SCIENCE
PASSION
TECHNOLOGY

Architecture of ML Systems
09 Data Acquisition and Preparation

Matthias Boehm

Graz University of Technology, Austria
Computer Science and Biomedical Engineering
Institute of Interactive Systems and Data Science
BMK endowed chair for Data Management

Last update: May 18, 2022

Announcements/Org

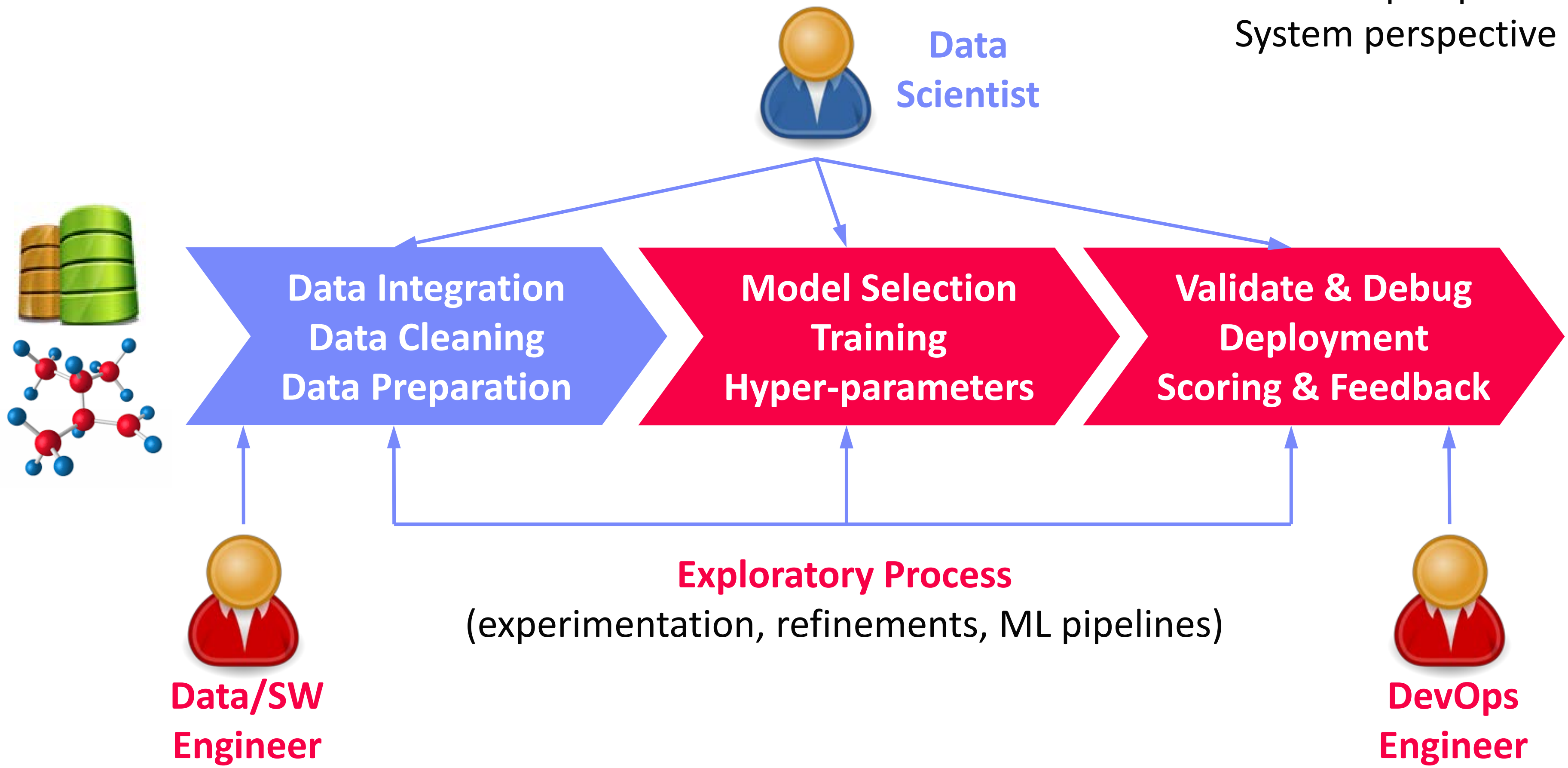
- **#1 Video Recording**
  - Link in **TeachCenter** & **TUbe** (lectures will be public)
  - Hybrid: HSi13 / https://tugraz.webex.com/meet/m.boehm
  - **Apr 25:** no more COVID restrictions at TU Graz

