Architecture of ML Systems (AMLS)
10 Data Acquisition and Preparation

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Last update: Jun 26, 2025

Announcements / Org

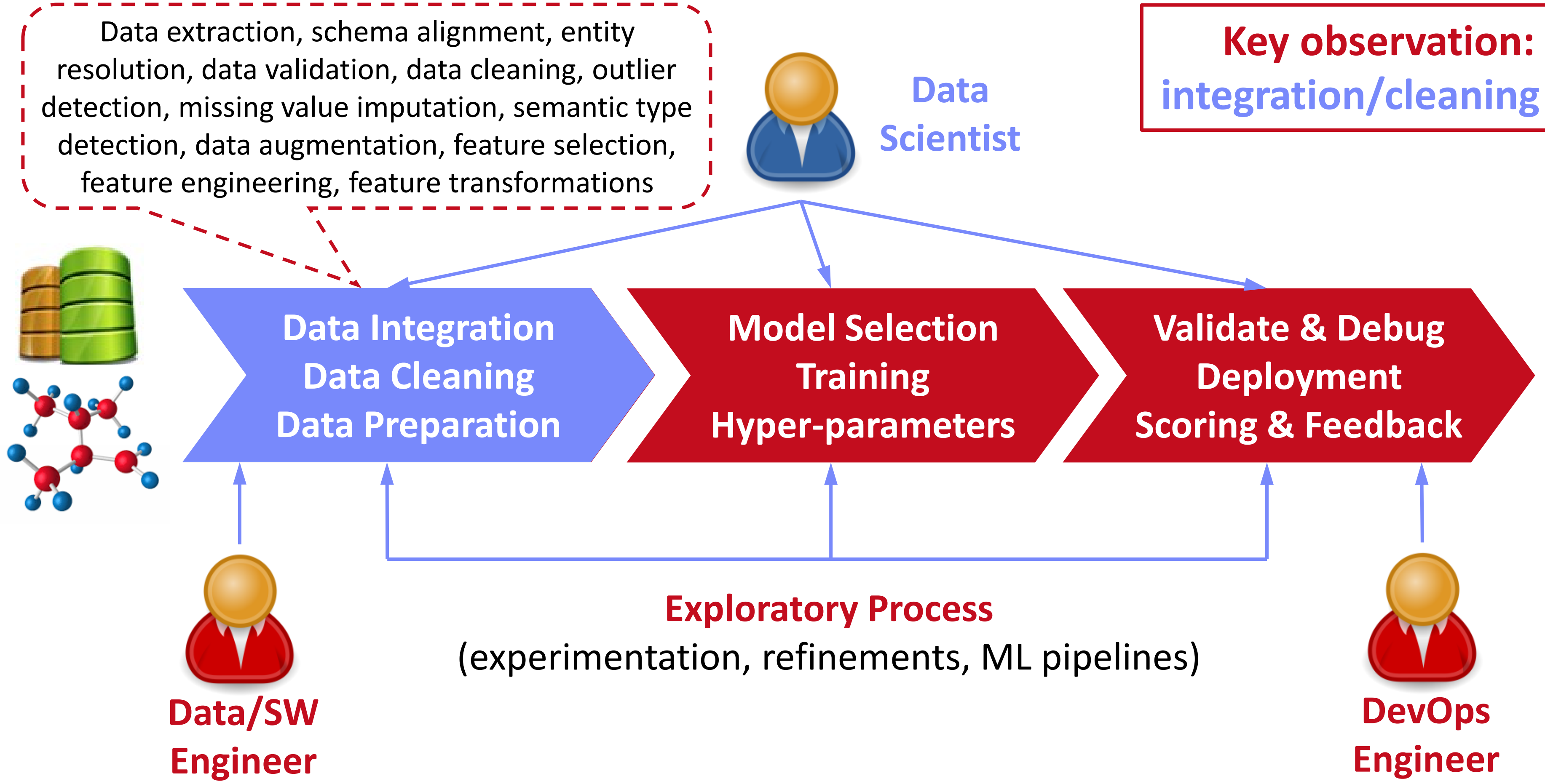
- **#1 Hybrid & Video Recording**
  - Hybrid lectures (in-person, zoom) with optional attendance
    https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09
  - Zoom **video recordings**, links from website
    https://mboehm7.github.io/**teaching**/ss25_amls/index.htm

