

DSGA 3001.009: Data Engineering For Machine Learning

# 09 - Data Validation and Data Cleaning

Sebastian Schelter Center for Data Science, New York University

### Course Topics



#### Introduction

- Intro & Real World Machine Learning Systems
- Systems Foundations & ML Engineering
- Case Study: A Demand Forecasting System at Amazon
- Guest Lecture on Practical Feature Extraction

#### Systems for Machine Learning

- Machine Learning on Distributed Dataflow Systems
- Distributed Machine Learning with Parameter Servers
- Deep Learning Engines
- Model Serving Systems

#### Data Management for Machine Learning

- Model Management
- Data Validation and Data Cleaning
- Fairness in Machine Assisted Decision Making
- Research in Data Management for Machine Learning

### Overview



- Announcements
- Introduction & Overview
- Exemplary Error Detection and Data Cleaning Techniques
  - Quantitative Data: Robust Univariate Outlier Detection
  - Categorical Data: String Normalization
  - Candidate Key Detection at Scale with Hyperloglog Sketches
  - Missing Value Imputation using Supervised Learning
  - Data Unit Testing with Deequ
- Summary & References

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# Solution for Assignment 3



- Forward pass in Neural Network
- Dataflow Graph Extraction

## Project Topics & Teams



- Assigned topics to 12 teams, chose topics from student preferences
- One very popular topic: 4x Fair AutoML
- Will reserve last two lectures on 12/5 and 12/12 for project presentations
  - 10min presentation +5min questions from me and class
  - Teams working on the same topic should present on the same day
- Lab will become "project consulting hour" from 11/20 on
  - Additionally office hours or appointment with me

### Gong Show next week 11/14



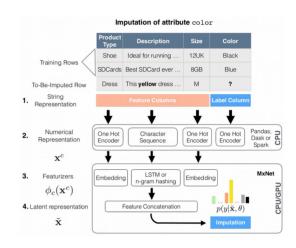
- First deliverable for each group project (worth 5 points)
- Single slide per team, to be presented by one person from the team in 2 minutes
  - Add the slide to a provided Google Doc until 11/13 at 12pm
  - Please provide the following information on the slide
    - (1) Two-sentence **summary** of the project
    - (2) **Description of the data** used during your project
    - (3) Description of how you will **measure the outcome** of your project
    - (4) Description of the **biggest problem** you will have to solve in your project
- Potentially answer 1 or 2 questions about your project (2min max)

# Datawig – Missing Value Imputation for Non-ML Experts



#### Project Description:

- Goal: Build an easy-to-use missing value imputation tool for categorical data
- Details: Automatically train an imputation model for CSV data without requiring the user to specify an algorithm or hyperparameters
- Data: Amazon customer reviews dataset (reviews written on amazon.com and associated metadata from 1995 until 2015)
  - https://s3.amazonaws.com/amazon-reviews-pds/readme.html
- **Evaluation:** Comparison against the SimpleImputer from scikit-learn, measuring the accuracy and F1-scores of the imputed values compared to the true values
- Biggest problem: Need to find a way to automatically compute features from heterogeneous data



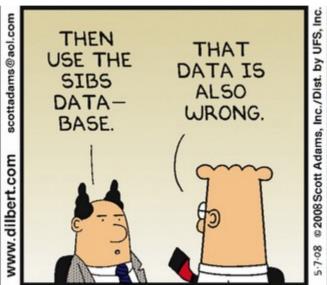
```
CREATE EXTERNAL TABLE amazon reviews parquet
  review id string,
  product id string
  product parent string
  product title string.
  helpful votes int
  review body string,
  review date bigint
  year int)
PARTITIONED BY (product_category string)
ROW FORMAT SERDE
 'org.apache.hadoop.hive.ql.io.parquet.serde.ParquetHiveSerDe
STORED AS INPUTFORMAT
 'org.apache.hadoop.hive.gl.io.parguet.MapredParguetInputForma
OUTPUTFORMAT
 'org.apache.hadoop.hive.ql.io.parquet.MapredParquetOutputFormat
LOCATION
  's3://amazon-reviews-pds/parquet/
```

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https://dilbert.com/strip/2008-05-07