- **#2 Projects and Oral Exams**
  - Precondition: completed exercise/project by **Jun 17 EOD**
  - Created doodle for exam slot selection (~35): https://doodle.com/meeting/participate/id/eER4P10a

Q&A

Recap: The Data Science Lifecycle

Data-centric View:
Application perspective
Workload perspective
System perspective

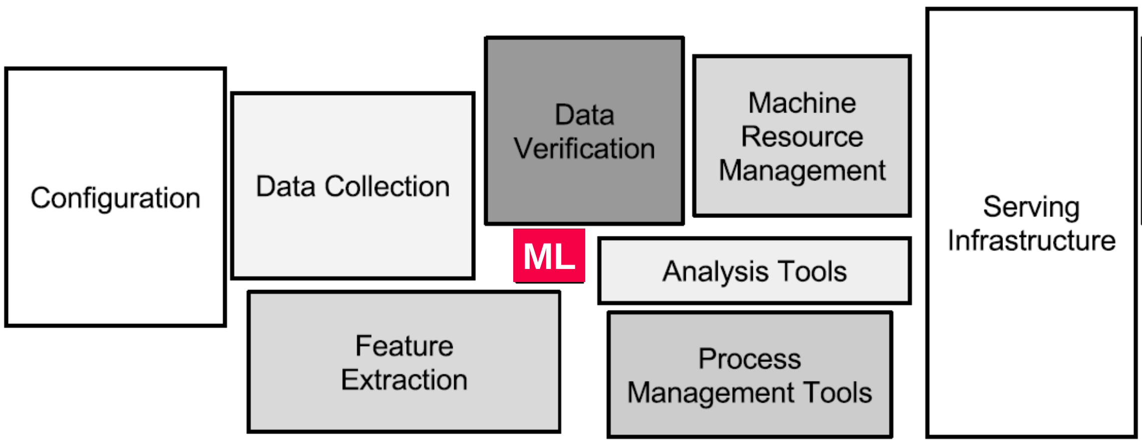


The 80% Argument

- **Data Sourcing Effort**
  - Data scientists spend **80-90% time** on finding, integrating, cleaning datasets

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

- **Technical Debts in ML Systems**



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

  - 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

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)
(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

[**Credit:** Albert Maier]

- **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
- **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

```
%%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
```

- **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)

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 relevant datasets in **data lakes**
  - **Metadata and provenance**
  - Augment data with open and linked data sources

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

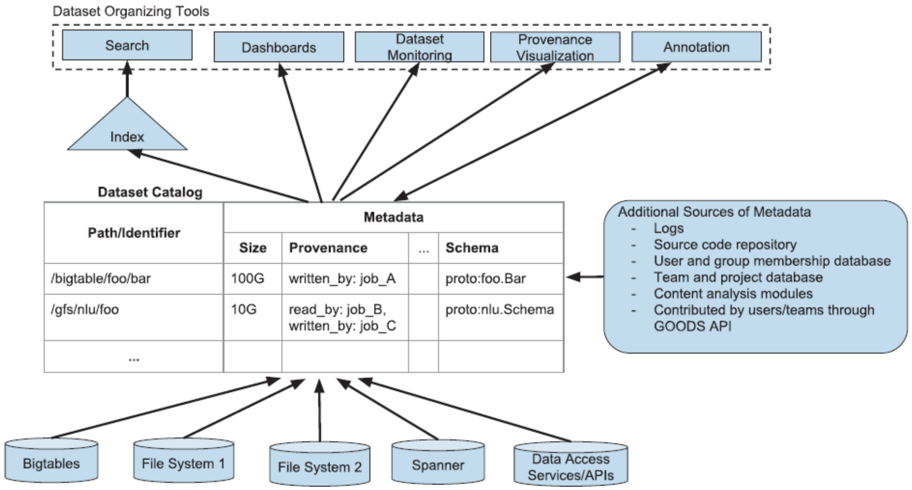
[Dan Brickley, Matthew Burgess, Natasha F. Noy: Google Dataset Search: Building a search engine for datasets in an open Web ecosystem. **WWW 2019**]