- **#2 Exam Registration**
  - Thu **July 24, 4-6pm** (A 151, **max 50**) → 14 registrations
  - Thu **July 31, 4-6pm** (EW 201, **max 47**) → 28 registrations
  - Thu **Aug 14, 4-6pm** (A 151, **max 50**) → 13 registrations

- **#3 Projects & Exercises**
  - **Submission deadline: Jul 15 EOD**
  - Get started, use the **office hour** (Tue 4pm-5.30), and mentor meetings

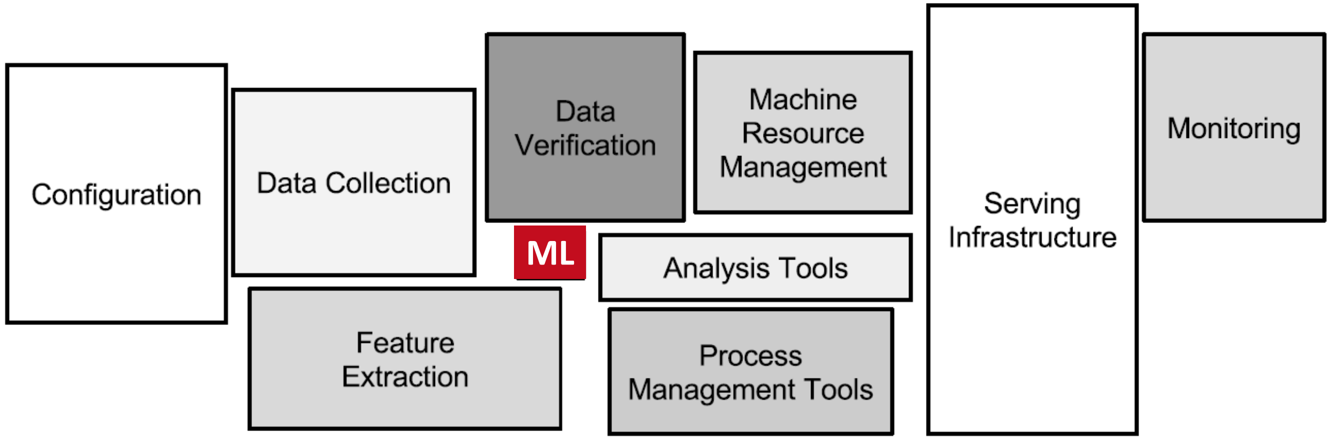
Recap: The Data Science Lifecycle (aka KDD Process, aka CRISP-DM)

Key observation: SotA data integration/cleaning based on ML



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)

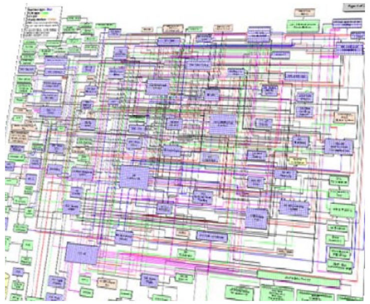
Data Acquisition, Integration, and Data Validation

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
- **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)

[**Credit:** Albert Maier]



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/Lists
  11. Attribute name w/o semantics
  12. Attribute composition

Column Name	% Distinct	Feature Type	Samples
Experience	100	Sentence	[12 Months, two years, ...]
Skills	100	Sentence	["Python,Java", ...]
Gender	60	Categorical	[F, Female, M]
Address	100	Sentence	[7050 CA, TX 7871, CA, ...]
Experience	60	Categorical	[1 year, 2 years, 3 years]
Skills	–	List	[SQL, Java, C++, ...]
Gender	40	Categorical	[Male, Female]
State	40	Categorical	[CA, TX]
Zip	40	Categorical	[7050, 7871]

Data Catalog

[Saeed Fathollahzadeh, Essam Mansour, Matthias Boehm: CatDB: Data-catalog-guided, LLM-based, Generation of Data-centric ML Pipelines, **PVLDB 2025 + SIGMOD 2025 Demo**]

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**]

