Data Management in Machine Learning: Challenges, Techniques, and Systems

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SIGMOD 2017

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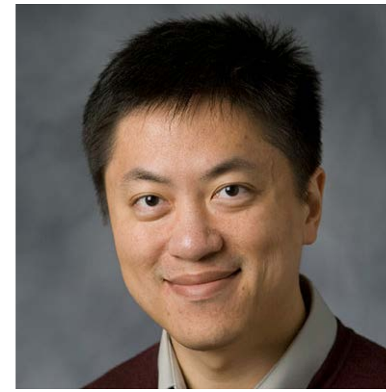
Apache SystemML™



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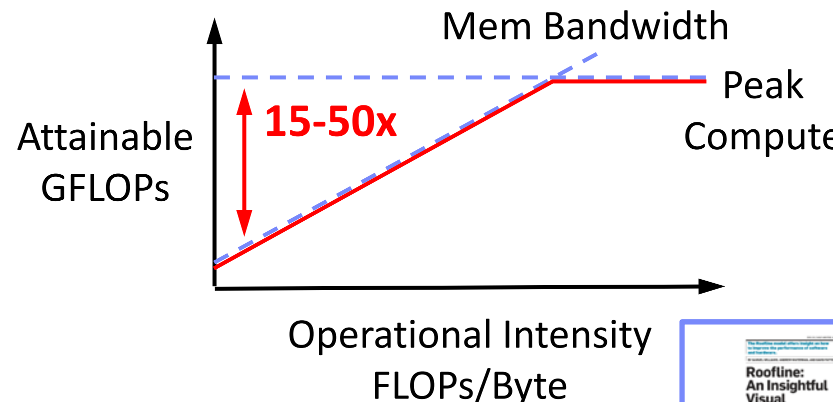
Motivation: A Data-Centric View of ML

- **Application Perspective**
  - Machine learning / advanced analytics / deep analytics
  - ➔ **Modern data-driven applications** (e.g., BI, e-commerce, healthcare)

- **Workload Perspective**
  - Repetitive ML workflows
  - Often **iterative ML algorithms**
  - Often **I/O-bound operations** (e.g., matrix-vector multiplications)




Roofline: An Insightful Visual Performance Model for Multicore Architectures

CACM'09

- **Systems Perspective**
  - **ML in data systems**
  - **DB-inspired ML systems**
  - **ML Lifecycle Systems**

This Tutorial

Motivation: Systems Landscape

TUPAQ Mlbase Tupleware GraphLab HP Distributed R Kasen Emma Cümülön(-D) OptiML Glade Cumulon RIOT-DB DMac LINVIEW Photon ML SystemML RIOT Hemingway Mahout Samsara SAP HANA MS (Rev) R Velox F Brainwash BigR SciDB ORE Longview TensorDB DeepDive AzureML Fa R4ML Columbus SimSQL Orion Zombie ScalOps MXNet BUDS R Matlab Santoku LibFM KeystoneML Torch Julia scikit-learn Sherlock ModelHub BigDL TensorFlow Weka ModelDB Hamlet Mahout CNTK Theano SPSS Spark ML MADlib VW Bismarck Keras Singa SAS Spark R Flink ML Caffe DL4J

Motivation: Tutorial Goals

- **Overall Goal:** Comprehensive review of systems and techniques that tackle data management challenges in the context of ML workloads

- **#1 Categorize Existing Systems**
  - ML in data systems, DB-inspired ML systems, ML lifecycle systems
- **#2 Survey State-of-the-Art Techniques**
  - Query gen, UDFs, factorized learning, deep DBMS integration
  - Optimization and runtime techniques, incl. resource elasticity
  - Model selection and model management

➔ **Intended Takeaways**
  - Awareness of existing systems and techniques
  - Survey of effective optimization and runtime techniques
  - Overview of open research problems

What this Tutorial is NOT

- **Introduction to Machine Learning**

- **Tutorial on General-Purpose Systems**
  - Dataflow systems
  - Graph-focused systems

[SIGMOD’13]

[SIGMOD’16]

- **Tutorial on Deep Learning**
  - Deep learning algorithms
  - Deep learning systems (e.g., Torch, Theano, BigDL, TensorFlow, MXNet, CNTK, Singa, Keras, Caffe, DL4J)

[SIGMOD Record’16]

- **Tutorial on ML for RDBMS Internals**
  - Cost models
  - Workload prediction (e.g., in Peloton)

[CIDR’17]

Tutorial Outline

ML in Data Systems

- **2 Query Generators and UDFs** 14min JY
- **3 Factorized Learning and Deep RDBMS Integration** 8min AK

DB-Inspired ML Systems

- **4 Rewrites, Operator Selection, and Fusion** 14min MB
- **5 Compression, Scan Sharing, and Index Structures** 10min MB
- [**6 Cloud Resource Elasticity** 10min JY]

ML Lifecycle Systems

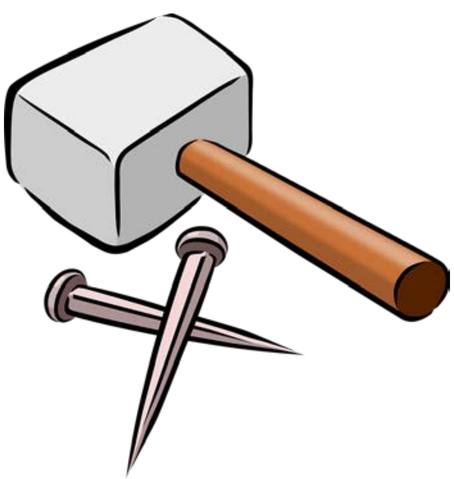
- **7 Feature Engineering, Model Selection/Management** 16min AK

Open Problems and Q&A

Part 2: ML with SQL & UDF

"I suppose it is tempting, if the only tool you have is a hammer, to treat everything as if it were a nail."

Abraham Maslow, 1966



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ML in Database – Why?

