TECHNISCHE UNIVERSITÄT BERLIN

Data Integration and Large-scale Analysis (DIA)
07 Data Provenance and Data Catalogs

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Last update: Nov 28, 2024

BIFOLD

Announcements / Administrative Items

- **#1 Video Recording**
  - Hybrid lectures: in-person H 0107, zoom live streaming, video recording
  - https://tu-berlin.zoom.us/j/9529634787?pwd=R1ZsN1M3SC9BOU1OcFdmem9zT202UT09

- **#2 Exercises/Projects**
  - **Reminder:** exercise/project submissions by **Jan 30** (no extensions)
  - Make use of **virtual** office hours **Wed 4.30pm-6pm**

- **#3 Lecture Dec 05**
  - FONDA II CRC (Foundations of Workflows for Large-Scale Scientific Data Analysis) **retreat Dec 04 – 06**
  - Virtual lecture on **Dec 05, 4pm** (start 4.15pm) from hotel room

Agenda

- **Motivation and Terminology**
- **Data Provenance**
- **Data Catalogs**

Motivation and Terminology

Excursus: FAIR Data Principles

[https://www.go-fair.org/fair-principles/]

- **#1 Findable**
  - Metadata and data have globally unique **persistent identifiers**
  - Data describes w/ rich **meta data**; registered/indexes and searchable
- **#2 Accessible**
  - Metadata and data retrievable via open, free and universal **commnication protocols**
  - Metadata accessible even when data no longer available
- **#3 Interoperable**
  - Metadata and data use a formal, **accessible, and broadly applicable format**
  - Metadata and data use FAIR vocabularies and qualified references
- **#4 Reusable**
  - Metadata and data described with plurality of accurate and relevant attributes
  - Clear license, **associated with provenance**, meets community standards

Terminology of Provenance/Lineage

- **Data Provenance**
  - Track and understand data origins and transformations of data (**where?**, **when?**, **who?**, **why?**, **how?**)

  - Contains meta data, context, and modifications (transform, enrichment)
  - **Synonyms:** **data provenance** (arts) **data lineage** (royals), **data pedigree** (horses)

- **Blockchain**
  - Data structure logging transactions in **verifiable** and **permanent way**

- **Data Catalogs** (curation/**governance**)
  - Directory of datasets including data provenance (meta data, artifacts)
  - Raw/original, curated datasets, derived data products

Application and Goals of Provenance

a) High-Level Goals

- **#1 Versioning and Reproducibility** (analogy experiments)
- **#2 Explainability, Interpretability, Verification**

b) Low-Level Goals

- **#3 Full and Partial Reuse of Intermediates**
- **#4 Incremental Maintenance of MatViews, Models, etc**
- **#5 Tape/log of Executed Operations** → Auto Differentiation
- **#6 Recomputation for Caching / Fault Tolerance**
- **#7 Debugging via Lineage Query Processing**

Data Provenance

Overview Data Provenance

- **Def Data Provenance**
  - Information about the **origin** and **creation process** of data
- Example
  - Debugging suspicious query results

```
SELECT Customer, sum(O.Quantity*P.Price)
  FROM Orders O, Products P
  WHERE O.PID = P.PID
  GROUP BY Customer
```

Customer	Sum
A	7620
B	120
C	130
D	75

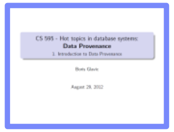
OID	Customer	Date	Quantity	PID
1	A	2019-06-22	3	2
2	B	2019-06-22	1	3
3	A	2019-06-22	101	4
4	C	2019-06-23	2	2
5	D	2019-06-23	1	4
6	C	2019-06-23	1	1

PID	Product	Price
1	X	100
2	Y	15
4	Z	75
3	W	120

Overview Data Provenance, cont.

- **An Abstract View**
  - **Data:** schema, structure → data items
  - **Data composition** (granularity): attribute, tuple, relation
  - **Transformation:** consumes inputs, produces outputs
  - **Hierarchical transformations:** query w/ views, query block, operators
  - **Additional:** env context (OS, libraries, env variables, state), users

[Boris Glavic: CS595 Data Provenance – Introduction to Data Provenance, **Illinois Institute of Technology, 2012**]



- **Goal: Tracing of Derived Results**
  - Inputs and parameters
  - Steps involved in creating the result
  - → Store and query data & provenance
  - General Data Protection Regulation (**GDPR**)?

```
1. Read file1
2. Sort rows
3. Compute median
4. Write to file2
```

Prov.

[Zachary G. Ives: Data Provenance: Challenges, Benefits, Research, **NIH Webinar 2016**]

Classification of Data Provenance

- **Overview**
  - Base query $Q(D) = O$ with database $D = \{R_1, \ldots, R_n\}$
  - **Forward lineage query:** $L_f(R_i'', O')$ from subset of input relation to output
  - **Backward lineage query:** $L_b(O', R_i)$ from subset of outputs to base tables

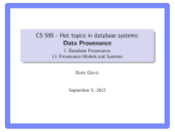
- **#1 Lazy Lineage Query Evaluation**
  - Rewrite (**invert**) lineage queries as relational queries over input relations
  - No runtime overhead but slow lineage query processing

- **#2 Eager Lineage Query Evaluation**
  - Materialize **annotations** (data/transforms) during base query evaluation
  - Runtime overhead but fast lineage query processing
  - Lineage capture: **Logical** (relational) vs **physical** (instrumented physical ops)

[Fotis Psallidas, Eugene Wu: Smoke: Fine-grained Lineage at Interactive Speed. **PVLDB 2018**]

Why-Provenance

[Boris Glavic: CS595 Data Provenance – Provenance Models and Systems, **Illinois Institute of Technology, 2012**]



- **Overview Why**
  - **Goal:** Which input tuples contributed to an output tuple t in query Q
  - Representation: Set of witnesses w for tuple t (**set semantics!**)
    - $w \subseteq I$ (subset of all tuples in instance I)
    - $t \in Q(w)$ (tuple in result of query over w)

- **Example Witnesses**

```
SELECT Customer, Product
  FROM Orders O, Products P
  WHERE O.PID=P.PID
```