- **Examples**

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 models

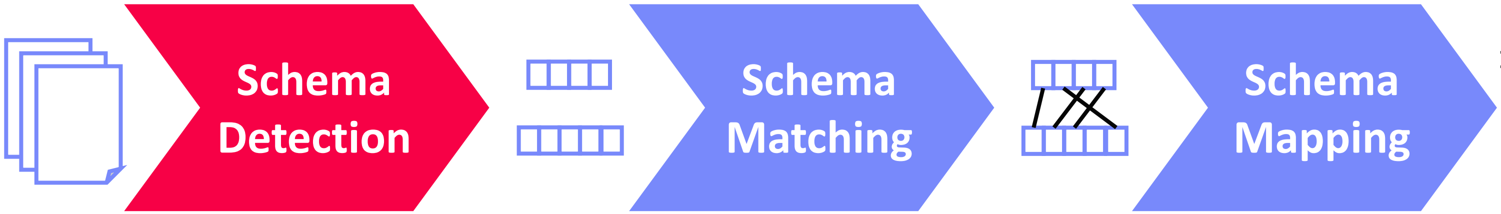
[Vraj Shah, Jonathan Lacanlale, Premanand Kumar, Kevin Yang, Arun Kumar: Towards Benchmarking Feature Type Inference for AutoML Platforms, **SIGMOD 2021**]

- **Semantic Type Detection**
  - Extract common feature types (e.g., location, date, rank, name)

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

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

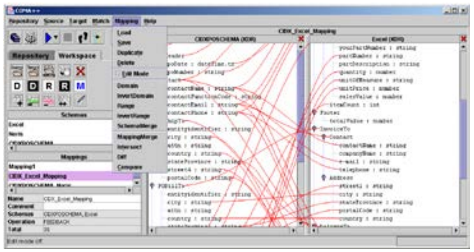
Schema Detection and Integration, cont.




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

- **Schema Matching**
  - Semi-automatic mapping of schema S1 to schema S2
    → **output:** schema correspondences
  - **Approaches:** Schema- vs instance-based; element- vs structure-based; linguistic vs rules
  - Global schema matching
    - One-to-one: stable marriage problem
    - Many-to-one: 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]

<u>ID</u>	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)**

Commits on Apr 21, 2019

- [MINOR] Fix 2002 match final scores, squad club
  mboehm7 committed on Apr 21
- [MINOR] Fixed mapping hansa rostock, and cons
  mboehm7 committed on Apr 21
- [MINOR] Fix null in match type (due to input file
  mboehm7 committed on Apr 21

Commits on Apr 19, 2019

- Fixed squads issues (resolved null clubs, non-unique clubs, player name)
  mboehm7 committed on Apr 19

Commits on Apr 18, 2019

- [MINOR] Fix squad club-country mapping, unique player names
  mboehm7 committed on Apr 18
- [MINOR] Fix squad club-country mapping, and spurious spaces
  mboehm7 committed on Apr 18

- **DM WS'19/20 (Airports and Airlines)**

Commits on Oct 7, 2019

- New airports and flights datasets (cleaned) ...
  OlgaOvcharenko authored and mboehm7 committed

Commits on Oct 30, 2019

- Fix data issues: redundant plane types in routes
  mboehm7 committed 14 days ago

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

- Fix data issues: referential integrity country names
  mboehm7 committed 14 days ago

```
- Oyo Ollombo Airport,Oyo,Congo (Brazzaville),O
- Beni Airport,Beni,Congo (Kinshasa),BNC,FZNP,0.575,
+ Beni Airport,Beni,Democratic Republic of Congo,BNC,
```