- **Convenience**
  - "Elephants" (octopi?) have shown remarkable flexibility
  - A single platform for not only data management, transformation, and querying, but also ML and application of insights
- **Efficiency**
  - Move the analysis, not data
  - Can co-optimize various steps involved in the "big data pipeline"
- **Declarativeness**
  - Simplifies development
  - Enables effective automatic optimization, which helps scalability/efficiency
  - One area where the DB community has plenty to offer

Roadmap

- **First, examples of what SQL can do for ML, at various levels of abstraction:**
  - Matrix multiply
  - Ordinary least squares
  - Gradient descent

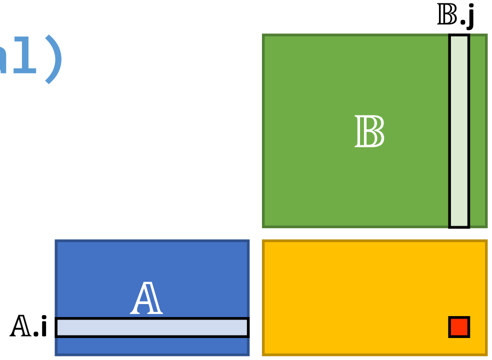
  (See backup slides for
  - k-means
  - Markov-chain Monte-Carlo)

- **Then, a brief discussion of approaches to using SQL for ML**

Matrix Multiply: Take 1

MAD Skills [VLDB'09]

- **Data:** `A(i,j,val)`, `B(i,j,val)`
  - Basically a sparse representation
- ```
  SELECT A.i, B.j, SUM(A.val*B.val)
  FROM A, B
  WHERE A.j = B.i
  GROUP BY A.i, B.j;
  ```



- **Works pretty well for sparse matrices**
- **Not so good for dense matrices, but still beats "small-data" platforms when data doesn't fit in memory**
  ```

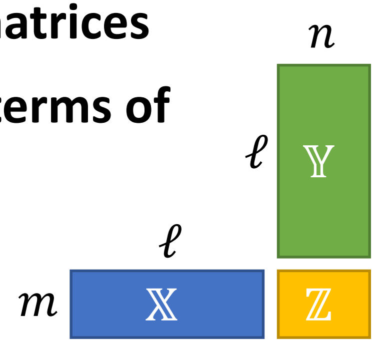
Matrix Multiply: Take 2

MAD Skills [VLDB'09]

- **Data:** `A(i,row), B(j,col)`
  - `row` and `col` are `ARRAY` types or user-defined vector types
  - Basically a row-/column-major representation
- **UDF (user-defined function):** `dotproduct(`v_1`,`v_2`)` **computes the dot product of two vectors**