	Customer	Date	PID
o1	A	2019-06-22	2
o2	B	2019-06-22	3
o3	A	2019-06-22	2

	PID	Product
p1	1	X
p2	2	Y
p3	4	Z
p4	3	W

	Customer	Product
t1	A	Y
t2	B	W

Witnesses for **t1**:
w1 = {o1,p2}, w2 = {o3,p2},
w3 = {o1,o3,p2}, …, wn = I

Minimal witnesses for t1:
w1 = {o1,p2}, w2 = {o3,p2}

How-Provenance

[Boris Glavic: CS595 Data Provenance – Provenance Models and Systems, **Illinois Institute of Technology, 2012**]

- **Overview**
  - Model how tuples where combined in the computation
  - **Alternative use:** need one of the tuples (e.g., union/projection)
  - **Conjunctive use:** need all tuples together (e.g., join)
- **Provenance Polynomials**
  - **Semi-ring annotations** to model provenance $(\mathbb{N}[I], +, \times, 0, 1)$
- **Examples**
  - $q = \pi_a(R)$

	a	b
r1	1	2
r2	1	3

a	Provenance
1	r1 + r2

  - $q = \pi_b(R \bowtie S)$

	a	b
r1	1	P
r2	2	G
	3	M

	c	a
s1	S	1
s2	S	2
s3	W	2

b	Provenance
P	r1 x s1
G	(r2 x s2) + (r2 x s3)

Provenance Polynomials

How-Provenance, cont.

- **Example Exam Question:**
  Given below tables R and S (with tuples r_i and s_j), query Q and results O, specify the provenance polynomials for every tuple in O. [3 points]

R

	A	B
r_1	X	1
r_2	Y	2
r_3	Z	1

S

	C	D
s_1	1	A
s_2	2	B
s_3	2	A
s_4	2	C

```
SELECT DISTINCT S.D
  FROM R, S
  WHERE R.B=S.C
```

⇒

O	Provenance Polynomials?
A	
B	
C	

A: r1 x s1 + r3 x s1 + r2 x s3
(equivalent: **(r1 + r3) x s1 + r2 x s3**)

B: r2 x s2

C: r2 x s4

Why Not?-Provenance

[Adriane Chapman, H. V. Jagadish: **Why not? SIGMOD 2009**]

- **Overview**
  - Why are items not in the results
  - **Example Problem:**
    "Window-display-books < $20"
    → (Euripides, Medea).
    → **Why not** (Hrotsvit, Basilius)?

<= 20$?

Not in book store?

Bug in the query / system?

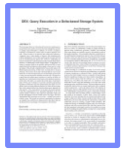
Author	Title	Price	Publisher
	Epic of Gilgamesh	$150	Hesperus
Euripides	Medea	$16	Free Press
Homer	Iliad	$18	Penguin
Homer	Odyssey	$49	Vintage
Hrotsvit	Basilius	$20	Harper
Longfellow	Wreck of the Hesperus	$89	Penguin
Shakespeare	Coriolanus	$70	Penguin
Sophocles	Antigone	$48	Free Press
Virgil	Aeneid	$92	Vintage

- **Evaluation Strategies**
  - Given a user question (why no tuple satisfies predicate S), dataset D, result set R, and query Q, leverage **why lineage**
  - **#1 Bottom-Up:** from leafs in topological order to find last op eliminating $d \in S$
  - **#2 Top-Down:** from result top down to find last op, **requires stored lineage**

Provenance for ML Pipelines (fine-grained)

- **DEX: Dataset Versioning**
  - **Versioning of datasets, stored with delta encoding**
  - Checkout, intersection, union queries over deltas
  - Query optimization for finding efficient plans

[Amit Chavan, Amol Deshpande: DEX: Query Execution in a Delta-based Storage System. **SIGMOD 2017**]



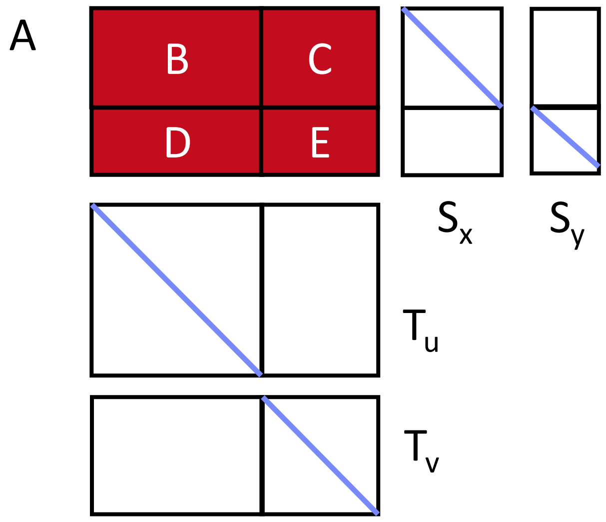
- **MISTIQUE: Intermediates of ML Pipelines**
  - Capturing, storage, querying of intermediates
  - **Lossy deduplication and compression**
  - Adaptive querying/materialization for finding efficient plans

[Manasi Vartak et al: MISTIQUE: A System to Store and Query Model Intermediates for Model Diagnosis. **SIGMOD 2018**]

- **Linear Algebra Provenance**
  - Provenance propagation by decomposition
  - Annotate parts w/ provenance polynomials (contributing inputs + impact)

[Zhepeng Yan, Val Tannen, Zachary G. Ives: Fine-grained Provenance for Linear Algebra Operators. **TaPP 2016**]

$$A = S_x B T_u + S_x C T_v$$
$$+ S_y D T_u + S_y E T_v$$



Provenance for ML Pipelines (coarse-grained)

- **MLflow**
  - Programmatic API for tracking parameters, experiments, and results
  - **`autolog()`** for specific params

[**Credit:** https://databricks.com/blog/2018/06/05]

```
import mlflow
mlflow.log_param("num_dimensions", 8)
mlflow.log_param("regularization", 0.1)
mlflow.log_metric("accuracy", 0.1)
mlflow.log_artifact("roc.png")
```

- **Flor (on Ground)**
  - DSL embedded in python for managing the workflow development phase of the ML lifecycle
  - DAGs of actions, artifacts, and literals
  - Data context generated by activities in Ground

https://rise.cs.berkeley.edu/projects/jarvis/

[Joseph M. Hellerstein et al: Ground: A Data Context Service. **CIDR 2017**]