- Fix data issue: spelling united kingdom
  mboehm7 committed 14 days ago

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

- **DM SS'20 (DBLP Publications)**

Commits on Mar 13, 2020

- Fix conf.csv header meta data (inconsistent number of
  mboehm7 committed on Mar 14
- Fix csv quoting (escaped quotes within fields)
  mboehm7 committed on Mar 14
- Fix publication titles (punctuation) and csv delimiters
  mboehm7 committed on Mar 14
- Updated dblp publications datasets (DB pubs only, clea
  mboehm7 committed on Mar 13

Commits on Mar 14, 2020

- Extract and clean city/country f
  mboehm7 committed on Mar 14
- Fix various columns by expecte
  mboehm7 committed on Mar 14
- Fix person/theses affiliation cou
  mboehm7 committed on Mar 14
- Fix conference title normalizati
  mboehm7 committed on Mar 14
- Fix normalization of conference
  mboehm7 committed on Mar 14
- Fix affiliation countries via robu
  mboehm7 committed on Mar 14

Commits on Apr 6, 2020

- Updated dblp publications rea
  mboehm7 committed on Apr 6
- Revert too aggressive matchin
  mboehm7 committed on Apr 6
- Additional cleaning of instituti
  mboehm7 committed on Apr 6
- Fix conference venues (consist
  mboehm7 committed on Apr 6
- Fix incorrect year in journal vol
  mboehm7 committed on Apr 6
- Fix handling of special characters beyond
  mboehm7 committed on Apr 6

Commits on Apr 5, 2020

- Initial deduplication of person affiliations and thesis schools
  mboehm7 committed on Apr 5
- Additional country cleaning (for person affiliations)
  mboehm7 committed on Apr 5
- Fix country name consistency (UK, Tunisia, The Netherlands, Autralia)
  mboehm7 committed on Apr 5
- Simplify dataset encoding (no quoting, no escaped quoates, etc)
  mboehm7 committed on Apr 5
- Fix head
  mboe

Commits on Apr 22, 2020

- Fix special character in french thesis
  mboehm7 committed on Apr 22

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

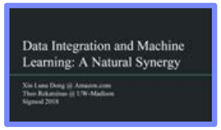
Misplaced data (wrong affiliation, MIT)

- **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

Sanity 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**]


Data Management Challenges in Production Machine Learning

(**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.

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

(**Amazon Research**)

- **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

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.

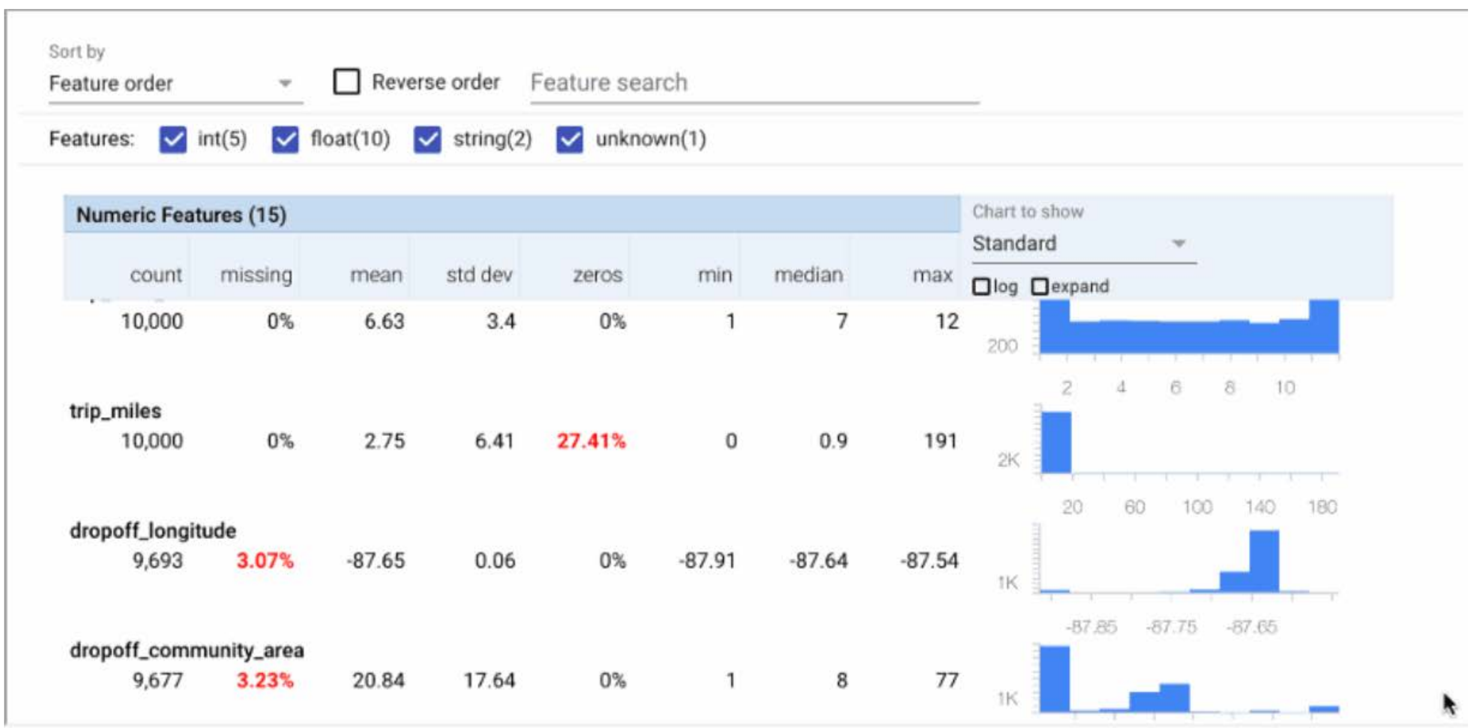
[Mike Dreves; Gene Huang; Zhuo Peng; Neoklis Polyzotis; Evan Rosen; Paul Suganthan: From Data to Models and Back. **DEEM 2020**]

