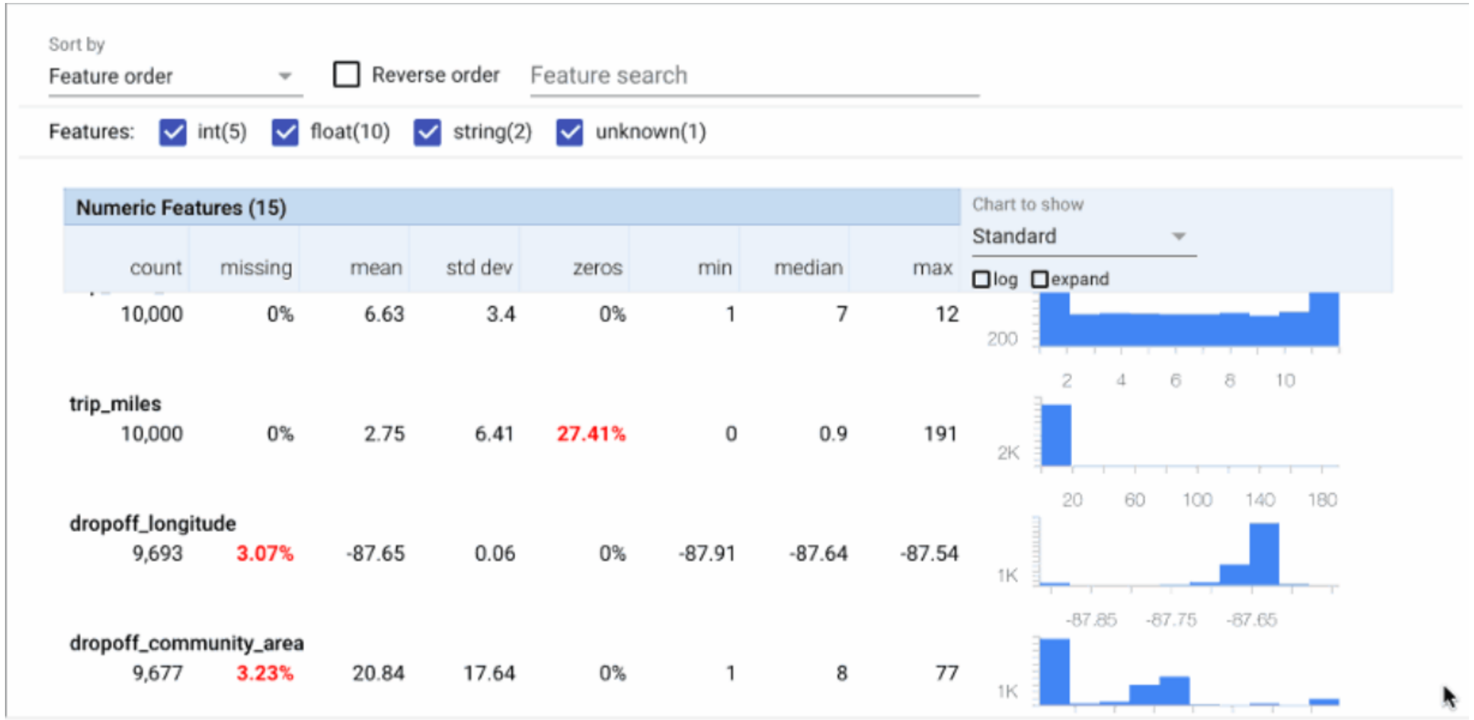
**Organizational Lesson:** benefit of shared vocabulary/procedures

**Technical Lesson:** fast/scalable; reduce manual and ad-hoc analysis

- **Approach**
  - **#1** Quality checks on basic metrics, computed in **Apache Spark**
  - **#2** **Incremental maintenance** of metrics and quality checks

# Data Validation, cont.

- **TensorFlow Data Validation (TFDV)**
  - Library or TFX components
  - Stats, schema extraction, validation checks, anomaly detection




[Mike Dreves; Gene Huang; Zhuo Peng; Neoklis Polyzotis; Evan Rosen; Paul Suganthan: From Data to Models and Back. **DEEM 2020**]

[Eric Breck, Neoklis Polyzotis, Sudip Roy, Steven Whang, Martin Zinkevich: Data Validation for Machine Learning. **MLSys 2019**]

[Emily Caveness et al: TensorFlow Data Validation: Data Analysis and Validation in Continuous ML Pipelines. **SIGMOD 2020**]

(**Google**)

TensorFlow



BIFOLD

# Feature Transformations and Feature Engineering

# Overview Feature Engineering

- **Terminology**
  - Matrix X of m observations (rows) and n features (columns)
  - **Continuous features:** numerical values (aka scale features)
  - **Categorical features:** non-numerical values, represent groups
  - **Ordinal features:** non-numerical values, associated ranking
  - Feature space: multi-dimensional space of features → curse of dimensionality
- **Feature Engineering**
  - Bring multi-modal data and features into numeric representation
  - Use domain expertise to expose predictive features to ML model training
- **Excursus: Representation Learning**
  - Neural networks combine representation learning and model training (pros and cons: learned, repeatable)
  - Mostly homogeneous inputs (e.g., image), research on multi-modal learning