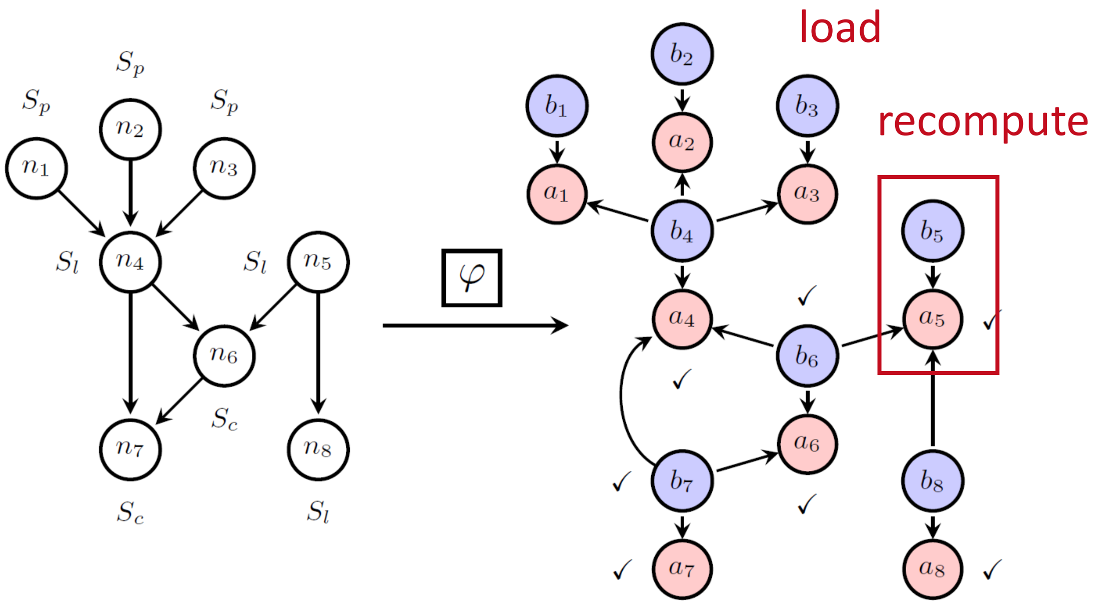
- **Vision: Dataset Relationship Management**
  - **Reuse**, **reveal**, **revise**, **retarget**, **reward**
  - Code-to-data relationships (data provenance)
  - Data-to-code relationships (potential transforms)

[Zachary G. Ives, Yi Zhang, Soonbo Han, Nan Zheng,: Dataset Relationship Management. **CIDR 2019**]

Provenance for ML Pipelines (coarse-grained), cont.

- **HELIX**
  - Goal: focus on iterative development w/ small modifications (trial & error)
  - Caching, reuse, and recomputation
  - Reuse as **Max-Flow problem** → **NP-hard** → heuristics
  - Materialization to disk for future reuse

[Doris Xin, Stephen Macke, Litian Ma, Jialin Liu, Shuchen Song, Aditya G. Parameswaran: Helix: Holistic Optimization for Accelerating Iterative Machine Learning. **PVLDB 2018**]



- **Collaborative Optimizer**

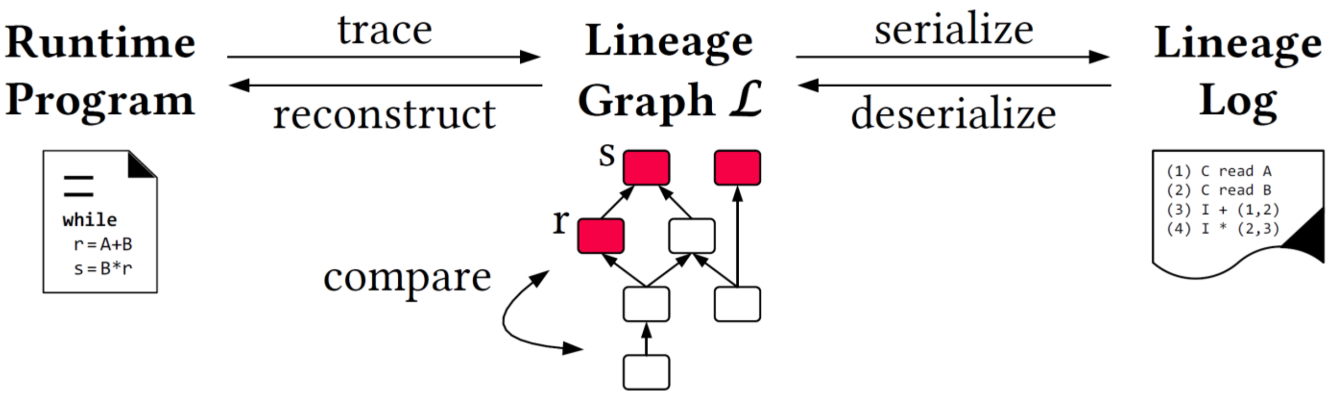
[Behrouz Derakhshan, Alireza Rezaei Mahdiraji, Ziawasch Abedjan, Tilmann Rabl, Volker Markl: Optimizing Machine Learning Workloads in Collaborative Environments. **SIGMOD 2020**]

Lineage Tracing & Reuse in SystemDS [CIDR’20, SIGMOD’21a, EDBT’25]

- **Problem**
  - **Exploratory data science** (data preprocessing, model configurations)
  - **Reproducibility** and **explainability** of trained models (data, parameters, prep)
  - ➔ **Lineage/Provenance as Key Enabling Technique:** Model versioning, reuse of intermediates, incremental maintenance, auto differentiation, and debugging (query processing over lineage)

[Arnab Phani, Benjamin Rath, Matthias Boehm: LIMA: Fine-grained Lineage Tracing and Reuse in Machine Learning Systems, **SIGMOD 2021**]

- **Efficient Lineage Tracing**
  - Tracing of inputs, literals, and **non-determinism**
  - **Trace lineage of logical operations**
  - **Deduplication** for loops/functions
  - Program/output reconstruction



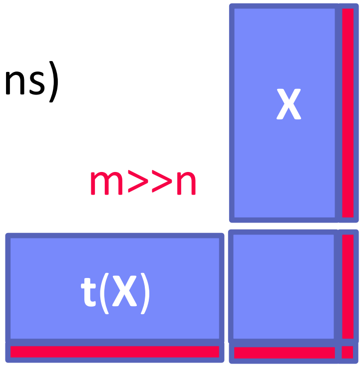
Lineage Tracing & Reuse in SystemDS, cont.