[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**]

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

(**Google**)



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 can be viewed as combined 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"

[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

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

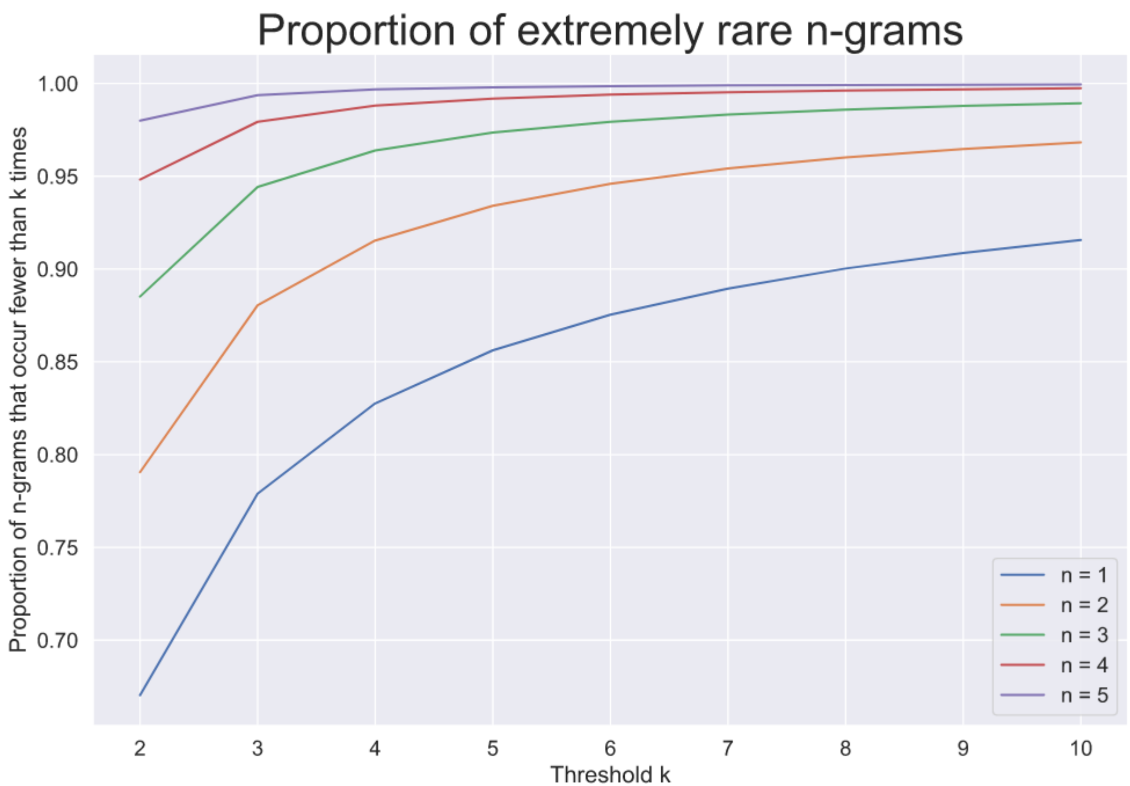
  - **Bi-grams:** bag-of-words for 2-sequences of words (order preserving)
  - **N-grams:** generalization of bi-grams to arbitrary-length sequences