➔ **Principle: If same accuracy, prefer simple model** (cheap, robust, explainable)

# Recoding

- **Summary**
  - Numerical encoding of categorical features (arbitrary strings)
  - Map distinct values to integer domain (potentially combined w/ one-hot)

| City | State |
|---|---|
| San Jose | CA |
| New York | NY |
| San Francisco | CA |
| Seattle | WA |
| New York | NY |
| Boston | MA |
| San Francisco | CA |
| Los Angeles | CA |
| Seattle | WA |

**Dictionaries**

```
{San Jose : 1,
New York : 2,
San Francisco : 3,
Seattle : 4,
Boston : 5,
Los Angeles : 6}

{CA : 1,
NY : 2,
WA : 3,
MA : 4}
```

| City | State |
|---|---|
| 1 | 1 |
| 2 | 2 |
| 3 | 1 |
| 4 | 3 |
| 2 | 2 |
| 5 | 4 |
| 3 | 1 |
| 6 | 1 |
| 4 | 3 |

# Feature Hashing

- **Summary**
  - Numerical encoding of categorical features (arbitrary strings)
  - Hash input to k buckets via hash(value) % k (often combined w/ one-hot)

| City |
|---|
| San Jose |
| New York |
| San Francisco |
| Seattle |
| New York |
| Boston |
| San Francisco |
| Los Angeles |
| Seattle |

**for k = 5:**

```
1993955031 % 5 → 1
1382994575 % 5 → 0
1540367136 % 5 → 1
-661909336 % 5 → 1
1993955031 % 5 → 1
1995575789 % 5 → 4
1540367136 % 5 → 1
-425347233 % 5 → 3
-661909336 % 5 → 1
```

**Efficient**, but **collisions**

| City |
|---|
| 1 |
| 0 |
| 1 |
| 1 |
| 1 |
| 4 |
| 1 |
| 3 |
| 1 |

# Binning (see also Quantization, Binarization)

- **Summary**
  - Encode of numerical features to integer domain (often combined w/ one-hot)
  - **Equi-width:** split (max-min)-range into k equal-sized buckets
  - **Equi-height:** compute data-driven ranges for k balanced buckets

| Sqft |
|---|
| 928.5 |
| 451 |
| 570.3 |
| 1,273 |
| 1,239 |
| 711.3 |
| 1,114 |
| 867 |

```
min = 451
max = 1,273
range = 822
```

**Equal-sized numerical buckets (with k=3)**

```
[451, 725) → 1
[725, 999) → 2
[999, 1,273] → 3
```

Allows modelling small, medium, large apartments

| Sqft-Bins |
|---|
| 2 |
| 1 |
| 1 |
| 3 |
| 3 |
| 1 |
| 3 |
| 2 |

# One-hot Encoding (see also Dummy Coding)

- **Summary**
  - Encode integer feature of cardinality d into sparse 0/1 vector of length d
  - Feature vectors of input features concatenated in sequence

| City | State |
|---|---|
| 1 | 1 |
| 2 | 2 |
| 3 | 1 |
| 4 | 3 |
| 2 | 2 |
| 5 | 4 |
| 3 | 1 |
| 6 | 1 |
| 4 | 3 |

→

| C1 | C2 | C3 | C4 | C5 | C6 | S1 | S2 | S3 | S4 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 |
| 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 0 |
| 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 |

# Hybrid Feature Transformations

- **Combinations**
  - Different encoders for different columns
  - Binning + one-hot encoding
  - Recoding + one-hot encoding
  - Feature hashing + one-hot encoding

**Pipelines of Encoders and Data Preparation Primitives**

- **Top-K Recoding/Feature Hashing**
  - Recoding top-k most frequent values (no collisions in frequent values)
  - Feature Hashing for others (collisions, but bounded #)
  - "Vocabulary encoding" w/ single code for N/A

[Doris Xin et al: Production Machine Learning Pipelines: Empirical Analysis and Optimization Opportunities, **SIGMOD 2021**]

| | City | Count |
|---|---|---|
| 1 | New York | 8,336,817 |
| 2 | San Jose | 1,026,350 |
| 3 | San Francisco | 883,305 |
| | Seattle | 704,352 |
| Feature Hashing k=2 | Boston | 684,379 |
| | … | … |
| | Graz | 291,072 |

- **Infrequent / Unknown Values**
  - E.g., **sk-learn** OneHotEncoder → values below min_frequency in single category

# Derived Features

- **#1 Intercept Computation**
  - Add a column of ones to X for computing the intercept as a weight
  - Applies to regression and classification