# Why is Data Quality Important?



- Impact on organisational decisions
  - Missing or incorrect data can result in wrong decision making
- Legal obligations in certain business scenarios
  - Plug type information required for selling electric devices in EU
- Impact on machine learning models
  - Cleaner data can greatly improve model performance
- Potential for causing biased decisions in ML-based systems
  - Not well understood, area of active research
- Operational stability: missing and inconsistent data can cause havoc in production systems
  - Crashes (e.g., due to "NullPointerExceptions" for missing attributes)
  - Wrong predictions (e.g., change of scale in attributes)

### Data: Academia vs the Real-World



#### Academic datasets

- Static
- Often down-sampled, cleaned and aggregated before publication
- Attributes typically well understood
- Most of time: size convenient for processing on desktop machines
- Example: UCI ML datasets

#### Real-world data

- Constantly changing
- Often hundreds of attributes
- Data originates from multiple sources / people / teams / systems
- Several potentially inconsistent copies
- Often too large to conveniently handle on a desktop machine
- Often difficult to access (e.g., data compressed and partitioned in a distributed filesystem)

# Changes in Data Collection Strategies



#### Pre-Internet Era

- Data collected in transactional, relational databases
- "Extract-Transform-Load" export to data warehouses for analysis
   (Relational databases optimized for analytical workloads)
- Modelling of the data and its schema before collection

#### Internet Era: "Collect first, analyze later"

- Advent of the internet gave rise to vast amount of semi-structured data
- New data stores established (key-value stores, document databases, data lakes)
  - Scale to very large datasets
  - Relaxed consistency (e.g. no distributed transactions)
  - Enforce fewer modelling decisions at collection time
  - "Schema-on-Read": application has to determine how to interpret data
- Economic incentives
  - Decreasing storage costs
  - Data becomes valuable as input to ML-based applications

### Sources of Error in Data



#### Data entry errors

- Typos in forms
- Different spellings for the same real-world entity (e.g., addresses, names)

#### Measurement errors

- Outside interference in measurement process
- Placement of sensors

#### Distillation errors

- Editorial bias in data summaries
- Domain-specific statistical analyses not understood by database manager

#### Data integration errors

- Resolution of inconsistencies w.r.t. duplicate entries
- Unification of units, measurement periods

### Dimensions of Data Quality



- Completeness
  - Degree to which data required to describe a real-world object is available
- Consistency: Intra-relation constraints (range of admissible values)
  - Specific data type, interval for a numerical column, set of values for a categorical column
- Consistency: Inter-relation constraints
  - Validity of references to other data entries (e.g., "foreign keys" in databases)
- Syntactic and semantic accuracy
  - Syntactic accuracy compares the representation of a value with a corresponding definition domain
    - E.g.: value *blue* for color attribute syntatically accurate for *red* product in online shop
  - Semantic accuracy compares a value with its real-world representation
    - E.g.: value XL for color attribute neither syntactically nor semantically accurate for this product

# Approaches to Improve Data Quality



#### Data entry interface design

- Enforce integrity constraints (e.g., constraints on numeric values, referential integrity)
- Can force users to "invent" dirty data

#### Organisational management

- Streamlining of processes for data collection and analysis
- Capturing of lineage and metadata

#### Automated data auditing and data cleaning

Application of automated techniques to identify and rectify data errors

#### Exploratory data analysis and data cleaning

- Human-in-the-loop approach necessary most of the time
- Interaction between data visualisation and data cleaning
- Iterative process

# Approaches to Improve Data Quality



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- Automated data auditing and data cleaning
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# Data Cleaning: Types and Techniques



#### Quantitative data

- Integers or floating point numbers in different shapes (sets, tensors, time series)
- Challenges: unit conversion (especially for volatile units like currency)
- Foundation of cleaning techniques: outlier detection

#### Categorical data

- Names or codes to assign data into groups, no ordering or distance defined
- Common problem: misspelling upon data entry
- Foundation of cleaning techniques: normalization / deduplication

#### Postal addresses

- Special case of categorical data, typically entered as free text
- Major challenge: deduplication

#### Identifiers / Keys

- Unique identifiers for data objects (e.g., product codes, phone numbers, SSNs)
- Challenge: detect reuse of identifier across distinct objects
- Challenge: Ensure referential integrity

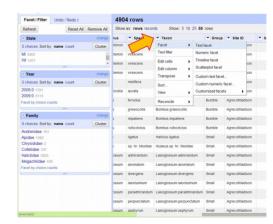
### The Need for the "Human in the Loop"