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

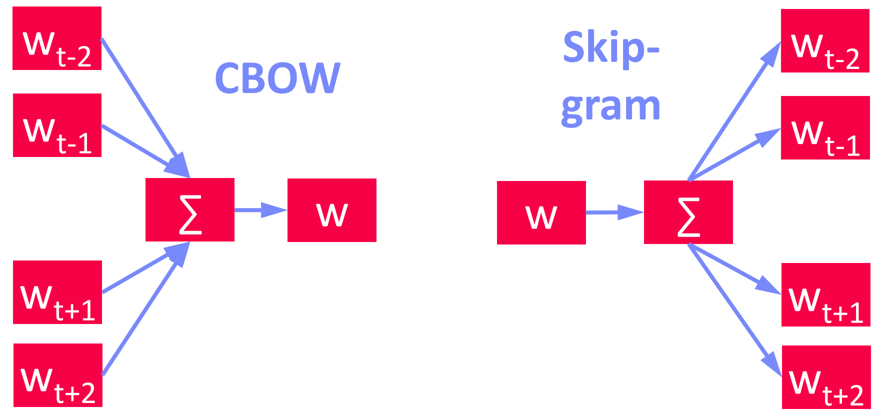


NLP Features, cont.

[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)

- **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**

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

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

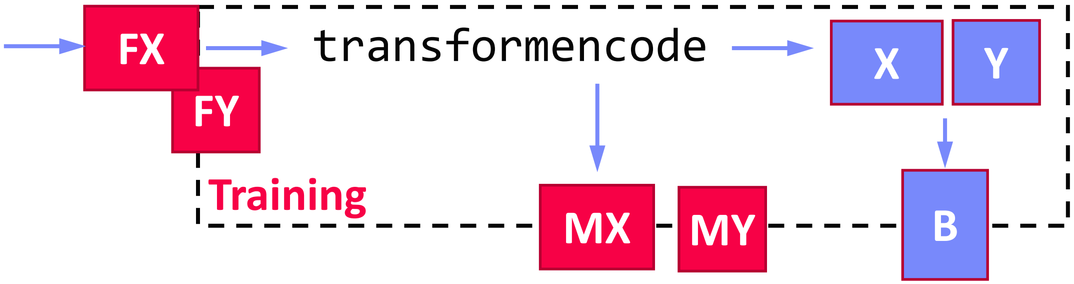
- **Example Pipeline**

```
// 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

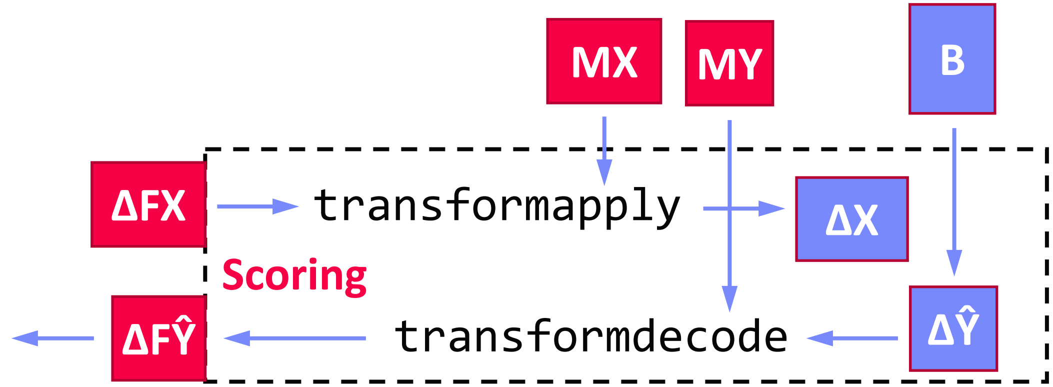
- **Feature Transformation during Training**