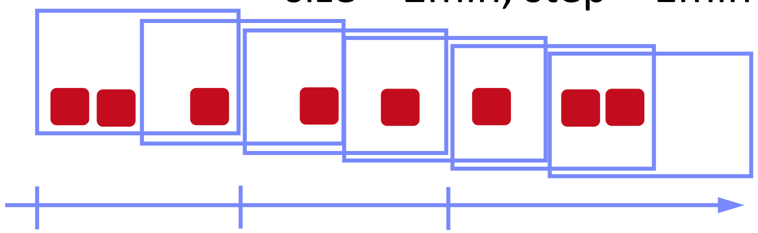
```
X = cbind(X,
  matrix(1, nrow(X), 1));
```

- **#2 Non-Linear Relationships**
  - Can be explicitly materialized as feature combinations
  - Example: Assumptions of underlying physical system
  - Arbitrary complex feature interactions: e.g., $X_1$^2 * $X_2$

```
// y ~ b1*X1 + b2*X1^2
X = cbind(X, X^2);
```

- **#3 Windowing**
  - Tumbling or sliding window over time series
  - Compute aggregates or existence of events

size = 2min, step = 1min



# NLP Features

- **Basic NLP Feature Extraction**
  - **Sentence/word tokenization:** split into sentences/words (e.g., via stop words)
  - **Part of Speech (PoS) tagging:** label words verb, noun, adjectives (syntactic)
  - **Semantic role labeling:** label entities with their roles in actions (semantic)

**Who** did **what** to **whom** at **where**?

- **Bag of Words (BOW) and N-Grams**
  - Represent sentences as **bag** (multisets)

A B C A B E.
A D E D E D.

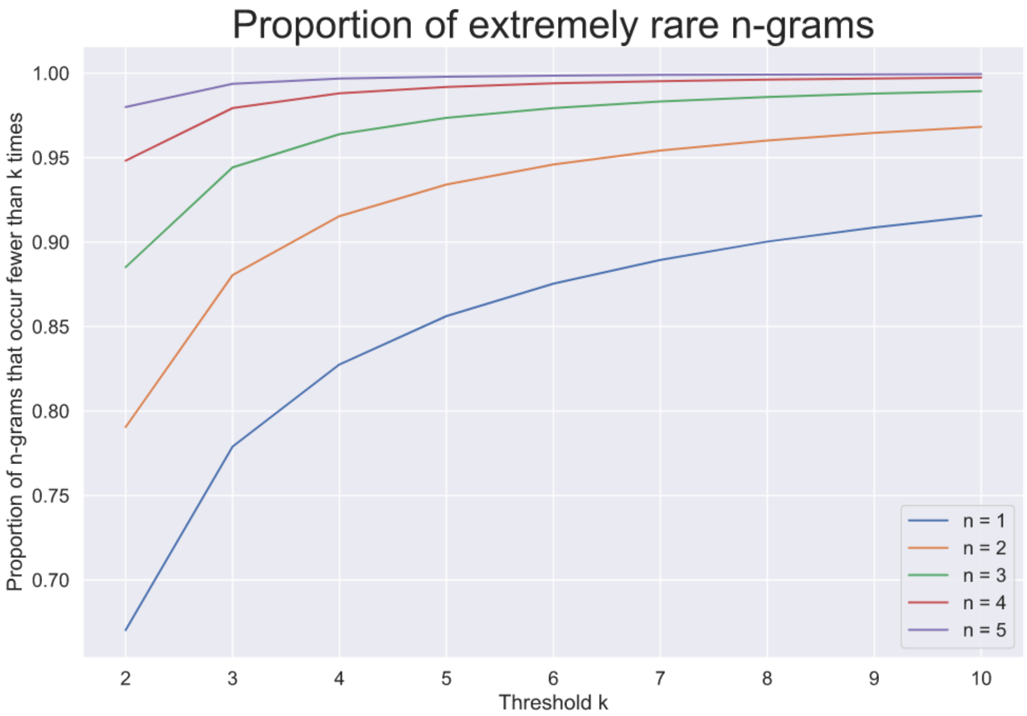
| A | B | C | D | E |
|---|---|---|---|---|
| 2 | 2 | 1 | 0 | 1 |
| 1 | 0 | 0 | 3 | 2 |

  - **Bi-grams:** bag-of-words for 2-sequences of words (order preserving)
  - **N-grams:** generalization of bi-grams to arbitrary-length sequences

# NLP Features, cont.

[John Hallman: Efficient Featurization of Common N-grams via Dynamic Programming. https://sisudata.com/blog/efficient-featurization-common-ngrams-via-dynamic-programming, 2021]

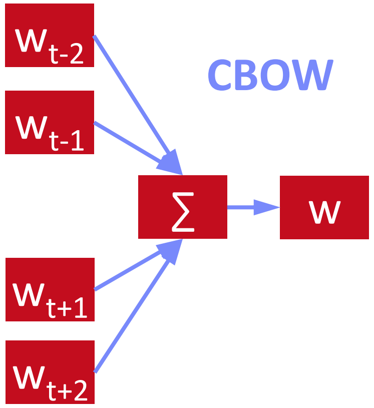
- **Common N-Grams**
  - Prune n-grams that appear <5 times, → 99.3% reduction
  - Lattice-based pruning (Apriori monotonicity property)
- **Example**
  - Amazon Reviews Dataset
  - 67% of words appear just once