```
SELECT A.i, B.j, dotproduct(A.row, B.col)
FROM A, B;
```

- **Works fine for dense matrices**
- **But still suboptimal in terms of compute-to-I/O ratio**



Computation: $O(\ell mn)$, or volume
I/O: $O(m\ell + \ell n + nm)$, or surface
☞ Want instead "blocky" units to maximize compute-to-I/O ratio

- **Also note the change in representation (from input to output)**

Matrix Multiply: Take 3

RIOT-DB [CIDR'09] *SimSQL* [ICDE'17]

- **Data:** `A(i,j,V)`, `B(i,j,V)`
  - V represents a submatrix; assume the dimensions are compatible
  - Basically a blocked representation
- **UDFs**
  - matmult(V_1,V_2) computes the product of two matrices
  - matsum(V) is a UDA (user-defined aggregate) that sums up input matrices

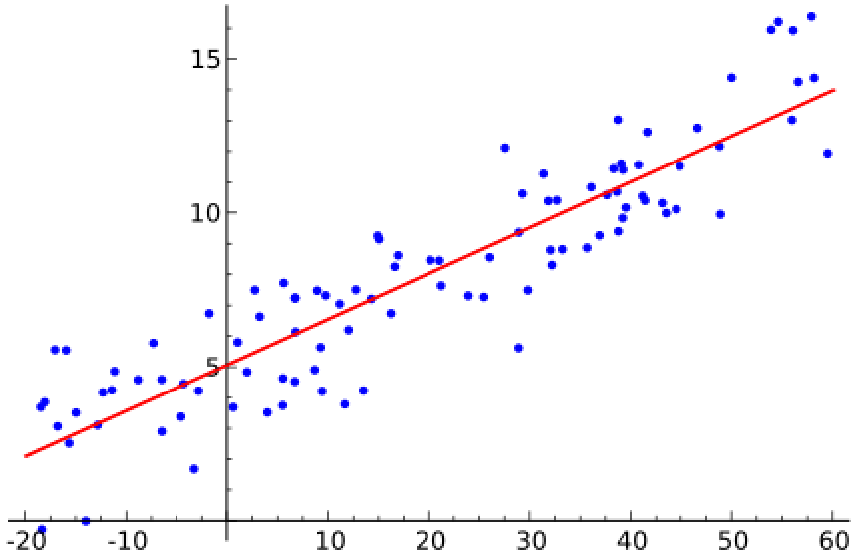
```
SELECT A.i, B.j, matsum(matmult(A.V, B,V))
FROM A, B
WHERE A.j = B.i
GROUP BY A.i, B.j;
```

- **Choose a "big enough" V with good aspect ratio**
  - E.g., square V's beat skinny V's
- **UDFs can use optimized libraries like BLAS**

Ordinary Least Squares

- **To fit data (X, y) to a linear model $y = X\beta + \epsilon$:**

$$\beta^{\star} = (X^T X)^{-1} X^T y$$



- **Computation involves basic matrix operators expressible in SQL with help of UDFs**
  - Inverse is tougher, but assuming the input matrix is small:
    - Code it as a UDF with memory-resident input
    - Processing won't benefit from DBMS though

MAD **[VLDB'09, '12]**
SimSQL **[ICDE'17]**

https://en.wikipedia.org/wiki/File:Linear_regression.svg

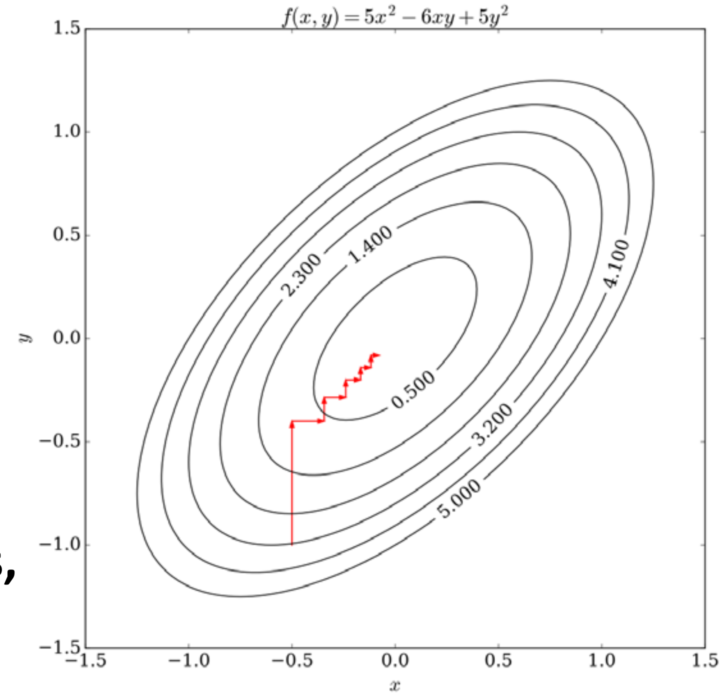
Observation

- **How far can UDF and UDA go? Surprisingly very!**
- **UDF (oftentimes coded in other languages, e.g., Python and R)**
  - Either on the tuple-level (invoked by SQL queries),
  - Or like an application program (invoking SQL queries)
- **UDA**
  - `Init(state)` initializes the state
  - `Accumulate(state, data)` computes updated state with new data
  - [optional] `Merge(state, state)` merges intermediate results computed over disjoint input subsets
  - `Finalize(state)` computes the final result from the state

☞This pattern covers lots of iterative computation in ML, e.g.
  - k-means (backup slides) ***GLADE* [LADIS'11,SIGMOD'12], *MADlib* [VLDB'12]**
  - Gradient descent (next)

Gradient Descent (GD)

- **Given a model with parameters w, we want to learn from data D, i.e., minimize a loss function $F(w; D)$**
  - E.g., sum of loss over all training data + a regularization term



- **Start with some guess w_0**
- **In each step $t+1$, update w in the direction of the gradient of the loss function at w_t, i.e., $F'(w_t)$**
- **Rinse and repeat**

- **Under certain (commonly held) conditions, GD converges to a local minimum**
  - If F is convex, that's its global minimum

https://zh.wikipedia.org/wiki/File:Coordinate_descent.svg

Stochastic GD (SGD)

- **Suppose $F(w; D)$ is linearly separable over D**
  - I.e., $F(w; D) = \sum_i f_i(w; d_i)$,
    where i iterates over the data points $D = \{d_i\}_i$
- **Instead of updating w using the "full gradient" computed over D in each GD step, just choose a single point in D**
  - I.e., use $f_i'(w)$ to approximate $F'(w)$
- **Remarkably, for convex $F(w)$, SGD also converges to the global minimum, even if we pick points from D in a fixed, arbitrary order**
  - Albeit at a slower rate

GD/SGD in SQL

- **GD (full gradient)**
  - Computation of full gradient over D can be done by a query using UDA
  - Several options for driving outer loop
    - ***MADlib*** **[VLDB'12]** uses Python UDF
    - ***ScalOps*** **[DeBull'12]** uses Datalog
      - Underlying implementation is MapReduce instead of SQL

- **SGD** ***Bismarck*** **[SIGMOD'12]**
  - The entire procedure can be written as a query over D using UDA—each `Accumulate()` corresponds to one step

MCMC in SQL

- **MCMC (Markov-Chain Monte-Carlo) is a key method in Bayesian ML**
- **Bayesian ML comes down to analyzing the "posterior" distribution**

  P(parameters, hidden variables | observations)
- **Direct analysis is often hard, so we use Monte-Carlo simulation**
  - Repeatedly sample from the posterior, and analyze the samples
- **But sampling directly from the posterior is often hard, so we use MCMC**
  - A sampler generates a Markov chain of samples, whose stationary distribution is the target posterior

☞**You can do Gibbs sampling (a form of MCMC) in *SimSQL* [SIGMOD'13]**
  - With user-define "value-generating" functions that draw samples
  - See backup slides for details

Approaches to SQL+ML

Backend choices

- **“On top of” (e.g., *RIOT-DB* [CIDR'09], *MAD* [VLDB'09,VLDB'12]) vs. “inside” DBMS (e.g., *SimSQL* [ICDE'17])**
- **Not DBMS, but still inspired by or rooted in DBMS**
  - General-purpose “big-data” platform (e.g., ***SystemML*** **[ICDE'11,VLDB'16]**, ***Cumulon*** **[SIGMOD'13]**)
  - Specialized system from ground up (e.g., ***RIOT*** **[ICDE'10]**, ***SciDB*** **[CSE'13]**)

Interface choices

- **SQL + libraries or extensions (e.g., *MAD* [VLDB'09,VLDB'12], *SimSQL* [ICDE'17], *Oracle Data Mining*, …)**
- **ML-oriented languages on top of SQL (e.g., *RIOT-DB* [CIDR'09], *BUDS/SimSQL* [SIGMOD'17], *Oracle R Enterprise*, …)**

Interface: SQL + Libraries/Extensions

- **Especially nice with integrated model management, e.g., *Oracle Data Mining***
  - Can create, store, update, and apply models in SQL

```
-- Create model settings:
CREATE TABLE svm_settings(
  setting_name VARCHAR2(30), setting_value VARCHAR2(30));
INSERT INTO svm_settings VALUES(
  dbms_data_mining.algo_name,
  dbms_data_mining.algo_support_vector_machines);
-- …
-- Build model:
DBMS_DATA_MINING.CREATE_MODEL(
  model_name => 'svm_model',
  mining_function => dbms_data_mining.classification,
  data_table_name => 'mining_data_build_v',
  case_id_column_name => 'cust_id',
  target_column_name => 'affinity_card',
  settings_table_name => 'svm_settings');
-- Apply model:
DBMS_DATA_MINING.APPLY(
  model_name => 'svm_model',
  data_table_name => 'mining_data_apply_v',
  case_id_column_name => 'cust_id',
  result_table_name => ’svm_apply_result');
```

Interface: no SQL

- **Let user write wh** … **R, Python, etc.)**
  - Provide a libra … ns implemented by the underlying …
  - SQL undernea … ***QL* [SIGMOD'17],** ***Oracle R Ente***…
  - Other "big-dat … **:DE'11,VLDB'16],** ***Spark R***, ***Mah***…

```
invGamma = externalFunction(...)...
invGaussian = externalFunction(...)...
multiNormal = externalFunction(...)...