```
# 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);
```

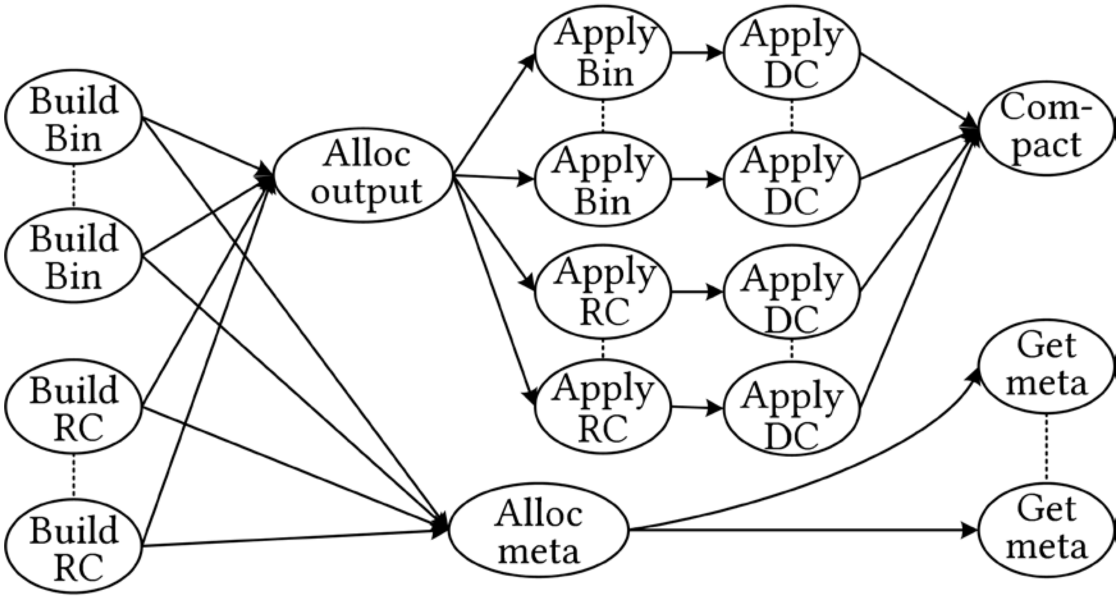
Parallelizing Feature Transformations

[**under submission**]

- **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**



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

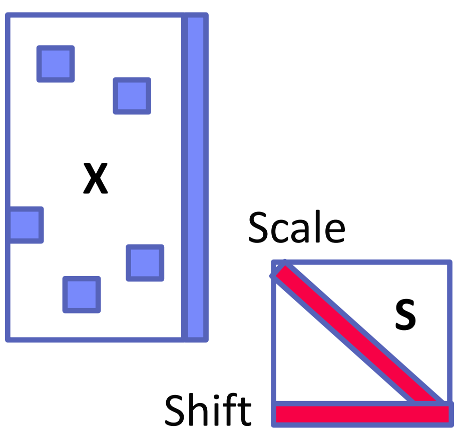
[Andreas C. Mueller: Preprocessing and Feature Transformations, **Applied ML Lecture 2020**, https://www.youtube.com/watch?v=XpOBSaktb6s]

Standardization/Normalization, cont.

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

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

Input w/ column of ones (intercept)



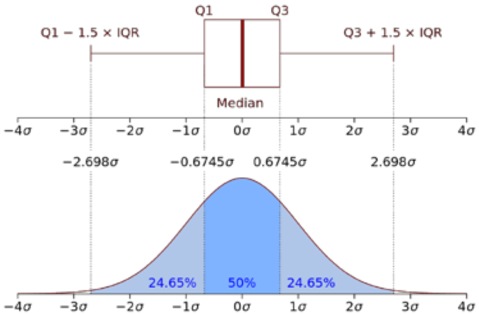