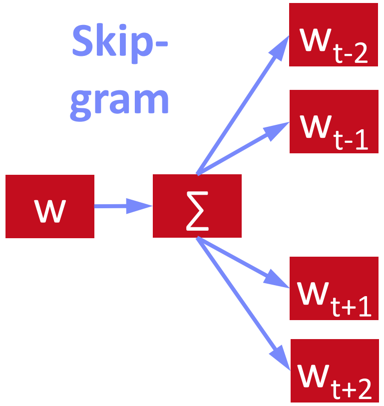


# NLP Features, cont.

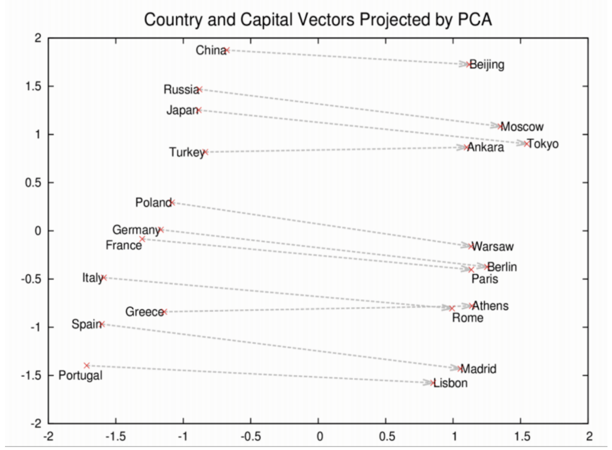
[Tomas Mikolov, Kai Chen, Greg Corrado, Jeffrey Dean: Efficient Estimation of Word Representations in Vector Space. **ICLR (Workshop) 2013**]
github.com/dav/word2vec

- **Word Embeddings**
  - Trained (word → vector) mappings (~ 50-300 dims)
  - **Word2vec:** continuous bag-of-words (CBOW) or continuous skip-gram
  - Subsampling frequent words
  - **Semantic preserving arithmetic operations** (+ ~ * of context distributions)




`vec(Paris) ≈ vec(Berlin) – vec(Germany) + vec(France)`




[https://wiki.pathmind.com/word2vec]

- **Follow-up Work**
  - Often pre-trained word embeddings; fine-tuning if necessary for task/domain
  - Various extensions/advancements: **Sentence2Vec**, **Doc2Vec**, **Node2Vec**
  - **BERT**, **RoBERTa**, **ALBERT**, **StructBERT** / **GPT**

[Jacob Devlin et al. : **BERT:** Pre-training of Deep Bidirectional Transformers for Language Understanding. **NAACL-HLT** (1) 2019]

[Tom B. Brown et al: Language Models are Few-Shot Learners. (**GPT-3**), **CoRR 2020**, https://arxiv.org/pdf/2005.14165.pdf]

# Example Spark ML

- **API Design**
  - **Transformers:** Feature transformations and learned models
  - **Estimators:** Algorithm that can be fit to produce a transformer
  - Compose ML pipelines from chains of transformers and estimators

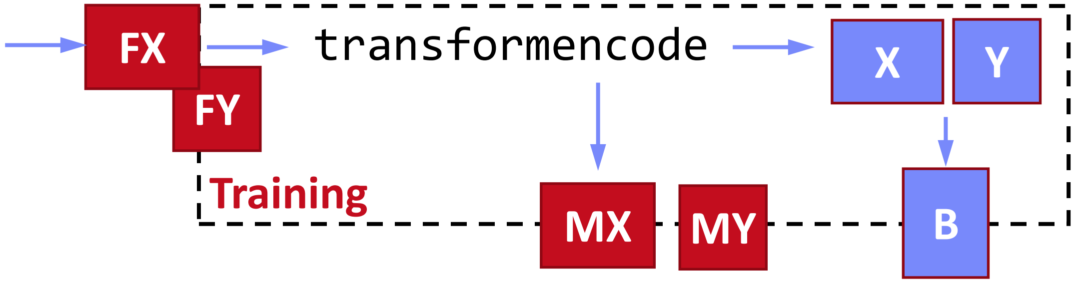
- **Example Pipeline**

```
// define pipeline stages
tokenizer = Tokenizer(inputCol="text", outputCol="words")
hashingTF = HashingTF(inputCol=tokenizer.getOutputCol(),
                      outputCol="features")
lr = LogisticRegression(maxIter=10, regParam=0.001)

// create pipeline transformer via fit
pipeline = Pipeline(stages=[tokenizer, hashingTF, lr])
model = pipeline.fit(training)

// use of resulting ML pipeline
prediction = model.transform(test)
```