X = read("test_data/xb.bin", format="binary")
y = read("test_data/yb.bin", format="binary")
y_avg = avg(y)
y = y - y_avg

# compute the matrix X'X, and X'Y
XX = t(X) %*% X
XY = t(X) %*% y

# number of data points and number of features
n = nrow(X)
m = ncol(X)

shape_prior = 1.0
scale_prior = 1.0
mean_prior = matrix(1.0, rows=1, cols=m)
sigma2= invGamma(shape_prior, scale_prior)
tau= invGaussian(mean_prior, shape_prior)

niter = 5

for (i in 1:niter) {

  A = XX + diag(t(tau))
  A_inv = inv(A)
  mu = A_inv %*% XY
  covariance = A_inv * sigma2
  beta = multiNormal(t(mu), covariance)
  remain_sum1 = (t(y) - beta %*% t(X))
    (y - X %*% t(beta)) / 2.0
  remain_sum2 = (beta * beta) %*% t(tau) / 2.0
  scale_m = 1.0 + remain_sum1 + remain_sum2
  scale = as.scalar(scale_m[1,1])
  shape = 1.0 + (n-1.0)/2.0 + m/2.0
  sigma2 = invGamma(shape, scale)
  tau_mu = sqrt(sigma2 / (beta * beta))
  tau = invGaussian(tau_mu, 1.0)
}
```

```
externalFunction(...)...
 = externalFunction(...)...
 = externalFunction(...)...

est_data/xb.bin", format="binary")
est_data/yb.bin", format="binary")
(y)
vg

he matrix X'X, and X'Y
*% X
*% y

 data points and number of features

 = 1.0
 = 1.0
= matrix(1.0, rows=1, cols=m)
Gamma(shape_prior, scale_prior)
ssian(mean_prior, shape_prior)