```
# operation w/ early standardized X
q = t(X) %*% diag(w) %*% X %*% B;
```

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);
```

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

- **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);
```

- **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

Route **Planes**

(Airline, From, To)

- **(Semi-)Automatic Approach: Expectations!**
  - PK → Values must be unique and defined (not null)

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

  - 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

Age=9999?

  - Invariant to capitalization
    Patterns → regular expressions

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

2019-11-15 vs Nov 15, 2019

- **Formal Constraints**
  - Functional dependencies (FD), conditional FDs (CFD), metric dependencies
  - Inclusion dependencies, matching dependencies
  - Denial constraints

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

- **Outlier Terminology**
  - **Outlier Detection:** detect and remove unwanted data points
  - **Anomaly Detection:** detect and extract rare/unusual/interesting events

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**]

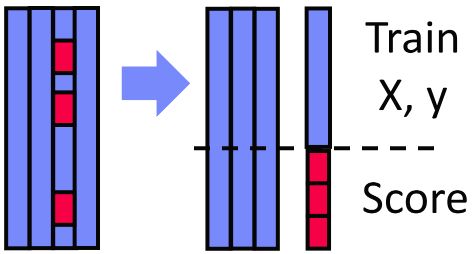
- **Types of Outlier Detection**
  - **Type 1 Unsupervised:** No prior knowledge of data, similar to unsupervised **clustering** → **expectations:** distance, # errors
  - **Type 2 Supervised:** Labeled normal and abnormal data, similar to supervised **classification**
  - **Type 3 Normal Model:** Represent 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**
  - MCAR **Continuous variables:** replace by **mean**
  - **Categorical variables:** replace by **median** or **mode**
- **Iterative Algorithms** (**chained-equation imputation**)
  - MAR 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

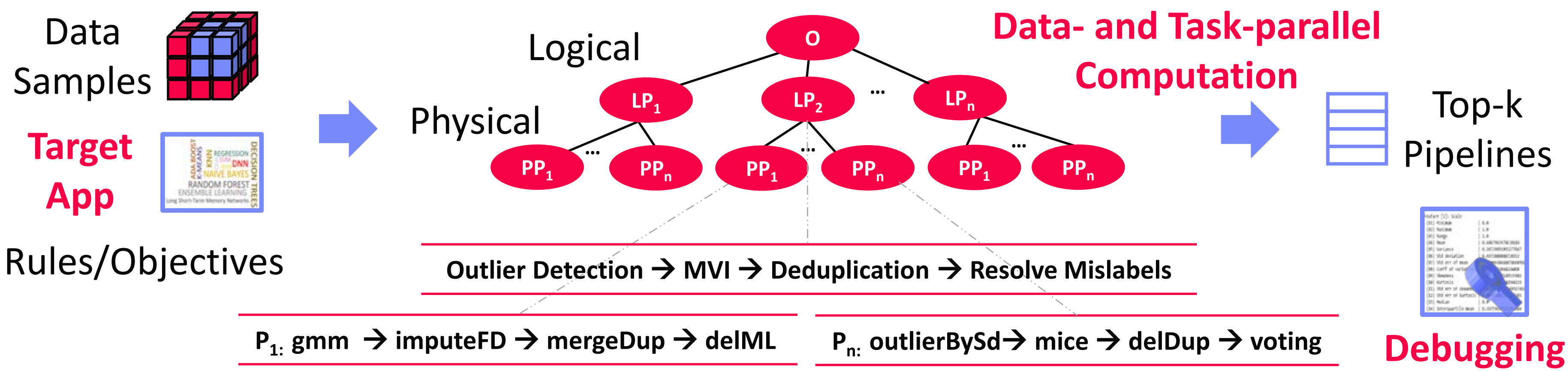
SystemDS: `mice()`



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

Data Cleaning Pipelines [under submission]

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



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 and Q&A

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

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

"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**
  - **May 26/27:** Ascension Day (Christi Himmelfahrt) + "Rektorstag"
  - **10 Model Selection and Management** [Jun 03]
    - Incl Data Augmentation
  - **11 Model Debugging Techniques** [Jun 10]
  - **12 Model Serving Systems and Techniques** [Jun 17]