- **Multi-level, Lineage-based Reuse**
  - Lineage trace uniquely identifies intermediates
  - Reuse intermediates at function / block / operation level
- **Full Reuse of Intermediates**
  - Before executing instruction, probe output lineage in cache `Map<Lineage, MatrixBlock>`
  - Cost-based/heuristic caching and eviction decisions (compiler-assisted)
- **Partial Reuse of Intermediates**
  - **Problem:** Often partial result overlap
  - Reuse partial results via dedicated rewrites (compensation plans)
  - Example: steplm
- **Next Steps:** multi-backend, unified mem mgmt

```
for( i in 1:numModels )
  R[,i] = lm(X, y, lambda[i,], ...)
```

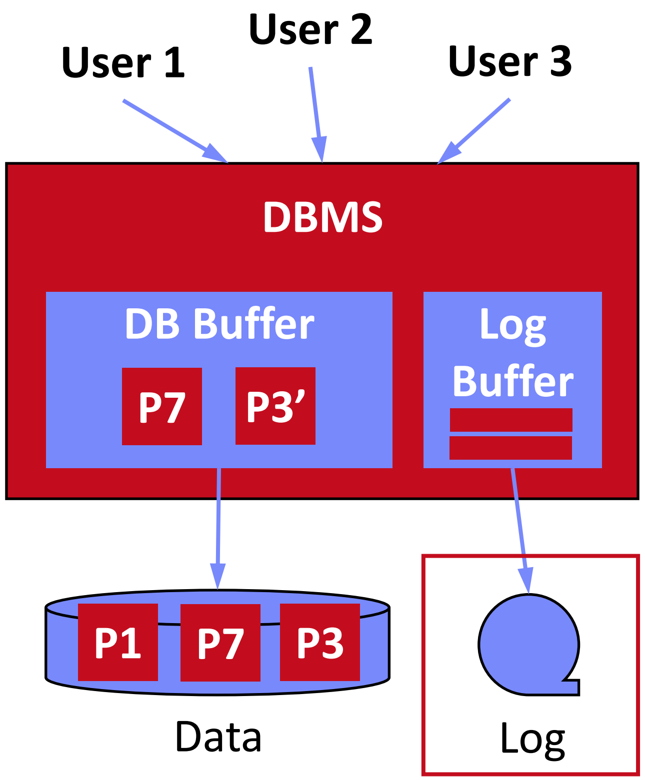
```
m_lmDS = function(...) {
  l = matrix(reg,ncol(X),1)
  A = t(X) %*% X + diag(l)
  b = t(X) %*% y
  beta = solve(A, b) ...}
```

```
m_steplm = function(...) {
  while( continue ) {
    parfor( i in 1:n ) {
      if( !fixed[1,i] ) {
        Xi = cbind(Xg, X[,i])
        B[,i] = lm(Xi, y, ...)
    } }
    # add best to Xg (AIC)
} }
```



Recap: Database (Transaction) Log

- **Database Architecture**
  - **Page-oriented storage** on disk and in memory (DB buffer)
  - Dedicated **eviction algorithms**
  - Modified in-memory pages marked as dirty, flushed by cleaner thread
  - **Log:** append-only TX changes
  - Data/log often placed on different devices and periodically archived (backup + truncate)



- **Write-Ahead Logging (WAL)**
  - The log records of changes to some (dirty) data page must be on **stable storage before the data page** (UNDO - atomicity)
  - **Force-log on commit** or full buffer (REDO - durability)
  - **Recovery:** forward (REDO) and backward (UNDO) processing
  - Log sequence number (LSN)

[C. Mohan, Donald J. Haderle, Bruce G. Lindsay, Hamid Pirahesh, Peter M. Schwarz: ARIES: A Transaction Recovery Method Supporting Fine-Granularity Locking and Partial Rollbacks Using Write-Ahead Logging. **TODS 1992**]

Bitcoin and Blockchain Fundamentals

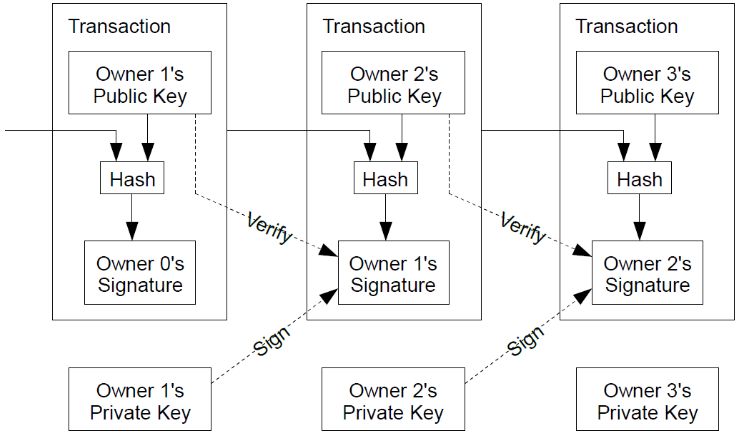
[**Satoshi Nakamoto**: Bitcoin: A Peer-to-Peer Electronic Cash System, **White paper 2008**]

- **Motivation**
  - Peer-to-peer (decentralized, anonymous) electronic cash/payments
  - **Non-reversible transactions** w/o need for trusted third party
  - **Statistics**

	Market Price (USD)	Average Block Size	Transactions per Day	Mempool Size
Nov 21 2019:	$7,862.72 USD	1.16 Megabytes	303,921 Transactions	11,304,890 Bytes
Nov 19 2020:	$17,975.24 USD	1.29 Megabytes	310,424 Transactions	19,920,773 Bytes

[https://www.blockchain.com/charts]

- **Transaction Overview**
  - Electronic coin defined as chain of digital signatures
  - Transfer by signing hash of previous TX and public key of next owner
  - **Double-spending problem** (without global verification)