- **Unrealistic assumptions about error detection in academia:** 
  - Existence of error detecting rules assumed: Integrity Constraints, Functional Dependencies, Conditional Functional Dependencies, Denial Constraints
  - Often focus on most efficient and accurate way to apply cleaning steps according to rules
- In practice: error detection already a very hard problem
  - Consequence: Human-in-the-loop solutions required
  - Data exploration and visualisation crucial
  - Iterative cleaning
  - Popular implementations: Open Refine, Trifacta



https://trifacta.com



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### Robust Univariate Outlier Detection



#### Univariate analysis

- Simple approach: investigate the set of values of a single attribute of our dataset
- Statistical perspective: values considered to be a sample of some data generating process

#### Center & Dispersion

- Set of values has a center that defines what is "average"
- Set of values has a dispersion that defines what is "far from average"

#### Outlier detection

- Assumption: erroneous values "far away" from typical values in the set
- Approach: identify outliers using statistical techniques
- Problem: How to reliably compute them when the data is dirty / erroneous?

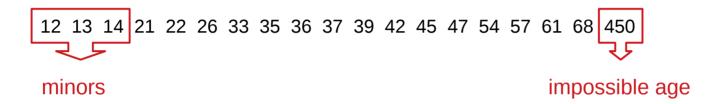


Set of age values of employees in a company:

12 13 14 21 22 26 33 35 36 37 39 42 45 47 54 57 61 68 450



Set of age values of employees in a company:





Set of age values of employees in a company:

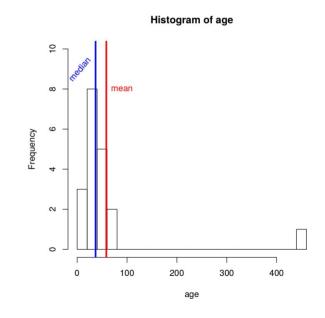
12 13 14 21 22 26 33 35 36 37 39 42 45 47 54 57 61 68 450

#### Potential approach:

- Assume normal distribution of age values
- Compute mean and standard deviation
- Flag values more 2 standard devations away from mean
- Interval is [96 2 \* 59, 9 + 2 \* 59] = [-22, 214]
- Misses first three values!

#### Problem: "Masking"

- Magnitude of one outlier shifts center and dispersion
- "Masks" other outliers



### **Robust Statistics**



- Idea: consider effect of corrupted data values on distribution
  - Estimators should be robust to such corruptions
  - Breakdown point: threshold of corrupt values before estimator produces arbitrarily erroneous results

#### Robust Centers

- *Median*: value for which half of the dataset is smaller (affected by position not magnitude of outliers)
- Trimmed Mean: remove k% of highest and lowest values, compute mean from rest

#### Robust Dispersion

- *Mean Absolute Deviation*: robust analogy to standard deviation
- Measures median distance of all values from the sample median



Set of age values of employees in a company:

```
12 13 14 21 22 26 33 35 36 37 39 42 45 47 54 57 61 68 450
```

Cleaned set of age values:

```
21 22 22 23 24 26 33 35 36 37 39 42 45 45 47 54 57 61 68
```

- Robust centers in example closer to center on clean data:
  - Median 37 (dirty) 39 (clean)
  - Mean ~96 (dirty) ~40 (clean)
  - 10%-Trimmed mean ~39 (dirty)
- Robust dispersion provides better interval on dirty data:
  - 1 standard deviation [37, 155] (includes six non-outliers)
  - 1.48 MAD [16, 61] (includes one non-outlier)

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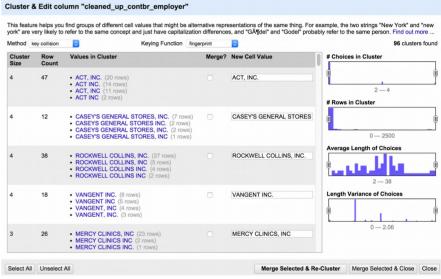


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### Normalization of String Data