:niter) {

diag(t(tau))
nv(A)
v %*% XY
nce = A_inv * sigma2
multiNormal(t(mu), covariance)
sum1 = (t(y) - beta %*% t(X))
X %*% t(beta)) / 2.0
sum2 = (beta * beta) %*% t(tau) / 2.0
 = 1.0 + remain_sum1 + remain_sum2
 as.scalar(scale_m[1,1])
 1.0 + (n-1.0)/2.0 + m/2.0
= invGamma(shape, scale)
= sqrt(sigma2 / (beta * beta))
nvGaussian(tau_mu, 1.0)
```

Bayesian LASSO in ***B***… … in ***SystemML***

(Examples from ***BUDS/SimSQL* [SIGMOD'17]**)

Summary

- **You can get a lot of mileage for machine learning with SQL+UDF (octopus + hammer)**

- **Deep roots in**
  - DBMS extensibility research
  - Array DBMS, e.g., ***SciDB*** **[CSE'13]**; see **Rusu & Cheng [arXiv 2013]** for survey

- **Next: more opportunities for deeper ML+DB integration**

http://www.bongpages.com/index.php?route=product/product&product_id=115

References for Part 2: ML with SQL & UDF

- ***Bismarck* [SIGMOD'12]** Feng et al. "Towards a Unified Architecture for in-RDBMS Analytics." SIGMOD 2012
- ***BUDS/SimSQL* [SIGMOD'17]** Gao et al. "The BUDS Language for Distributed Bayesian Machine Learning." SIGMOD 2017
- ***Cumulon* [SIGMOD'13]** Huang et al. "Cumulon: optimizing statistical data analysis in the cloud." SIGMOD 2013
- ***GLADE* [LADIS'11]** Rusu & Dobra. "GLADE: A Scalable Framework for Efficient Analytics." LADIS 2011
- ***GLADE* [SIGMOD'12]** Cheng et al. "GLADE: Big Data Analytics Made Easy." SIGMOD 2012
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- ***MADlib* [VLDB'12]** Hellerstein et al. "The MADlib Analytics Library or MAD Skills, the SQL." PVLDB 5(12), 2012
- ***RIOT-DB* [CIDR'09]** Zhang et al. "RIOT: I/O-efficient numerical computing without SQL." CIDR 2009
- ***RIOT* [ICDE'10]** Zhang et al. "I/O-efficient statistical computing with RIOT." ICDE 2010
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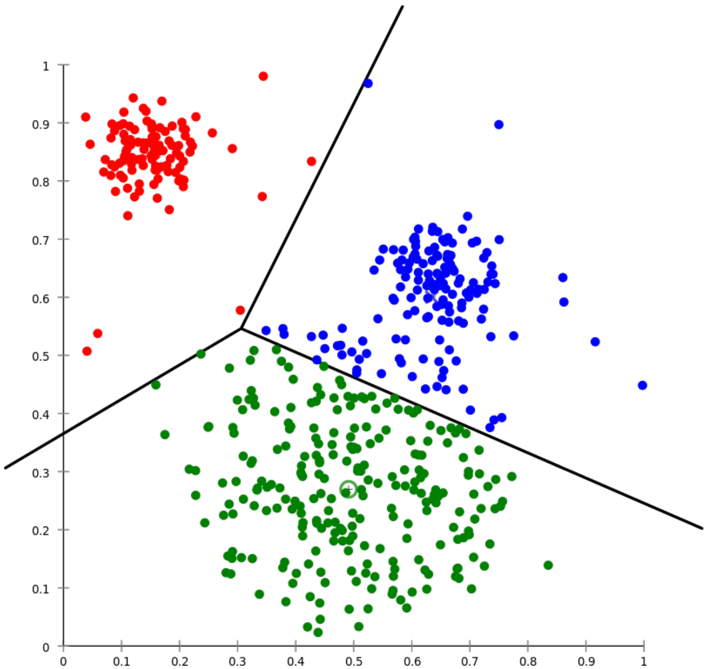
- ***SciDB* [CSE'13]** "SciDB: A Database Management System for Applications with Complex Analytics." Comp. Sci. Eng. 15(3), 2013
- ***SimSQL* [SIGMOD'13]** Cai et al. "Simulation of Database-Valued Markov Chains Using SimSQL." SIGMOD 2013
- ***SimSQL* [ICDE'17]** Luo et al. "Scalable Linear Algebra on a Relational Database System." ICDE 2017
- ***SystemML* [ICDE'11]** Ghoting et al. "SystemML: Declarative machine learning on MapReduce." ICDE 2011
- ***SystemML* [VLDB'16]** Boehm et al. "SystemML: Declarative machine learning on Spark." PVLDB 9(13), 2016

Part 2 Backup/Extra Slides

k-Means Clustering

- **Given n points, find k centroids to minimize sum of squared distances between each point and its closest centroid**



- **EM-style iterative algorithm:**
  1. Pick initial k candidate centroid locations
  2. Assign each point to the closest candidate
  3. Reposition each candidate as the centroid of its assigned points
  4. Repeat 2-3 above until assignment changes no more (or very little)

https://commons.wikimedia.org/wiki/File:KMeans-Gaussian-data.svg

k-Means as UDA

- **State: k candidates with locations + cluster info** $\{\langle \mathrm{loc}_i, \mathbf{sum}_i, \mathbf{cnt}_i \rangle\}_{1 \le i \le k}$
- `Init`**: given centroid locations, with sum and count of 0**
- `Accumulate`**: given a data point p, find the candidate i closest to p; increment $\mathbf{sum}_i$ by p's coordinates and $\mathbf{cnt}_i$ by one**
- `Merge`**: merge $\langle \mathrm{loc}, \mathbf{sum}, \mathrm{cnt} \rangle$ records by $\mathbf{loc}$; add sum and cnt**
- `Finalize`**: for each i, compute new loc_i as $\mathbf{sum}_i / \mathbf{cnt}_i$**
- **One SQL query with this UDA gives one iteration of the EM algorithm**
  - For the next iteration, the UDA will be initialized with the k locations computed from the previous
  - Can use a UDF to drive overall iterations
  - Termination condition can be evaluated in SQL too (see *MADlib*)

***GLADE* [LADIS'11,SIGMOD'12]**
***MADlib* [VLDB'12]**

Markov-Chain Monte-Carlo (MCMC)

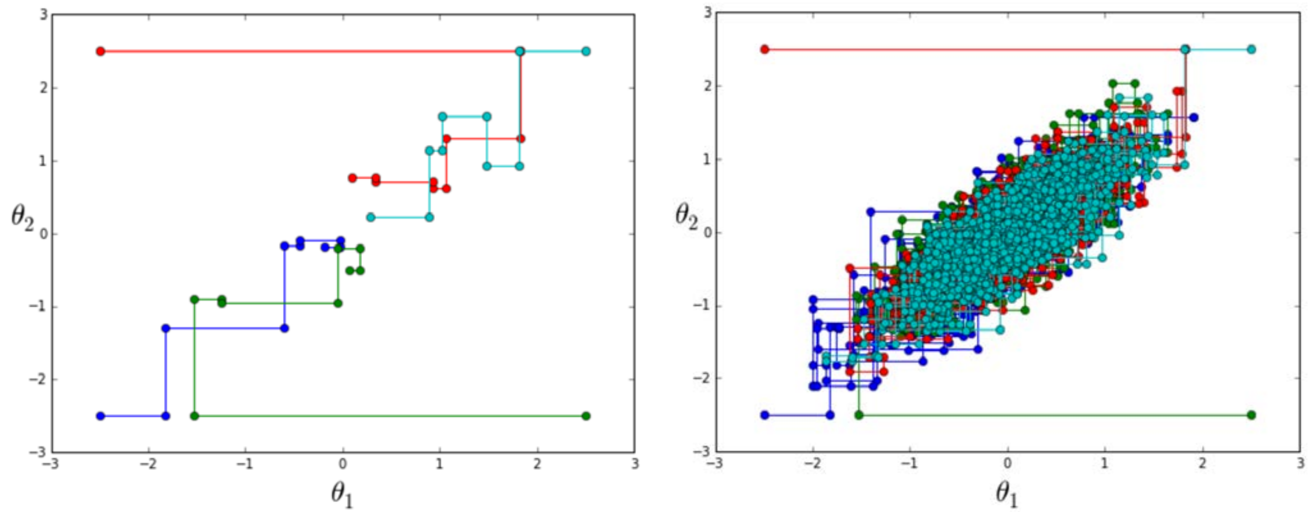
- **Bayesian ML comes down to analyzing the “posterior” distribution**

  P(parameters, hidden variables | observations)

- **Direct analysis is often hard, so we use Monte-Carlo simulation**
  - Repeatedly sample from the posterior, and analyze the samples
- **But sampling directly from the posterior is often hard, so we use MCMC**
  - A sampler generates a Markov chain of samples, whose stationary distribution is the target posterior

Example: Gibbs Sampling

- **Suppose we have an n-variate distribution, but the conditional distributions are easier to sample from**
- **Begin with some initial sample $\mathbb{z}^{(0)}$**
- **For the $(t+1)$-th sample $\mathbb{z}^{(t+1)}$, sample each component $z_i^{(t+1)}$ conditioned on all other components sampled most recently, i.e., $p\left(z_i^{(t+1)} \,\middle|\, z_1^{(t+1)}, \dots, z_{i-1}^{(t+1)}, z_{i+1}^{(t)}, z_n^{(t)}\right)$**
- **Rinse and repeat**



https://ga7g08.github.io/2015/02/09/Gibbs-sampler-with-a-bivariate-normal-distribution/

MCMC in SimSQL

SimSQL **[SIGMOD'13]**

- **Think of each sample as a table (tables)**
- **Write UDF to define "VG" (value-generating) functions that draw samples**
- **Write SQL with VG functions to define how to generate T$[t]$ (instance of table T in the t-th sample) from T$[t-1]$**
- **Write SQL to simulate multiple MCMC chains, and to compute compute distributional properties for variables of interest from T$[t]$'s across T's, t's, and chains**

☞**An example of staying true to the declarative roots of databases**

- But also need new techniques not in traditional DBMS, e.g.:
  - Plans are huge—cut them into "frames"; observe execution stats of last frame and to optimize the next
  - Use "tuple bundles" to instantiate/process multiple possible worlds simultaneously

Part 3: Learning Over Joins, SRL, and Deep RDBMS Integration

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Overview: Learning Over Joins

Problem: Many datasets are multi-table ⟷ ML toolkits assume single-table inputs → ML after joining tables

Overheads:
Extra storage