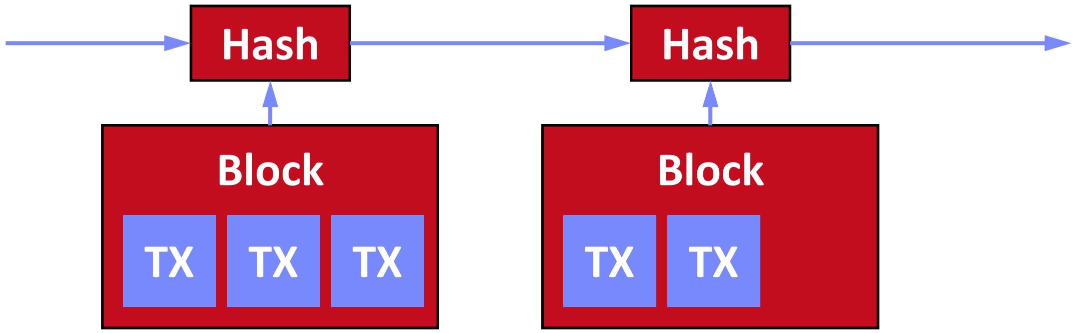


- **Permissioned/Private Blockchains**
  - Blockchain as shared, replicated, permissioned ledger (TX log): **consensus**, **provenance**, **immutability**

Blockchain Data Structure

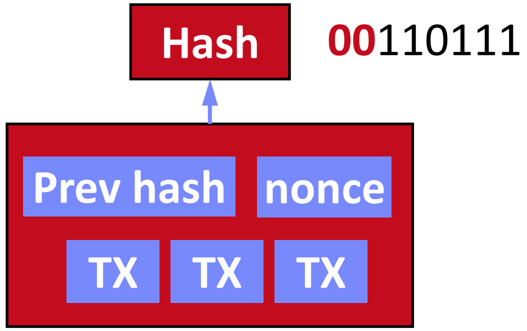
[**Satoshi Nakamoto**: Bitcoin: A Peer-to-Peer Electronic Cash System, **White paper 2008**]

- **Timestamp Server**
  - Decentralized timestamp server: chain of hashes ➔ **public ledger**



Enforces order dependency
➔ **No double-spending**

- **Proof-of-Work**
  - Scanning for value (nonce) whose **SHA-256 hash** begins with a number of zero bits → exponential in number of zeros
  - # zero bits determined by moving average of avg blocks/hour
  - Hard to recompute for chain, easy to check
  - **Majority decision:** CPU time, longest chain



Merkel tree (hash tree)

Blockchain Data Structure, cont.

- **Bitcoin Mining**
  - HW: from CPU to GPUs/FPGAs/ASICs (**10-70 TH/s** @ 2-3KW)
  - Usually mining pools → **"mining cartels"**
- **Hash Rate of Bitcoin Network**
  - **~10 min per block** (144 blocks per day)

@Malaysia

Nov 12, 2021: ~160 EH
Nov 25, 2023: ~494 EH
Nov 25, 2024: ~776 EH

[https://www.blockchain.com/en/charts/hash-rate?daysAverageString=7&timespan=180days, **Nov 12 2021**]

Blockchain Consensus Mechanisms

"means of showing that one invested a non-trivial amount of effort related to some statement"

- **Proof of Work (PoW)**
  - Validation by performing work, existence of HW resources
  - **High HW cost of attacks**
  - **Wasted work, resources, energy** (only first block, no real outcome, e-waste)

- **Proof of Stake (PoS)**
  - Validation by stake-weighted random node selection
  - **Intrinsic coin cost**, **less HW resources**/energy
  - **Untested attack mitigation?**

Ethereum 2.0
→ PoS/sharding over time

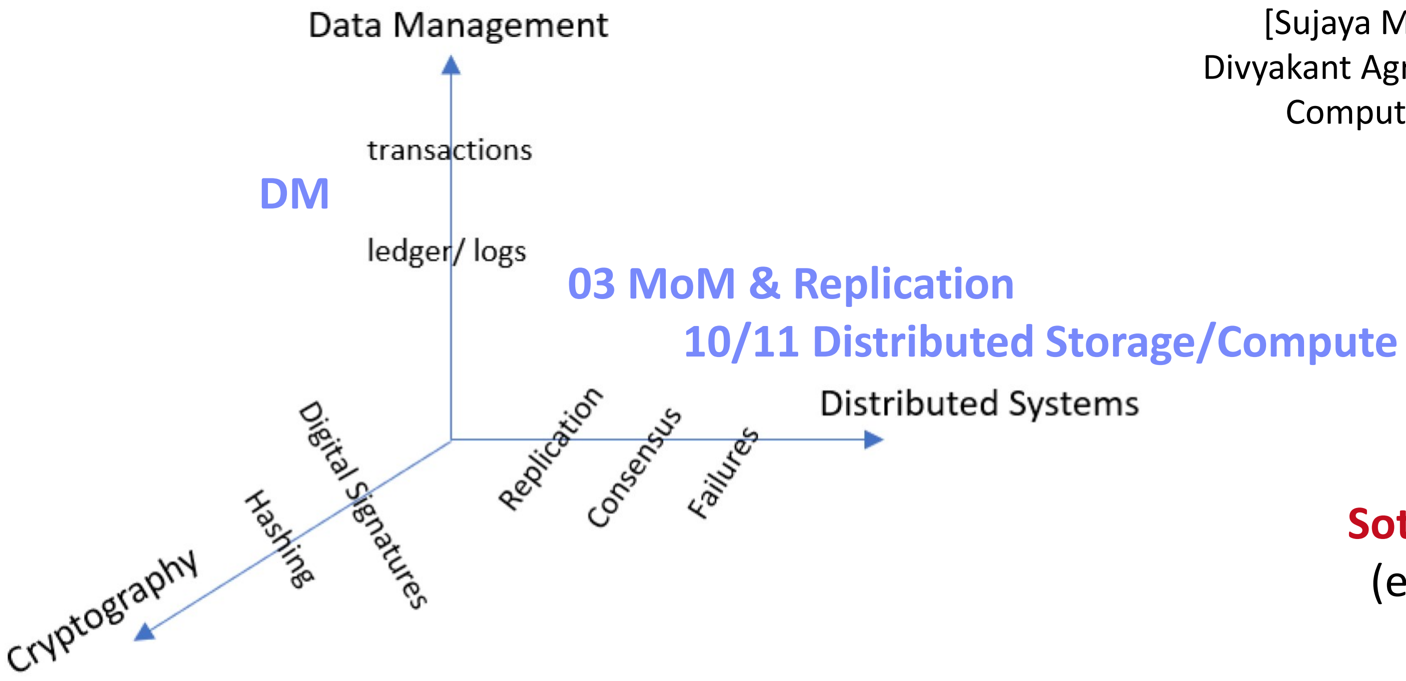
- **Proof of Space/Capacity**
  - Upfront creation of "plot files", store nonces+hashes, find solutions, occasional validation
  - **HW costs of attacks**, use of **unused space**
  - **Moderate adoption**