- Free-text entry of categorical attributes very error-prone:
  - Different spellings (Jérôme vs Jerome)
  - Different punctuation (ACME Inc. vs ACME, Inc)
  - Typos (Alice → Ailce)
  - Misunderstandings (Rupert → Robert)
- Normalization with simple heuristic clustering algorithm:
  - Keying function k
  - Compute key k(s) per string s
  - group pairs (s, k(s)) by k(s) and count pairs
  - Automatic: Replace all strings in a group with string with highest cardinality
  - Human-in-the-Loop: shows groups and statistics to user



http://www.padjo.org/files/tutorials/open-refine/fingerprint-cluster-popup.png

# String Normalization



- "Fingerprint keying": remove punctuation and case sensitivity
  - remove whitespace around the string
  - lowercase the string
  - remove all punctuation and control characters
  - find ASCII equivalents of characters
  - tokenize (split by whitespace)
  - order fragments and deduplicate them

```
ACT, INC. \rightarrow act inc
ACT INC \rightarrow act inc
ACT, Inc \rightarrow act inc
Act Inc \rightarrow act inc
```

# String Normalization



- "SOUNDEX": Algorithm for phonetic indexing of English strings
  - Save the first letter.
  - Remove all occurrences of a, e, i, o, u, y, h, w
  - Replace all consonants (include the first letter) with digits as follows:

b, f, p, 
$$v \rightarrow 1$$
; c, g, j, k, q, s, x,  $z \rightarrow 2$ ; d,  $t \rightarrow 3$ ,  $l \rightarrow 4$ ; m, n  $\rightarrow 5$ ; r  $\rightarrow 6$ 

- Replace all adjacent same digits with one digit.
- If the saved letter's digit is the same as the resulting first digit, remove the digit (keep the letter).
- Append 3 zeros if result contains less than 3 digits. Remove all except first letter and 3 digits after it

```
Robert → R163
```

Rupert → R163

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# Frequency Statistics of Categorical Data



- In some cases: frequency of values more important than actual values
  - Especially for categorical data attributes (where values have no ordering and no distance)
  - E.g. "species code" in a dataset of animal sightings
- Application: Discovery of "Candidate Keys"
  - Key: attribute or combination of attributes that uniquely identifies a tuple in a relation
  - In clean data:
    - Frequency of every value of the candidate key attribute should be 1
    - Number of distinct values equals number of tuples
  - Both conditions can be violated in case of dirty data

# Heuristics for Discovering "Dirty Keys"



- Idea: discover attributes intended to be used as keys in dirty data
- "Unique Row Ratio"
  - Ratio of distinct values of an attribute to the number of tuples
  - Attribute is potential key if heuristic close to 1.0
  - Problem: "frequency outliers": small number of values
     with very high frequency often caused by UIs forcing users to
     "invent" common "dummy values" like 00000 or 12345
- "Unique Value Ratio"
  - Ratio of unique values to number of distinct values
  - Attribute is potential key if heuristic close to 1.0
  - More robust against frequency outliers
- Problem of both approaches: high memory requirements during computation

item_id
1
3
000
4
5
6
8
10
000
000

### Cardinality Estimation with HLL Sketches



- Problem: exact counting requires memory linear in the number of distinct elements
  - E.g., to maintain a hashtable with values and counts
  - Does not scale to large or unbounded datasets
- HyperLogLog (HLL) Sketch
  - "Sketch" data structure: approximate counting with drastically less memory
  - Uses randomization to approximate the cardinality of a multiset

### HyperLogLog: Idea



- Apply hash function h to every element to be counted (h must produce uniformely distributed outputs)
- Keep track of the maximum number of leading zeros of the bit representations of all observed hash values

- $h("hello") \rightarrow 10011$   $h("world") \rightarrow 11011$   $h("hello") \rightarrow 10011$   $h("alice") \rightarrow 00101$  $h("world") \rightarrow 11011$
- Intuitively: hash values with more leading zeros are less likely and indicate a larger cardinality
- If bit pattern  $0^{q-1}1$  is observed at the beginning of a hash value, estimate size of multiset as  $2^q$

# HyperLogLog: Details



- Algorithm applies several techniques to reduce variability of these measurements
  - Input stream divided into m substreams  $S_i$  with  $m = 2^p$
  - p number of bits of hash values to store
  - array of registers M, M[i] stores max number of leading zeros + 1 from stream  $S_i$
  - Final estimate uses bias-corrected harmonic mean of the estimations on the substreams

$$\alpha_m m^2 \sum_{i=1}^m 2^{-M[i]}$$

- Extremely powerful in practice
  - Low memory requirements: e.g., SparkSQL implementation uses less than 3.5 KB for the registers,
     works on billions of elements
  - Easy to parallelize as registers can be cheaply merged via max function
  - Allows to run **cardinality estimation** on multiple columns of huge tables **with a single scan**
- Basis of key detection in data validation library "deequ" https://github.com/awslabs/deequ