Computational redundancy
Join time
Maintenance headaches

Learning Over Joins: "Push Down" ML through joins

1) Over standard data systems: Orion, Santoku, Morpheus
2) Over a "factorized database" system: FDB-F
3) Special-purpose tools: libFM, TensorDB, Compressed ML

Related but orthogonal: Statistical relational learning (DeepDive, etc.)

Learning Over Joins

Over standard data systems: Orion, Morpheus, Santoku

Example: GLMs with gradient descent (GD)

$$L(w) = \sum_{i=1}^{n} f(w'x_i, y_i) \qquad \nabla L(w) = \sum_{i=1}^{n} g(w'x_i, y_i)x_i$$

$$w'x = w'_S x_S + w'_R x_R \qquad x = [x_S \ x_R]$$

$$T = S \bowtie R$$

Orion [SIGMOD'15]:

Introduced the scalable "factorized learning" idea

Easy UDA implementation on existing data systems (RDBMS/Hive/Spark)

Morpheus [VLDB'17]:

Generalizes factorized learning to any ML algorithm in *linear algebra*

"Push down" rewrites for matrix-vector mult., gramian, ginv, etc.

Santoku [VLDB'15]: Discrete features (Naive Bayes, trees, etc.)

Learning Over Joins

Over a "factorized database" system: **FDB-F [SIGMOD'16]**

Generalized semiring-based aggregates over "factorized joins"

Sales

P	S
p_1	s_1
p_1	s_2
p_2	s_3
p_2	s_4
p_3	s_5

Branch

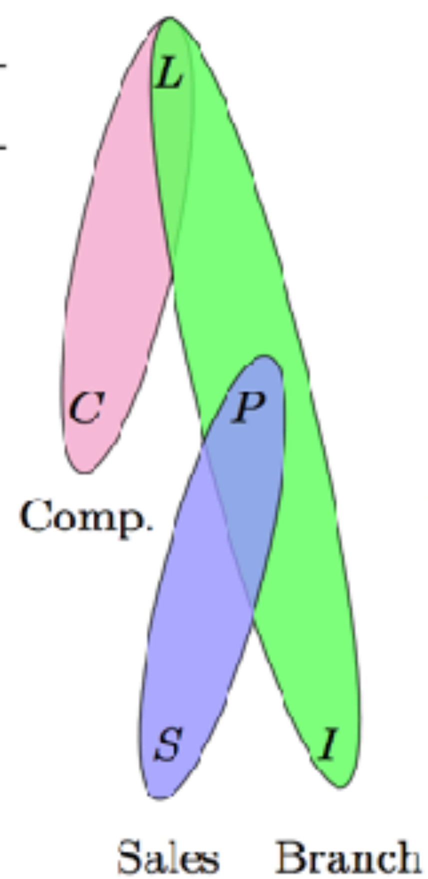
L	P	I
l_1	p_1	i_1
l_1	p_1	i_2
l_1	p_2	i_3
l_2	p_2	i_4
l_2	p_3	i_5

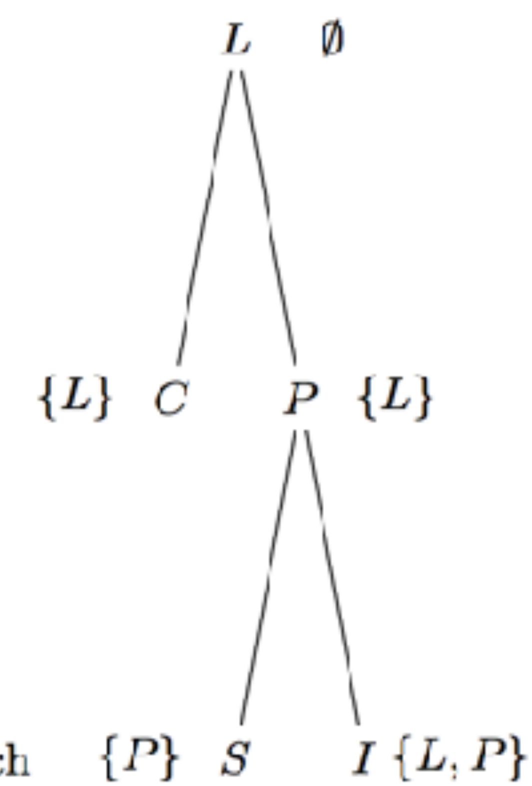
Competition

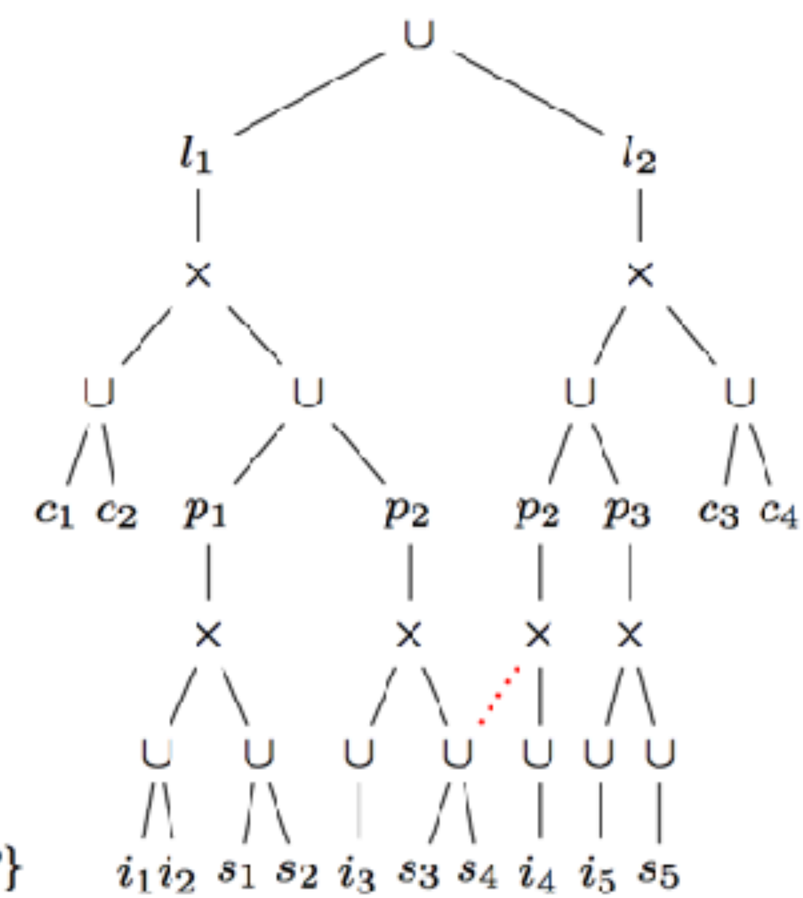
L	C
l_1	c_1
l_1	c_2
l_2	c_3
l_2	c_4

Natural Join

L	C	P	I	S
l_1	c_1	p_1	i_1	s_1
l_1	c_1	p_1	i_1	s_2
l_1	c_1	p_1	i_2	s_1
l_1	c_1	p_1	i_2	s_2
l_1	c_1	p_2	i_3	s_3
l_1	c_1	p_2	i_3	s_4
....				
above block for c_2				
....				
l_2	c_3	p_2	i_4	s_3
l_2	c_3	p_2	i_4	s_4
l_2	c_3	p_3	i_5	s_5
....				
above block for c_4				







SRL; Deep RDBMS Integration

SRL combines statistical learning with logic-based rules/constraints

"Non-IID" ML models
(MVDs, EMVDs, JDs)

NIPS'12 tutorial by Lise Getoor
Book with Ben Taskar

Inference and learning often perform joins internally!

Scalable grounding using RDBMS: **Tuffy [VLDB'10]**
Incremental maintenance: **IncrementalDeepDive [VLDB'15]**

Increasing interest in deeper integration of ML into DBMS kernel!

SAP HANA SLACID: Linear algebra kernels in an RDBMS **[SSDBM'14]**
New compressed sparse row/col. representations
Integrated API for basic access patterns and lin. alg. ops
OpenMP-based shared memory parallelism in DBMS task scheduler

References: Part 3

Columbus [SIGMOD'14]: Materialization Optimizations for Feature Selection Workloads

DeepDive [DataEng'14]: Feature Engineering for Knowledge Base Construction

FDB-F [SIGMOD'16]: Learning Linear Regression Models over Factorized Joins

IncrementalDeepDive [VLDB'15]: Incremental Knowledge Base Construction Using DeepDive

Morpheus [VLDB'17]: Towards Linear Algebra over Normalized Data

Orion [SIGMOD'15]: Learning Generalized Linear Models Over Normalized Data

Santoku [VLDB'15]: Demonstration of Santoku: Optimizing Machine Learning over Normalized Data

SLACID [SSDBM'14]: SLACID - Sparse Linear Algebra in a Column-Oriented In-Memory Database System

Tuffy [VLDB'10]: Tuffy: Scaling up Statistical Inference in Markov Logic Networks using an RDBMS

Backup Slides

Statistical Relational Learning Systems

Captures logical dependencies between between entities/variables

"Non-IID" ML models
(MVDs, EMVDs, JDs)

PODS tutorial by Lise Getoor on Tue!
(also NIPS'12; book with Taskar)

Example: Markov Logic Network (MLN); used by DeepDive

	weight	rule		wrote('Joe', 'P1')
paper(PaperID, URL)	5	$\texttt{cat}(p, c1), \texttt{cat}(p, c2) \Rightarrow c1 = c2$	(F_1)	wrote('Joe', 'P2')
wrote(Author, Paper)	1	$\texttt{wrote}(x, p1), \texttt{wrote}(x, p2), \texttt{cat}(p1, c) \Rightarrow \texttt{cat}(p2, c)$	(F_2)	wrote('Jake', 'P3')
refers(Paper, Paper)	2	$\texttt{cat}(p1, c), \texttt{refers}(p1, p2) \Rightarrow \texttt{cat}(p2, c)$	(F_3)	refers('P1', 'P3')
cat(Paper, Category)	$+\infty$	$\texttt{paper}(p, u) \Rightarrow \exists x.\ \texttt{wrote}(x, p)$	(F_4)	cat('P2', 'DB')
	-1	$\texttt{cat}(p, \text{'Networking'})$	(F_5)	...
Schema		A Markov Logic Program		Evidence

MLN inference (MAP) computes "most probable world" by plugging values of variables to predict

$\boxed{\text{Grounding}}$ + Search

Involves joins!

Scalable grounding using RDBMS: **Tuffy [VLDB'10]**

Scalable Gibbs sampling: **Elementary [SIGMOD'13]**

Incremental maintenance: **IncrementalDeepDive [VLDB'15]**

Deep RDBMS Integration

Integrating linear algebra kernels into an RDBMS: SAP HANA

SLACID [SSDBM'14]: Mutable columnar layout for sparse matrices

Compressed sparse row/col. representation + incr. delta

Integrated API for basic access patterns and lin. alg. ops

OpenMP-based shared memory parallelism in DBMS task scheduler

Time series-specific systems: Fa, F2DB

Fa [VLDB'07]: "Declarative forecasting" queries for time series

Projection and shift-based time series feature transformations

Feature ranking and subset selection heuristics

Lin. reg., Bayesian networks, SVM, CART, Random Forest

Both one-time and continuous forecasting

Part 4: Rewrites, Operator Selection, and Operator Fusion

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SIGMOD 2017

Overview Optimizing Compilers for ML Algorithms

- **Comparison Query Optimization**
  - **Rule- and cost-based rewrites and operator ordering**
  - **Physical operator selection and query compilation**
  - Linear algebra / other ML operators, DAGs, control flow, sparse/dense formats

PL → **Compilers for Large-scale ML**
DB → **Compilers for Large-scale ML**
HPC → **Compilers for Large-scale ML**

- **#1 Interpretation** (operation at-a-time)
  - Examples: **Morpheus** [PVLDB'17]
- **#2 Lazy Expression Compilation** (DAG at-a-time)
  - Examples: **RIOT** [CIDR'09], **Mahout Samsara** [MLSystems'16]
  - Examples w/ control structures: **Weld** [CIDR'17], **OptiML** [ICML'11], **Emma** [SIGMOD'15]
- **#3 Program Compilation** (entire program)
  - Examples: **SystemML** [PVLDB'16], **Cumulon** [SIGMOD'13], **Tupleware** [PVLDB'15]

Optimization Scope