[https://www.chia.net/]

[Stefan Dziembowski, Sebastian Faust, Vladimir Kolmogorov, Krzysztof Pietrzak: Proofs of Space. IACR Cryptol. 2013]

Discussion Blockchain

[Sujaya Maiyya, Victor Zakhary, Mohammad Javad Amiri, Divyakant Agrawal, Amr El Abbadi: Database and Distributed Computing Foundations of Blockchains. **SIGMOD 2019**]



Many established techniques

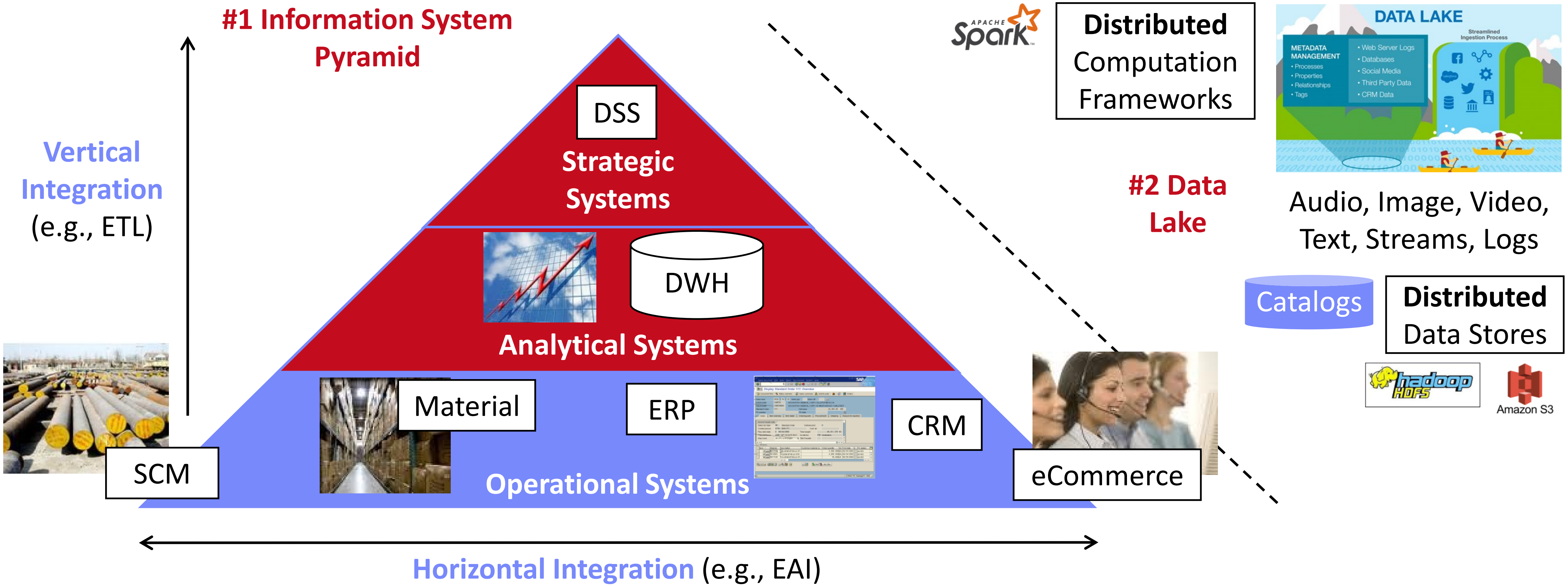
SotA toward scalable/efficient blockchains

(especially for permissioned blockchains)

➔ **Recommendation: Investigate business requirements/context, decide on technical properties and acceptable trade-offs**

Data Catalogs

Recap: Complementary System Architectures



Overview Data Catalogs

- **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**]

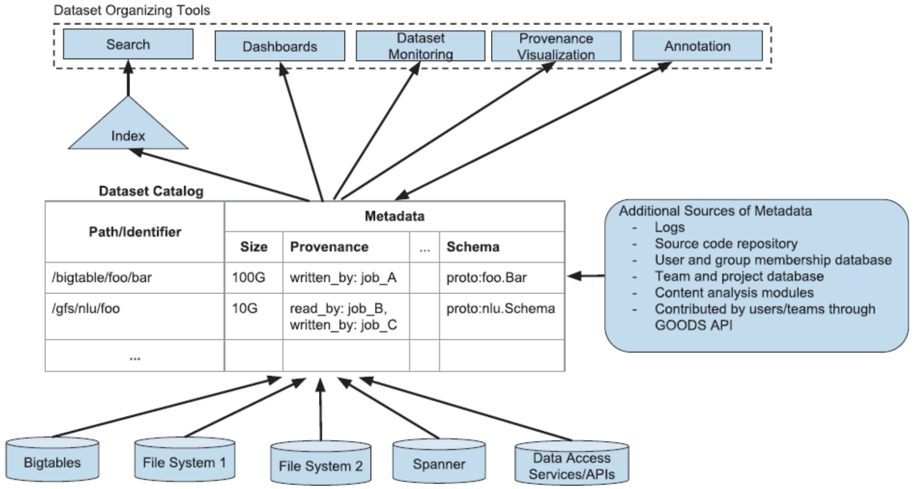
[Dan Brickley, Matthew Burgess, Natasha F. Noy: Google Dataset Search: Building a search engine for datasets in an open Web ecosystem. **WWW 2019**]