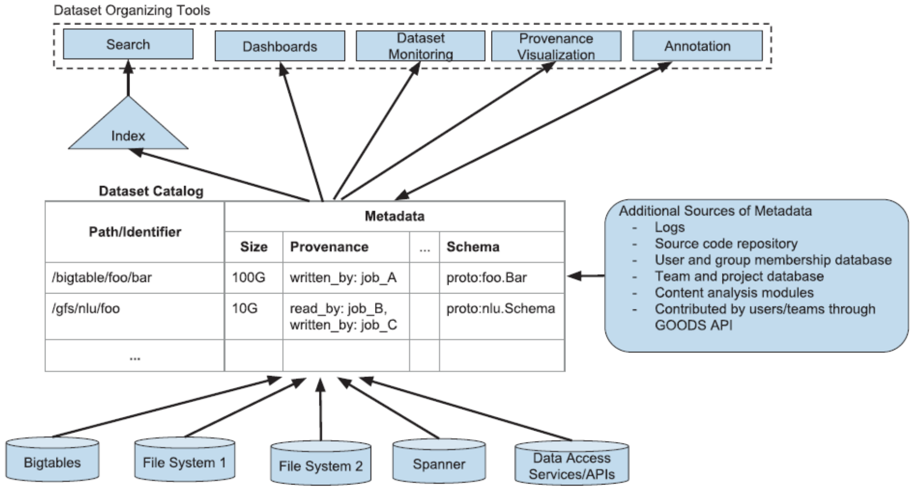
[Dan Brickley, Matthew Burgess, Natasha F. Noy: Google Dataset Search: Building a search engine for datasets in an open Web ecosystem. **WWW 2019**]

[Omar Benjelloun, Shiyu Chen, Natasha Noy: Google Dataset Search by the Numbers, https://arxiv.org/pdf/2006.06894]

SAP Data Hub

[SAP Sapphire Now 2019]

Google Dataset Search



Category	Number of datasets	% of total	Sample formats
Tables	7,822K	37%	CSV, XLS
Structured	6,312K	30%	JSON, XML, OWL, RDF
Documents	2,277K	11%	PDF, DOC, HTML
Images	1,027K	5%	JPEG, PNG, TIFF
Archives	659K	3%	ZIP, TAR, RAR
Text	623K	3%	TXT, ASCII
Geospatial	376K	2%	SHP, GEOJSON, KML
Computational biology	110K	<1%	SBML, BIOPAX2, SBGN
Audio	27K	<1%	WAV, MP3, OGG
Video	9K	<1%	AVI, MPG
Presentations	7K	<1%	PPTX
Medical imaging	4K	<1%	NII, DCM
Other categories	2,245K	11%	

500K → 30M datasets

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))
```

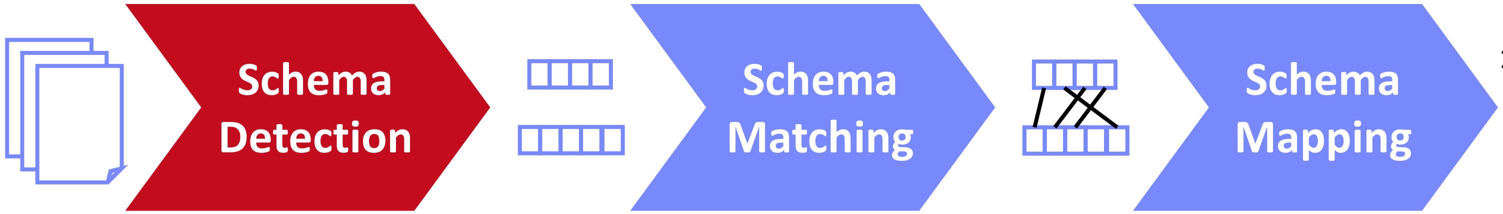
- **Feature Type Detection**
  - Numerical vs Categorical vs Ordinal
  - Rules and trained ML model
- **Semantic Type Detection**
  - Extract common semantic feature types (e.g., location, date, rank, name)

[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/

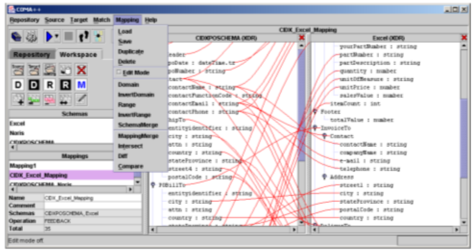
Schema Detection and Integration, cont.