[https://spark.apache.org/docs/2.4.3/ml-pipeline.html]

# Example SystemML/SystemDS

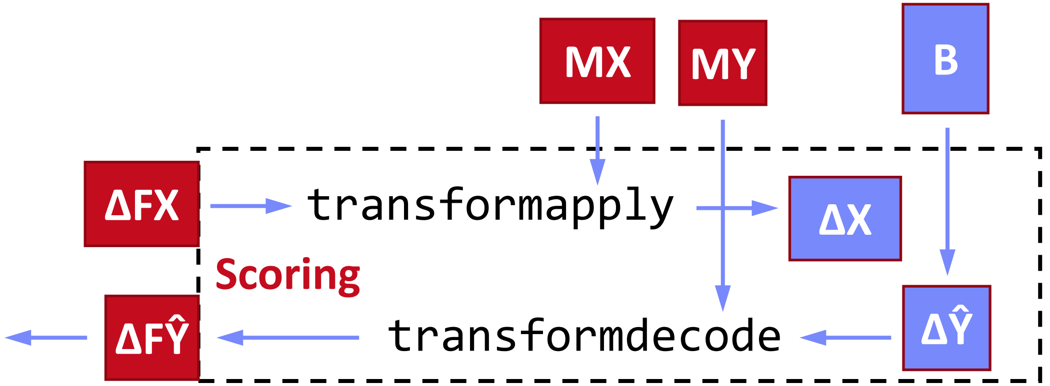
- **Feature Transformation during Training**




```
# read tokenized words
FX = read(“./input/FX”, data_type=FRAME); # sentence id, word, count
FY = read(“./input/FY”, data_type=FRAME); # sentence id, labels

# encode and one-hot encoding
[X0, MX] = transformencode(target=FX, spec=“{recode:[2]}”);
[Y0, MY] = transformencode(target=FY, spec=“{recode:[2]}”);
X = table(X0[,1], X0[,2], X0[,3]); # bag of words
Y = table(Y0[,1], Y0[,2]);         # bag of words

# model training via multi-label, multi-nominal logical regression
B = mlogreg(X, Y);
```

# Example SystemML/SystemDS, cont.

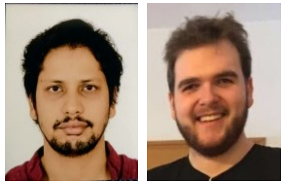
- **Feature Transformation during Scoring**




```
# read tokenized words of test sentences
dFX = read("./input/dFX", data_type=FRAME); # sentence id, word, count

# encode and one-hot encoding
dX0 = transformapply(target=dFX, spec="{recode:[2]}", meta=MX);
dX = table(dX0[,1], dX0[,2], dX0[,3]); # bag of words

# model scoring and postprocessing (reshape, attach sentence ID, etc)
dYhat = (X %*% B) >= theta; ...;

# decode output labels: sentence id, label word
dFYhat = transformdecode(target=dYhat, spec="{recode:[2]}", meta=MY);
```

# Parallelizing Feature Transformations

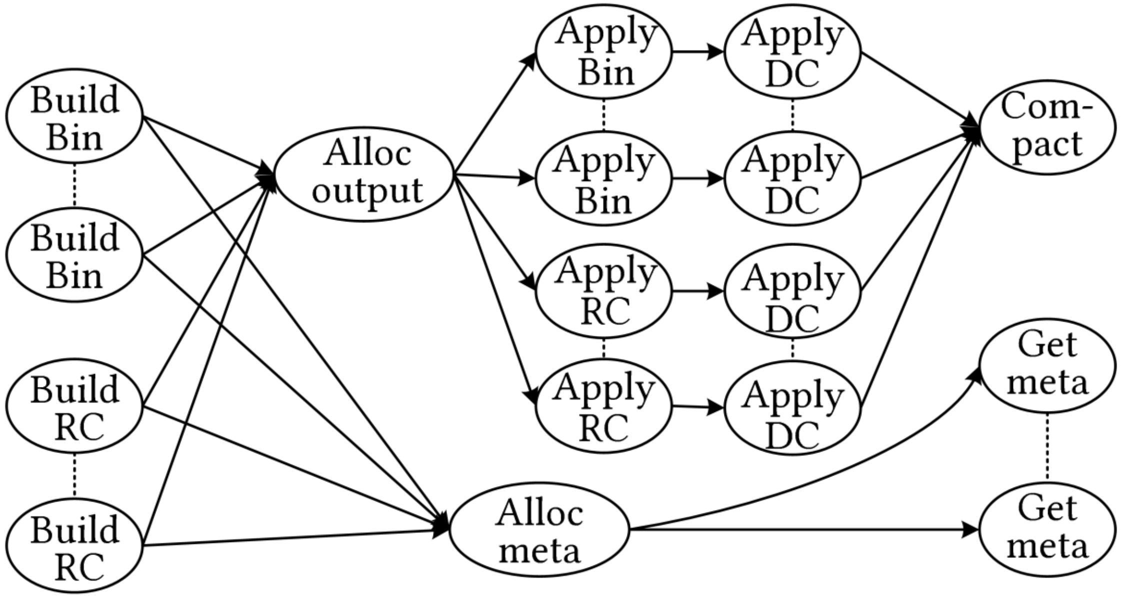
[Arnab Phani, Lukas Erlbacher, Matthias Boehm: UPLIFT: Parallelization Strategies for Feature Transformations in Machine Learning Workloads, **PVLDB 2022**]