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## Missing Value Imputation



- Missing data is a central data quality problem
- Missing for various reasons: Missing Completely at Random (MCAR),
   Missing at Random (MAR), Not Missing at Random (NMAR)
- Example: Questionaire about income
  - MCAR: missingness completely random (as if we lost some questionaires by chance)
  - MAR: Missingness random within certain subgroups (manager more likely to not share income then engineers)
  - MNAR: Reason for missing data depends on missing data itself (e.g., people with less than \$1000 do not want to share their income)
- Various ways to handle missing data for ML applications
  - Complete-case analysis (remove examples with missing attributes)
  - Add placeholder symbol for missing values
  - Impute missing values
    - Often implemented with techniques from popular ML libraries, like mean and mode imputation
    - ML: supervised learning for missing value imputation

# Imputation of Categorical Data (1)



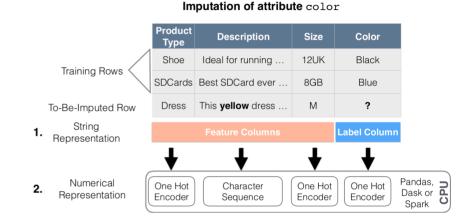
- Assume tabular data
- Want to impute missing values in a column with categorical data
- Idea: apply techniques from supervised learning
- Example: product catalog, colors missing
   p(color=yellow | other columns, imputation model)
- Treat imputation problem as multi-class classification problem

Product Type	Description	Size	Color
Shoe	Ideal for running	12UK	Black
SDCards	Best SDCard ever	8GB	Blue
Dress	This <b>yellow</b> dress	М	?

# Imputation of Categorical Data (2)



- Must encode table data from feature columns to a numerical representation
- Standard encoding techniques
  - "One-hot" encoding of categorical columns
     (zero vector with as many dimensions as distinct values, 1 in corresponding dimensions)
  - Standardisation of numerical columns
     (substract mean, divide by standard deviation)
  - Character sequences for textual columns



# Imputation of Categorical Data (3)



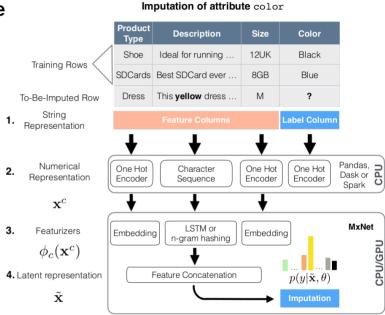
Train neural network to predict likelihood of values to impute

$$p(y|\tilde{\mathbf{x}}, \boldsymbol{\theta}) = \operatorname{softmax} [\mathbf{W}\tilde{\mathbf{x}} + \mathbf{b}]$$

Concatenation of featurizers into single feature vector

$$\tilde{\mathbf{x}} = [\phi_1(\mathbf{x}^1), \phi_2(\mathbf{x}^2), \dots, \phi_C(\mathbf{x}^C)] \in \mathbb{R}^D$$

- Standard featurization techniques
  - Embeddings for one-hot encoded categories
  - Hashed n-grams or LSTMs for character sequences
- Open source implementation "datawig" available at https://github.com/awslabs/datawig



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#### **Unit Tests for Data**



- Inspiration from software engineering:
  - Unit tests, integration tests, deployment pipelines
- 'Unit Tests for Data'
  - Assume **structured data** (database table, CSV file, flattened ison file, ...)
  - Users should be able to easily define 'unit tests' for data in a **declarative** manner
  - 'Unit-Tests' consist of constraints on statistics of the data combined with user-defined validation code
  - Data pipelines can 'quarantine' data in case of failing validations

# Example: a Unit Test for the Quality of Video Logs



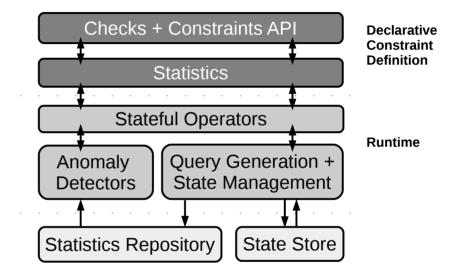
```
val check = Check()
  // Data integrity
  .isComplete("customerId", "title", "impressionStart", "impressionEnd", "deviceType", "priority")
  .isUnique("customerId", "countryResidence", "deviceType", "title")
  .hasApproxCountDistinct("title", _ <= callRestService(...))
  .isNonNegative("count")
  .isInValidRange("priority", ("hi", "lo"))
  // No anomalies over time
  .hasNoAnomalies(OnlineNormal(stdDevs=3), Size)
  // Relaxed functional dependencies
  .isPredictableFrom("countryResidence", ("zipCode", "cityResidence"), precision=0.98)

Verification.run(check, data)</pre>
```