```
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)

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 normalizatio
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 matching
mboehm7 committed on Apr 6

Additional cleaning of instituti
mboehm7 committed on Apr 6

Fix conference venues (consiste
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

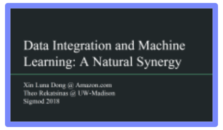
Misplaced data (wrong affiliation, MIT)

- **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

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 *consistenc*	
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**)

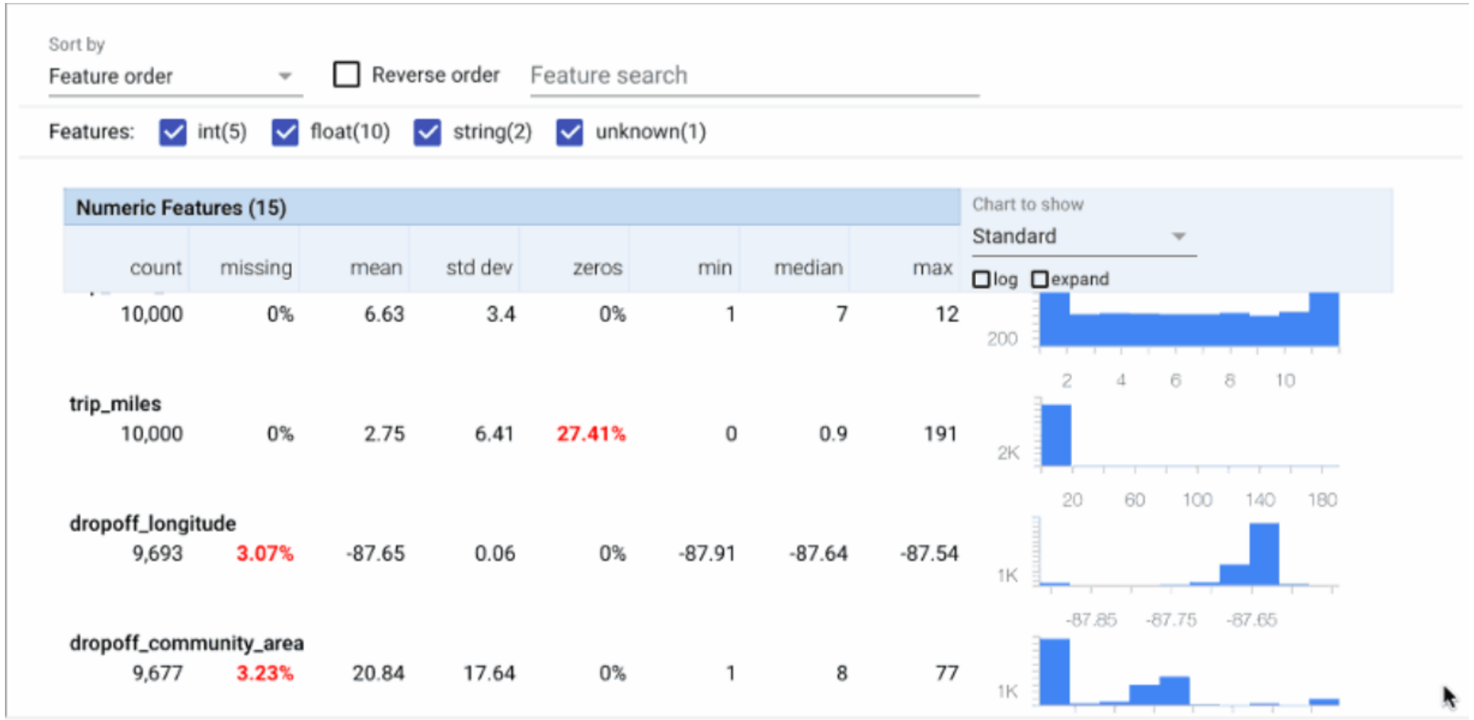
Organizational Lesson: benefit of shared vocabulary/procedures

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

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)

for k = 5:

City	hash % k	City
San Jose	1993955031 % 5 → 1	1
New York	1382994575 % 5 → 0	0
San Francisco	1540367136 % 5 → 1	1
Seattle	-661909336 % 5 → 1	1
New York	1993955031 % 5 → 1	1
Boston	1995575789 % 5 → 4	4
San Francisco	1540367136 % 5 → 1	1
Los Angeles	-425347233 % 5 → 3	3
Seattle	-661909336 % 5 → 1	1