```
X = read($1); # n x m matrix
y = read($2); # n x 1 vector
maxi = 50; lambda = 0.001;
intercept = $3;
...
r = -(t(X) %*% y);
norm_r2 = sum(r * r); p = -r;
w = matrix(0, ncol(X), 1); i = 0;
while(i<maxi & norm_r2>norm_r2_trgt)
{
   q = (t(X) %*% X %*% p)+lambda*p;
   alpha = norm_r2 / sum(p * q);
   w = w + alpha * p;
   old_norm_r2 = norm_r2;
   r = r + alpha * q;
   norm_r2 = sum(r * r);
   beta = norm_r2 / old_norm_r2;
   p = -r + beta * p; i = i + 1;
}
write(w, $4, format="text");
```

Logical Simplification Rewrites

- **Traditional PL Rewrites** (e.g., TensorFlow, OptiML, SystemML)
  - CSE, constant folding, branch removal

- **Algebraic Simplification Rewrites** (e.g., SystemML, FAQ [PODS'16])
  - `t(X) %*% y` → `t(t(y) %*% X)`
  - `trace(X %*% Y)` → `sum(X * t(Y))`
  - `sum(X + Y)` → `sum(X) + sum(Y)`
  - `sum(X^2)` → `t(X) %*% X, iff ncol(X)=1`

- **Loop Vectorization** (e.g., OptiML, SystemML)