## **Execution using Aggregation Queries**



- (1) Identification of required data quality statistics
- (2) Translation of statistics computations to aggregation queries in SQL (optimized for scan-sharing)
- (3) Invocation of **user-defined validation code** to query results to evaluate constraints



Implementation internally supports huge variety of quality statistics on which constraints can be defined, e.g.,
 Completeness, ApproxCountDistinct, UniqueValueRatio, RegexCompliance, Minimum, Maximum,
 Mean, StandardDeviation, Entropy, Correlation, ApproxQuantiles, TypeCompliance, Predictability,
 ValueRangeCompliance

## Stateful Computation of Data Quality Statistics



- Data is seldomly static, many systems continuously produce data
- Support scenarios with regular ingestion/update of new data partitions
- Goal: update data quality statistics without requiring access to previously processed data
  - Allows to scale computations with the size of delta

#### Approach:

- (1) Compute "mergeable states" on data partitions
- (2) Compute statistics from merged states
- (3) In light of changes, only re-compute states for changed partitions

#### Toy Example



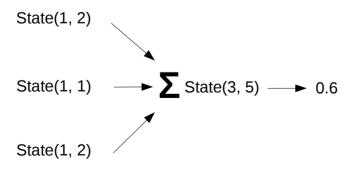
```
val check = Check()
   .hasCompleteness("origin", _ > 0.7)

Verification
   .runOnPartitionedData(check, Map(
    "US" -> dataUS,
    "IN" -> dataIN,
    "EU" -> dataEU))
   .saveStatesTo("s3://...")
```

item	origin	market
item1	US	US
item3	NULL	US

item	origin	market
item4	US	IN

item	origin	market
item5	NULL	EU
item6	DE	EU

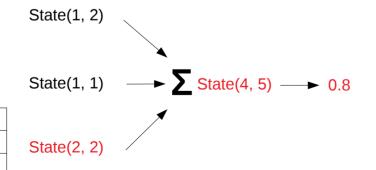


## Toy Example



```
val check = Check()
   .hasCompleteness("origin", _ > 0.7)

Verification
   .runOnPartitionedData(check, Map("EU" -> newDataEU))
   .loadStatesFrom("s3://...")
```



Implementation via adjusted catalyst-based aggregation functions in Spark

item	origin	market
item5	IT	EU
item6	DE	EU

## Algebraic Foundations



Define states and merge functions for data statistics using commutative monoids as algebraic basis

Monoid 
$$(\mathcal{S},\oplus,\mathbb{O})$$
 Merge function for states  $\oplus:\mathcal{S} imes\mathcal{S} o\mathcal{S}$ 

Incremental statistics computation 
$$m(s)$$

$$m(s(d_1 \cup d_2)) = m(s(d_1) \oplus s(d_2))$$

- Applicable to a wide variety of statistics, e.g.:
  - Completeness: ratio of non-null values in a column, corresponding monoid is  $(N^2, +, [0, 0])$
  - Maximum value in a column, corresponding monoid is (R, max, -∞)
  - Approximate cardinality of a column, (computed with hyperloglog sketches),
     corresponding monoid is ({0,1}<sup>d</sup>, v, [0,...,0])

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## Summary



- Data quality important for: decision making, conforming to legal obligations, improving the performance of ML models, operation of data processing systems
- Real-world data is always messy and difficult to handle
- Dimensions of data quality: completeness, consistency, syntactic & semantic accuracy
- Data cleaning techniques
  - Quantitative data: outlier detection
  - Categorical data: normalisation / deduplication
  - Postal addresses: deduplication
  - Identifiers / keys: ensuring referential integrity
- Error detection is already a very hard problem: typically requires iterative cleaning, visualisation and a human-in-the-loop

#### References



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- Batini, Carlo, et al. "Methodologies for data quality assessment and improvement."
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