Efficient, but **collisions**

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

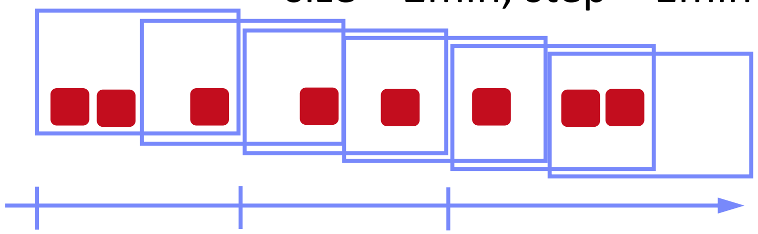
- **#1 Intercept Computation**
  - Add a column of ones to X for computing the intercept as a weight
  - Applies to regression and classification

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

- **#2 Non-Linear Relationships / Interaction Features**
  - 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 + b3*X1*X2
X = cbind(X1, X1^2, X1*X2);
```

- **#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

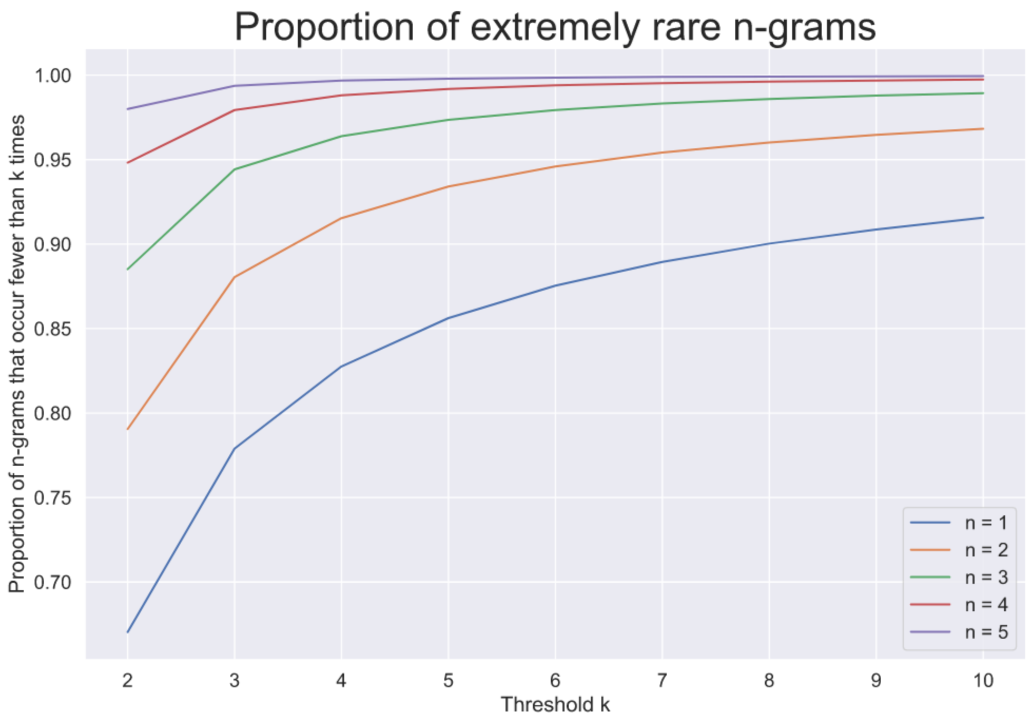
  - **Bi-grams:** bag-of-words for 2-sequences of words (order preserving)
  - **N-grams:** generalization of bi-grams to arbitrary-length sequences

NLP Features, cont.

- **Common N-Grams**
  - Prune n-grams that appear <5 times, → 99.3% reduction
  - **Lattice-based pruning** (Apriori monotonicity property)

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

- **Example**
  - Amazon Reviews Dataset
  - 67% of words appear just once

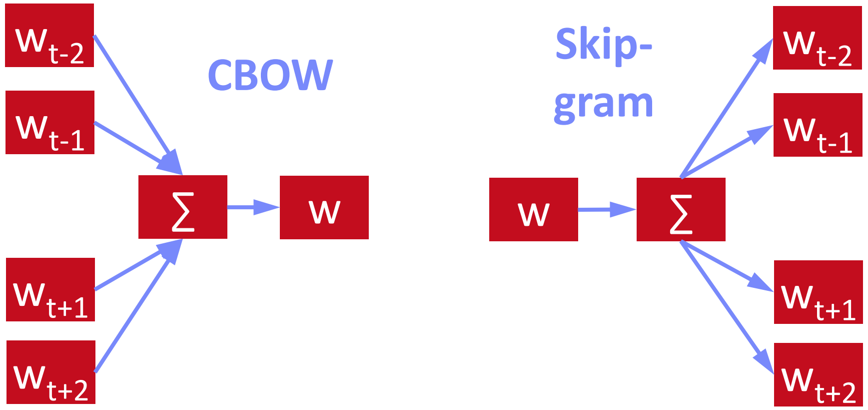


NLP Features, cont.

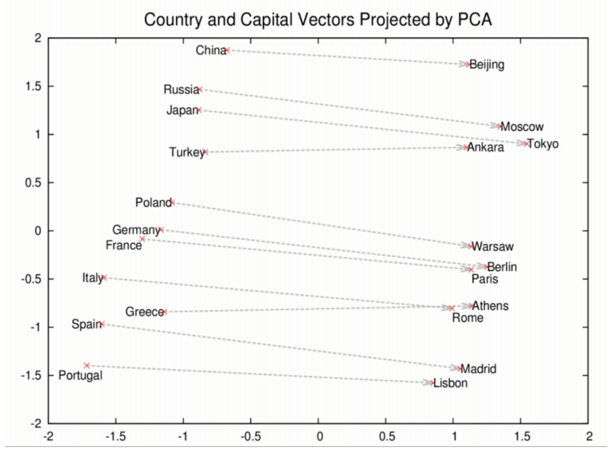
[Tomas Mikolov, Kai Chen, Greg Corrado, Jeffrey Dean: Efficient Estimation of Word Representations in Vector Space. **ICLR (Workshop) 2013**]

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

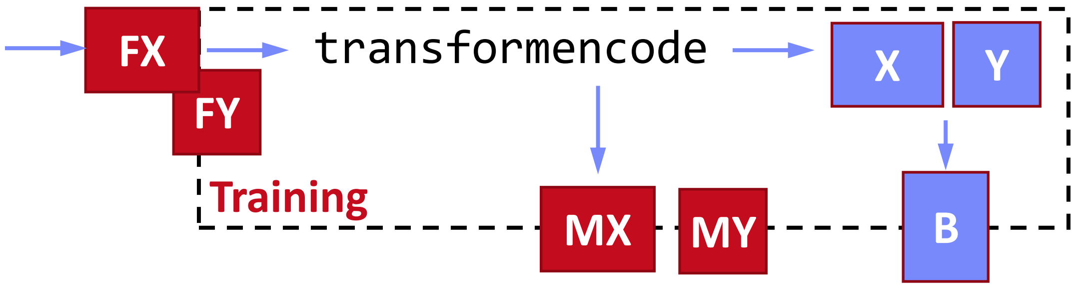
- **Example Pipeline**