- **Feature Transformations**
  - **Numeric:** pass-through, H/W binning + one-hot
  - **Categorical:** recoding, feature hashing + one-hot
  - **Text/Graph embeddings**

large dictionaries; many build (groupby, sort) and apply (FK-PK join) ops

- **Parallelization**
  - Fine-grained, **future-based task graph**
  - Optimization via task graph rewrites (s.t. mem budget)
  - Different operations and **parallelization strategies**




- **FTBench**
  - 15 feature transformation use cases

# Data Preparation and Cleaning

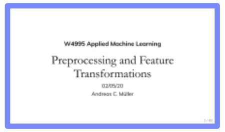
# Standardization/Normalization

- **#1 Standardization**
  - Centering and scaling to mean 0 and variance 1
  - **Ensures well-behaved training** (and distance computation)
  - **Densifying operation** / **NaNs**
  - **Batch normalization** in DNN: standardization of activations

```
X = X - colMeans(X);
X = X / sqrt(colVars(X));

X = replace(X, pattern=NaN,
  replacement=0); #robustness
```

- **#2 (Min-Max) Normalization**
  - Rescale values into common range [0,1]
  - **Avoid bias to large-scale features**
  - Does not handle outliers

```
X = (X - colMins(X))
  / (colMaxs(X) - colMins(X));
```




**Recommended Reading**

[Andreas C. Mueller: Preprocessing and Feature Transformations, **Applied ML Lecture 2020**, https://www.youtube.com/watch?v=XpOBSaktb6s]

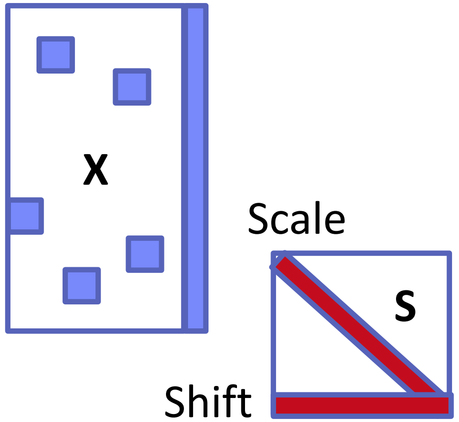
# Standardization/Normalization, cont.

- **#3 Deferred Standardization**
  - Avoid densifying dataset upfront by pushing standardization into inner loop iterations
  - Let matrix-multiplication chain optimization + rewrites do the rest

[**Credit:** Alexandre (Sasha) V. Evfimievski]

- **Example GLM/lmCG**

Input w/ column of ones (intercept)



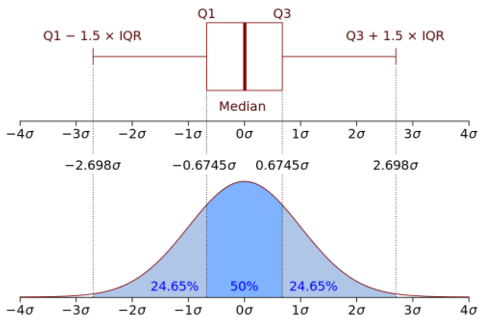

```
# operation w/ early standardized X
q = t(X) %*% diag(w) %*% X %*% B;
```

**Substitute X with X %*% S**

```
# operation w/ deferred standardization
q = t(S) %*% t(X) %*% diag(w)
   %*% X %*% S %*% B;
```

```
q = t(S) %*% (t(X) %*% (diag(w)
   %*% (X %*% (S %*% B))));
```

# Winsorizing and Trimming




[**Credit:** https://en.wikipedia.org]

- **Recap: Quantiles**
  - Quantile $Q_p$ w/ $p \in (0,1)$ defined as $P[X \leq x] = p$

- **Winsorizing**
  - **Replace** tails of data distribution at user-specified threshold
  - Quantiles / std-dev ➔ Reduce skew

```
# compute quantiles for lower and upper
ql = quantile(X, 0.05);
qu = quantile(X, 0.95);

# replace values outside [ql,qu] w/ ql and qu
Y = ifelse(X < ql, ql, X);
Y = ifelse(Y > qu, qu, Y);
```

- **Truncation/Trimming**
  - **Remove** tails of data distribution at user-specified threshold

```
# remove values outside [ql,qu]
I = X < qu | X > ql;
Y = removeEmpty(X, “rows”, select = I);
```