[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



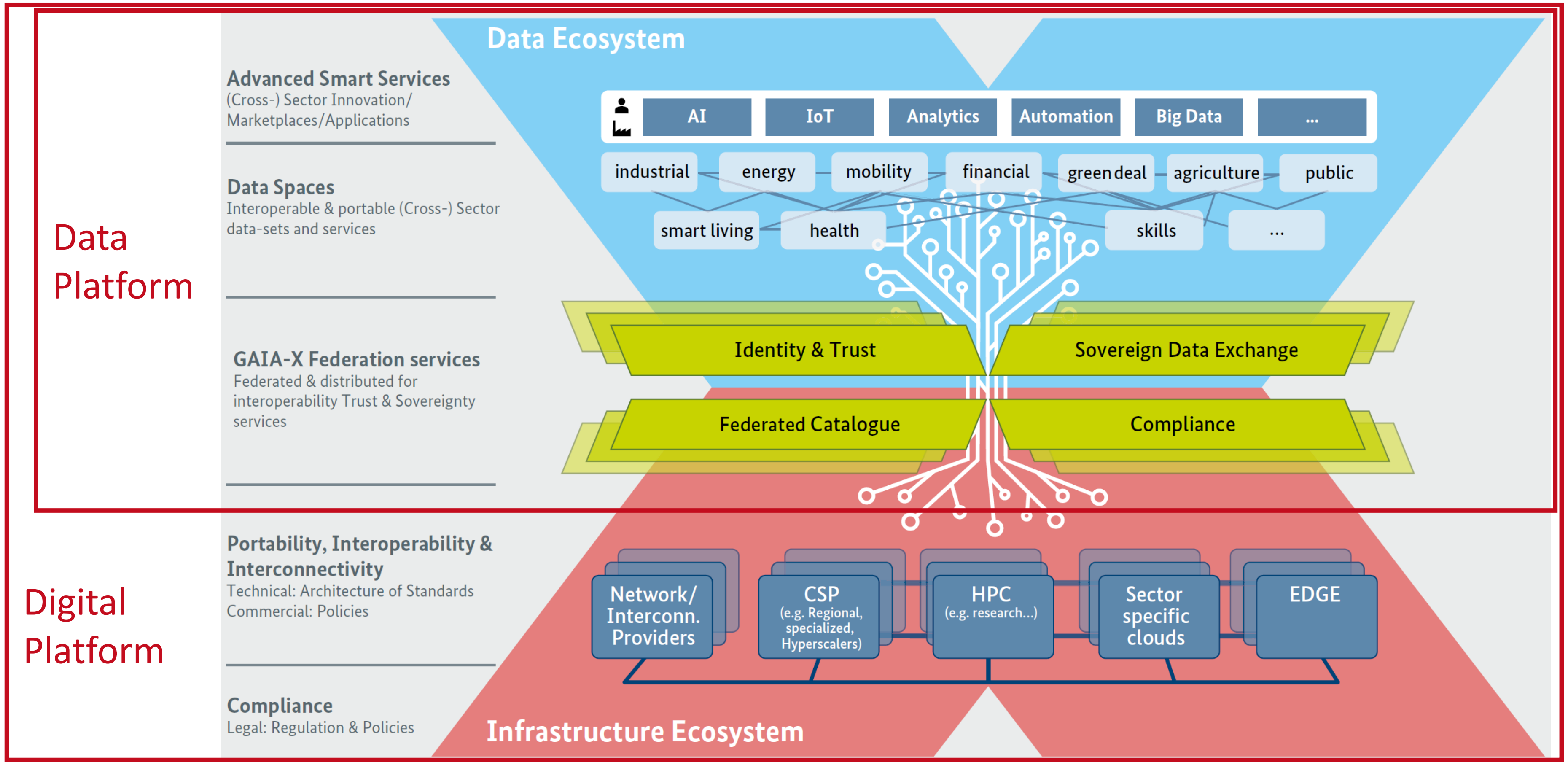
Category	Number of datasets	% of total	Sample formats
Tables	7,822K	37%	CSV, XLS
Structured	6,312K	30%	JSON, XML, OWL, RDF
Documents	2,277K	11%	PDF, DOC, HTML
Images	1,027K	5%	JPEG, PNG, TIFF
Archives	659K	3%	ZIP, TAR, RAR
Text	623K	3%	TXT, ASCII
Geospatial	376K	2%	SHP, GEOJSON, KML
Computational biology	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

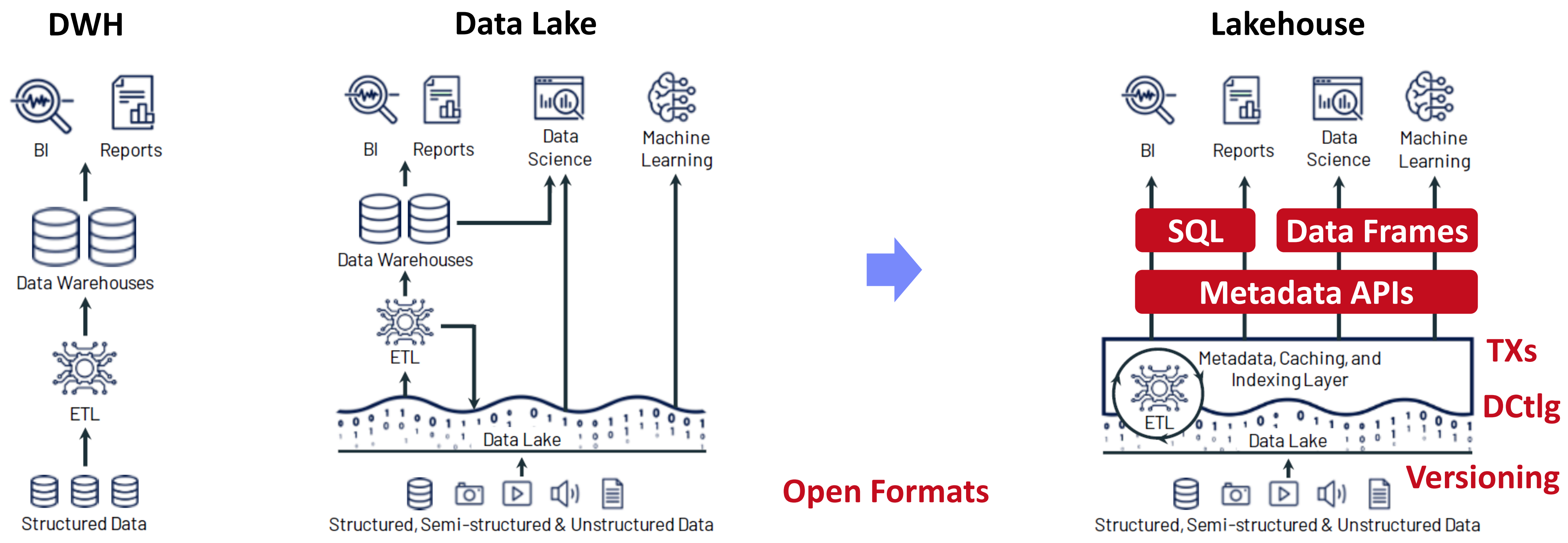
GAIA-X Initiative & Integration

[BMWi: GAIA-X: Driver of digital innovation in Europe – Featuring the next generation of data infrastructure, **2020**]