```
// 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

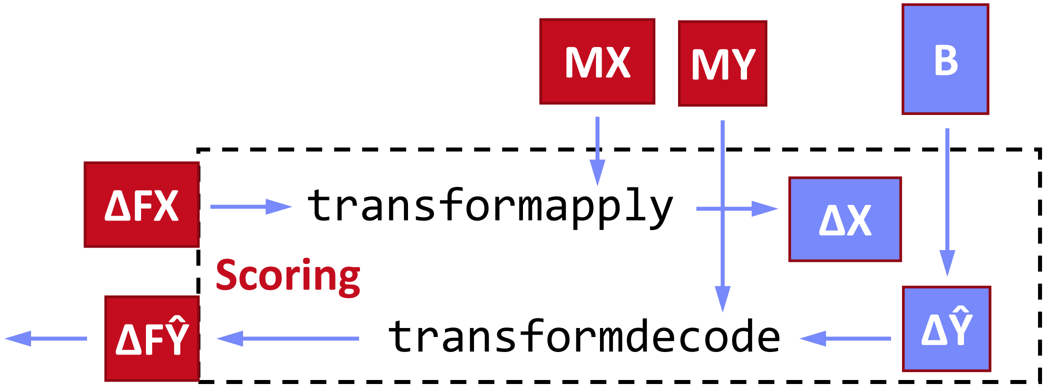
- **Feature Transformation during Training**




```
# 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);
```