**SystemDS:**
`winsorize()`
`outlier()`
`outlierByIQR()`
`outlierBySd()`

- **Largest Difference from Mean**

```
# determine largest diff from mean
I = (colMaxs(X)-colMeans(X))
  > (colMeans(X)-colMins(X));
Y = ifelse(xor(I,op), colMaxs(X), colMins(X));
```

# Constraints and Outliers

- **(Semi-)Automatic Approach: Expectations!**
  - PK → Values must be unique and defined (not null)
  - Exact PK-FK → Inclusion dependencies
  - Noisy PK-FK → Robust inclusion dependencies |R[X]∈S[Y]| / |R[X]| > δ
  - Semantics of attributes → Value ranges / # distinct values
  - Invariant to capitalization: Patterns → regular expressions
- **Formal Constraints**
  - Functional dependencies (FD), conditional FDs (CFD), metric dependencies
  - Inclusion dependencies, matching dependencies
  - Denial constraints
- **Outlier Terminology**
  - **Outlier Detection:** detect and remove unwanted data points
  - **Anomaly Detection:** detect and extract rare/unusual/interesting events

**Route** **Planes**
(Airline, From, To)

```
- US,DFW,LIT,ER4;M83;M83
+ US,DFW,LIT,ER4;M83
```

Age=9999?

```
- RAF St Athan,4Q,STN,UNited Kingdom,N
+ RAF St Athan,4Q,STN,United Kingdom,N
```

2019-11-15 vs Nov 15, 2019

$$\forall t_\alpha t_\beta \in R: \neg(t_\alpha.Role = t_\beta.Role \wedge t_\alpha.City = 'NYC' \wedge t_\beta.City \neq 'NYC' \wedge t_\alpha.Salary < t_\beta.Salary)$$

# Outliers and Outlier Detection

- **Types of Outliers**
  - **Point outliers:** single data points far from the data distribution
  - **Contextual outliers:** noise or other systematic anomalies in data
  - **Sequence (contextual) outliers:** sequence of values w/ abnormal shape/agg
  - Univariate vs multivariate analysis
  - Beware of underlying assumptions (distributions)

[Varun Chandola, Arindam Banerjee, Vipin Kumar: Anomaly detection: A survey. **ACM Comput. Surv. 2009**]

- **Types of Outlier Detection**
  - **Type 1 Unsupervised:** No prior knowledge of data, similar to unsupervised **clustering** → **expectations:** distance, # errors
  - **Type 2 Supervised:** Labeled normal and abnormal data, similar to supervised **classification**
  - **Type 3 Normal Model:** Represent normal behavior, similar to **pattern recognition** → **expectations:** rules/constraints

[Victoria J. Hodge, Jim Austin: A Survey of Outlier Detection Methodologies. **Artif. Intell. Rev. 2004**]

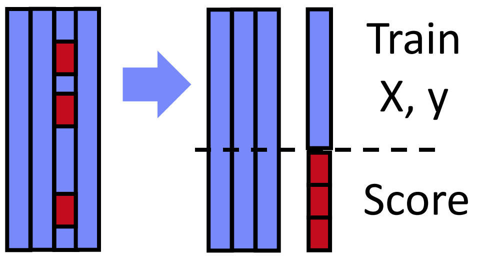
# Missing Value Imputation

- **Missing Value**
  - Application context defines if 0 is missing value or not
  - If differences between 0 and missing values, use NA or NaN
- **Basic Value Imputation**
  - General-purpose: replace by user-specified **constant**
  - **Continuous variables:** replace by **mean**
  - **Categorical variables:** replace by **median** or **mode**
- **Iterative Algorithms** (**chained-equation imputation**)
  - Train ML model to predict missing information (feature k → label, split data into observed/missing)
  - Noise reduction: feature subsets + averaging
- **Dynamic Imputation**
  - Data exploration w/ on-the-fly imputation
  - Optimal placement of imputation operations

MCAR

MAR

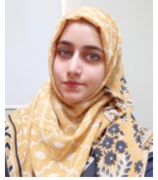
**SystemDS:**
`mice()`




[Jose Cambronero, John K. Feser, Micah Smith, Samuel Madden: Query Optimization for Dynamic Imputation. **PVLDB 2017**]

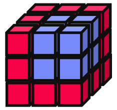
# Data Cleaning Pipelines

[Shafaq Siddiqi, Roman Kern, Matthias Boehm: SAGA: A Scalable Framework for Optimizing Data Cleaning Pipelines for Machine Learning Applications, **SIGMOD 2024**]