- **GAIA-X Architecture Overview**



Example Delta Lake (and Lakehouse Architecture)



[Michael Armbrust et al: **Delta Lake:** High-Performance ACID Table Storage over Cloud Object Stores. **PVLDB 13(12) 2020**]

[Michael Armbrust, Ali Ghodsi, Reynold Xin, Matei Zaharia: **Lakehouse:** A New Generation of Open Platforms that Unify Data Ware-housing and Advanced Analytics, **CIDR 2021**]

[Alexander Behm: Photon: A High-Performance Query Engine for the **Lakehouse**, **CIDR 2022**]

Key Features of a Data Catalog

- **#1 Dictionary of Datasets**
  - Basic overview, links, and curation of available datasets
  - Raw/original, curated datasets, derived data products
- **#2 Rich Meta Data Collection**
  - **Format, schema, and access information** of datasets
  - **Data profiling, data validation** results, and data quality scores
- **#3 Lineage/Provenance**
  - Coarse- **or fine-grained lineage**, incl applied **data integration and cleaning process**
  - Optionally **artifacts** to reproduce datasets from sources
- **#4 Data Discovery, Governance, and Sharing**
  - Find related "joinable" datasets (e.g., over spatial-temporal keys)
  - **Efficient discovery** and **sharing** of federated data sources

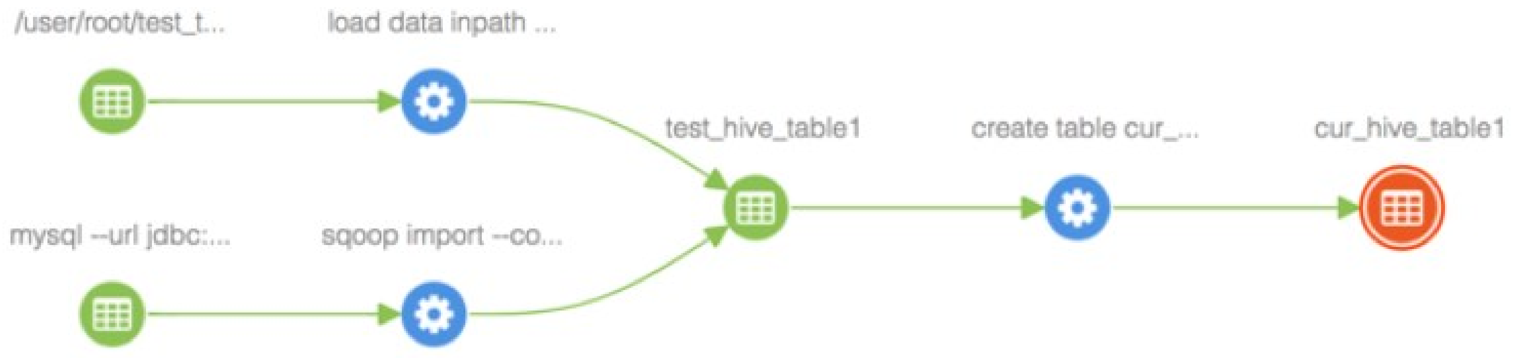
[Sonia Castelo, Rémi Rampin, Aécio S. R. Santos, Aline Bessa, Fernando Chirigati, Juliana Freire: Auctus: A Dataset Search Engine for Data Discovery and Augmentation. **PVLDB 2021**]

Apache Atlas

[https://atlas.apache.org]

- **Apache Atlas Overview**
  - Metadata management and governance capabilities
  - Build catalog (data classification, cross-component lineage)

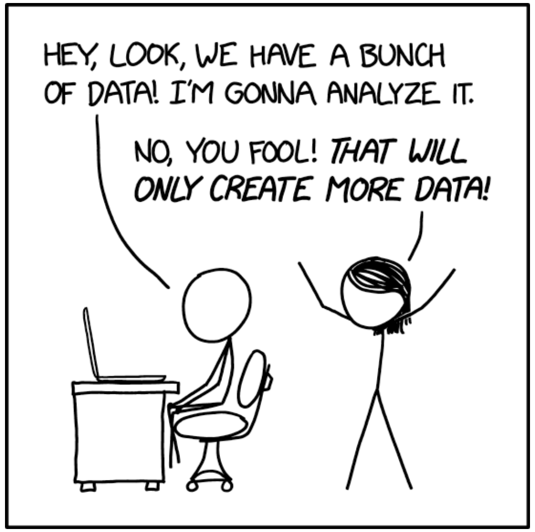
- **Example**
  - Configure Atlas hooks w/ Hadoop components
  - Automatic tracking of lineage and side effects



[https://www.cloudera.com/tutorials/cross-component-lineage-with-apache-atlas-across-apache-sqoop-hive-kafka-storm/.html]

Summary and Q&A

- **Motivation and Terminology**
- **Data Provenance**
- **Data Catalogs**



[https://xkcd.com/2582/]

- **Next Lectures (Large-scale Data Management and Analysis)**
  - **08 Cloud Computing Fundamentals** [Dec 05, **virtual only**]
  - **09 Cloud Resource Management and Scheduling** [Dec 12]
  - **10 Distributed Data Storage** [Dec 19]
  - **11 Distributed, Data-Parallel Computation** [Jan 09]
  - **12 Distributed Stream Processing** [Jan 16]
  - **13 Distributed Machine Learning Systems** [Jan 23]