Example Keras FeatureSpace

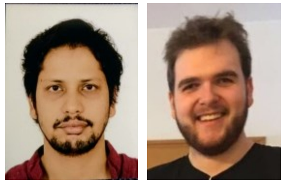
- **Feature Transformation, Normalization, and Interaction Features**

  [https://keras.io/examples/structured_data/feature_space_advanced/]

```
feature_space = FeatureSpace(
    features={
        # Categorical features encoded as integers
        "previously_contacted": FeatureSpace.integer_categorical(num_oov_indices=0),
        # Categorical features encoded as string
        "marital": FeatureSpace.string_categorical(num_oov_indices=0),
        "education": FeatureSpace.string_categorical(num_oov_indices=0),
        "housing": FeatureSpace.string_categorical(num_oov_indices=0),
        "loan": FeatureSpace.string_categorical(num_oov_indices=0),
        # Categorical features to hash and bin
        "job": FeatureSpace.string_hashed(num_bins=3),
        # Numerical features to hash and bin
        "pdays": FeatureSpace.integer_hashed(num_bins=4),
        # Numerical features to normalize and bin
        "age": FeatureSpace.float_discretized(num_bins=4),
        # Numerical features to normalize
        "campaign": FeatureSpace.float_normalized(),
        "previous": FeatureSpace.float_normalized(),
    },
    # Specify feature crosses with a custom crossing dim
    crosses=[
        FeatureSpace.cross(feature_names=("age", "job"), crossing_dim=8),
        FeatureSpace.cross(feature_names=("housing", "loan"), crossing_dim=6),
        FeatureSpace.cross(
            feature_names=("job", "previously_contacted"), crossing_dim=2
        ),
    ],
    output_mode="concat",
)

# Adapt the state of the FeatureSpace using a sample of inputs
train_ds_with_no_labels = train_ds.map(lambda x, _: x)
feature_space.adapt(train_ds_with_no_labels)

# Save the FeatureSpace for later reuse
feature_space.save("myfeaturespace.keras")

# Preprocess a Dataset using the FeatureSpace
preprocessed_train_ds = train_ds.map(
    lambda x, y: (feature_space(x), y), num_parallel_calls=8
)
```

Parallelizing Feature Transformations

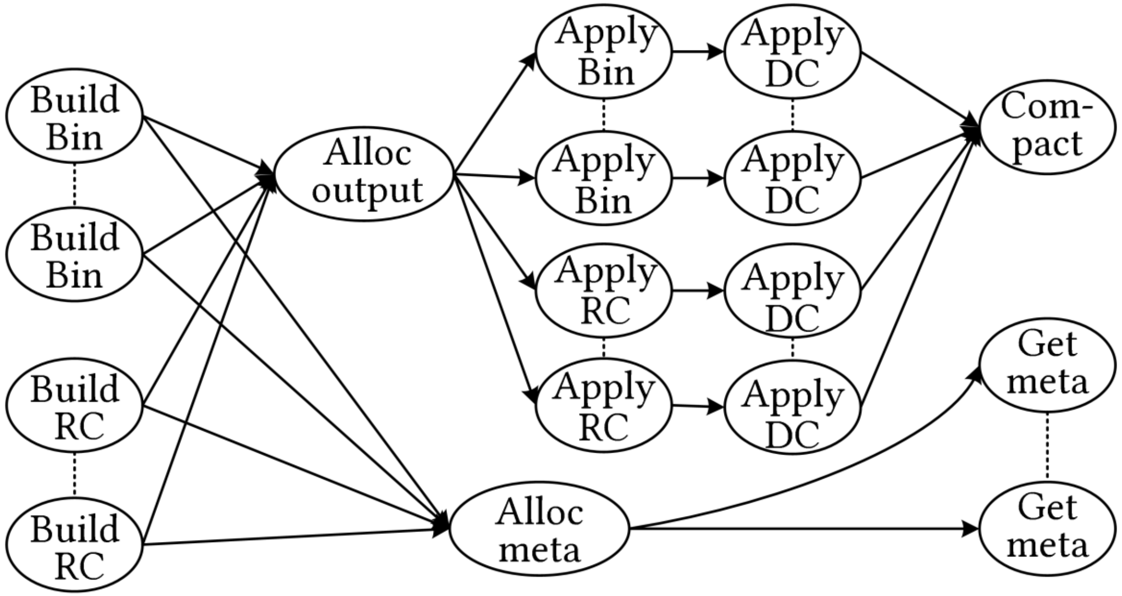
[Arnab Phani, Lukas Erlbacher, Matthias Boehm: UPLIFT: Parallelization Strategies for Feature Transformations in Machine Learning Workloads, **PVLDB 2022**]