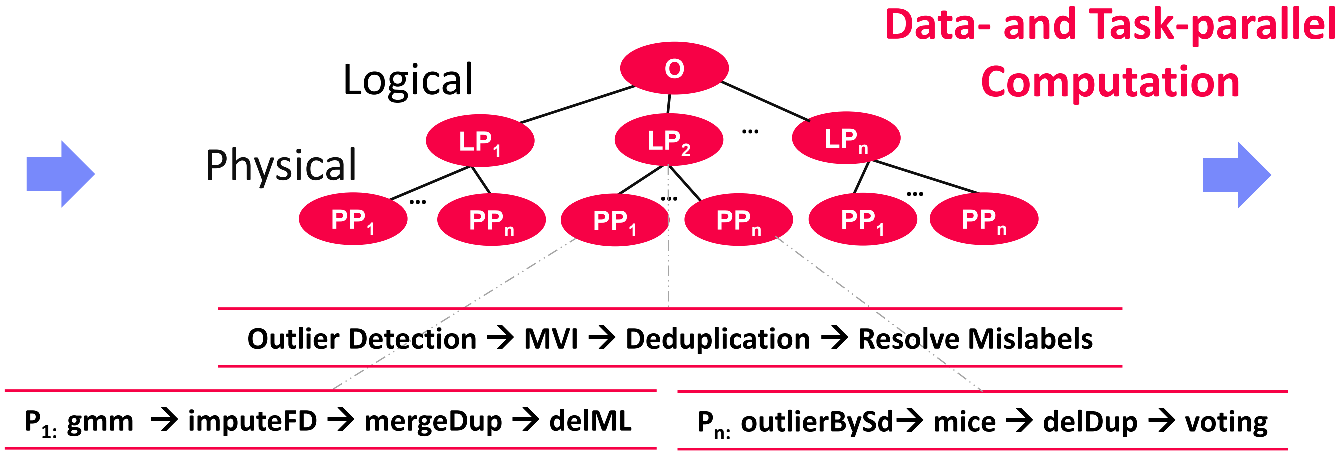
- **Automatic Generation of Cleaning Pipelines**
  - Library of robust, parameterized **data cleaning primitives**,
  - **Enumeration of DAGs** of primitives & **hyper-parameter optimization** (evolutionary, HB)

Data Samples



**Target App**

Rules/Objectives




Top-k Pipelines

**Debugging**

| University | Country |
|---|---|
| TU Graz | Austria |
| TU Graz | Austria |
| TU Graz | Germany |
| IIT | India |
| IIT | IIT |
| IIT | Pakistan |
| IIT | India |
| SIBA | Pakistan |
| SIBA | null |
| SIBA | null |

**Dirty Data**

| University | Country |
|---|---|
| TU Graz | Austria |
| TU Graz | Austria |
| TU Graz | Austria |
| IIT | India |
| IIT | India |
| IIT | India |
| IIT | India |
| SIBA | Pakistan |
| SIBA | Pakistan |
| SIBA | Pakistan |

After **imputeFD(0.5)**

| A | B | C | D |
|---|---|---|---|
| 0.77 | 0.80 | 1 | 1 |
| 0.96 | 0.12 | 1 | 1 |
| 0.66 | 0.09 | null | 1 |
| 0.23 | 0.04 | 17 | 1 |
| 0.91 | 0.02 | 17 | null |
| 0.21 | 0.38 | 17 | 1 |
| 0.31 | null | 17 | 1 |
| 0.75 | 0.21 | 20 | 1 |
| null | null | 20 | 1 |
| 0.19 | 0.61 | 20 | 1 |
| 0.64 | 0.31 | 20 | 1 |

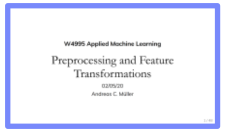
**Dirty Data**

| A | B | C | D |
|---|---|---|---|
| 0.77 | 0.80 | 1 | 1 |
| 0.96 | 0.12 | 1 | 1 |
| 0.66 | 0.09 | 17 | 1 |
| 0.23 | 0.04 | 17 | 1 |
| 0.91 | 0.02 | 17 | 1 |
| 0.21 | 0.38 | 17 | 1 |
| 0.31 | 0.29 | 17 | 1 |
| 0.75 | 0.21 | 20 | 1 |
| 0.41 | 0.24 | 20 | 1 |
| 0.19 | 0.61 | 20 | 1 |
| 0.64 | 0.31 | 20 | 1 |

After **MICE**

# Summary & QA

[Andreas C. Mueller: Preprocessing and Feature Transformations, **Applied ML Lecture 2020**]


W4995 Applied Machine Learning

Preprocessing and Feature Transformations

02/05/20

Andreas C. Müller

- **Data Acquisition, Integration, and Validation**
- **Feature Transformations and Feature Engineering**
- **Data Preparation and Cleaning**

"Coming up with features is difficult, time-consuming, requires expert knowledge. "Applied machine learning" is basically feature engineering"
– Andrew Ng

➔ **Trend towards "Data-centric AI"** (since 2021/2022)

- **Next Lectures** (Part B)
  - **10 Model Selection and Management** [Jun 29, **virtual only**]
  - **11 Model Debugging, Fairness, Explainability** [Jul 06]
  - **12 Model Serving Systems and Techniques** [Jul 13]