- **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

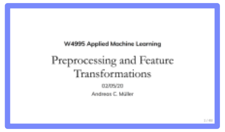
Standardization/Normalization

- **#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]

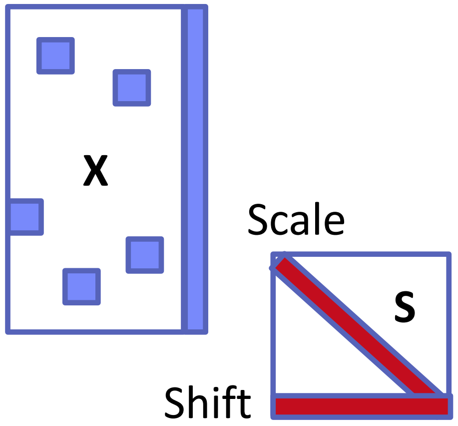
Standardization/Normalization, cont.

- **#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)



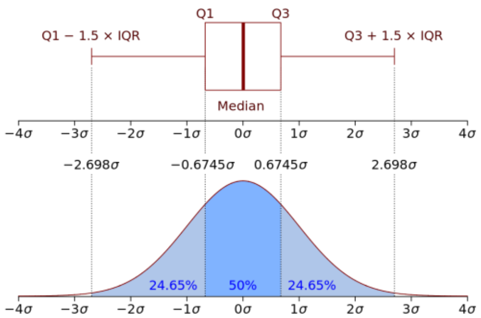

```
# operation w/ early standardized X
q = t(X) %*% diag(w) %*% X %*% B;
```

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 = min(qu, max(ql, X));
```

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

```
- 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

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

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**]

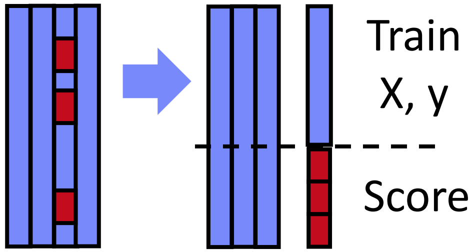
Missing Value Imputation

- **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

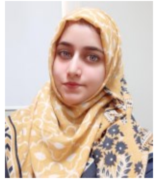
SystemDS:
`mice()`



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

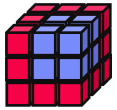
Data Cleaning Pipelines

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



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

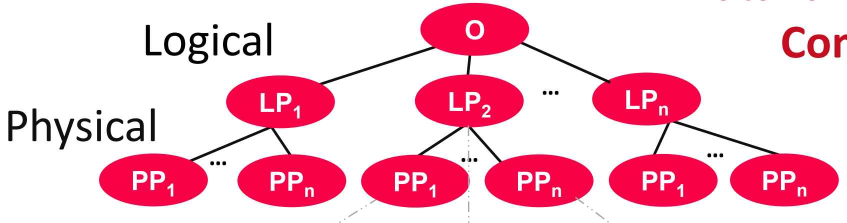
Data Samples



Target App

Rules/Objectives

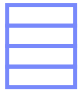
Data- and Task-parallel Computation



Outlier Detection → MVI → Deduplication → Resolve Mislabels

P_1: gmm → imputeFD → mergeDup → delML

P_n: outlierBySd → mice → delDup → voting



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

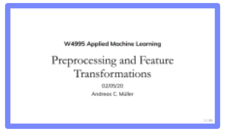
Dirty Data

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**]



- **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)
  - **11 Model Selection and Management** [Jul 03]
  - **12 Model Debugging, Fairness, Explainability** [Jul 10]
  - **13 Model Serving Systems and Techniques** [Jul 17]

    Q&A and Exam Preparation [Jul 17]