```
for(i in a:b)
   X[i,1] = Y[i,2] + Z[i,1]
```
→
```
X[a:b,1] = Y[a:b,2] + Z[a:b,1]
```

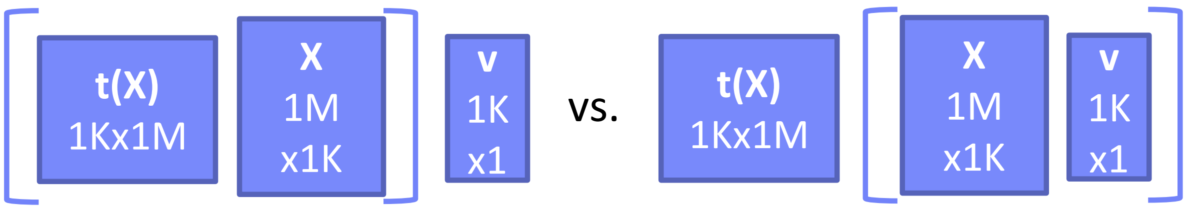
- **Incremental Computations**
  - Delta update rules (e.g., LINVIEW [SIGMOD'14], factorized [CoRR'17])
  - Incremental iterations (e.g., Flink)
  - Update-in-place (e.g., SystemML)

```
A = t(X) %*% X + t(ΔX) %*% ΔX
b = t(X) %*% y + t(ΔX) %*% Δy
```

Logical Simplification Rewrites Matrix Multiplication Chain Optimization

- **Optimization Problem**
  - Matrix multiplication chain of n matrices M_1, M_2, …M_n (associative)
  - Optimal parenthesization of the product M_1M_2 … M_n

Example
t(X) %*% X %*% v



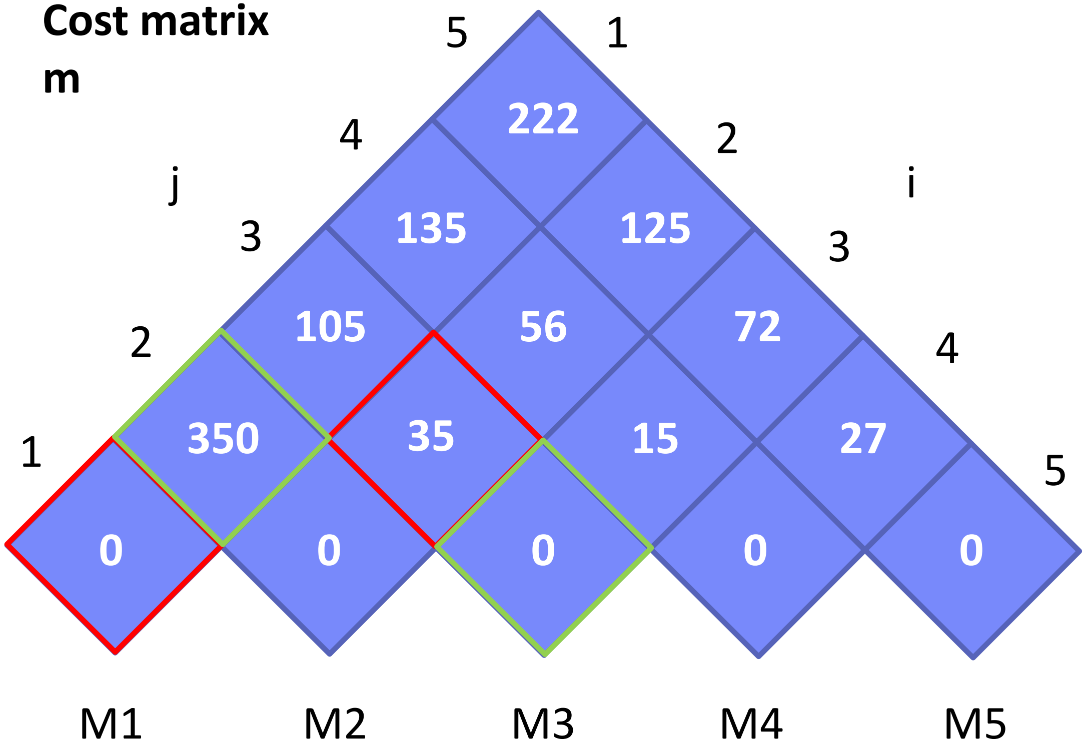
2,002 GFLOPs **4 GFLOPs**

- **Search Space Characteristics**
  - Naïve exhaustive: Catalan numbers → $\Omega(4^n / n^{3/2})$)
  - DP applies: (1) optimal substructure, (2) overlapping subproblems
  - Textbook DP algorithm [MIT Press'09]: $\Theta(n^3)$ time, $\Theta(n^2)$ space
    - Examples: **SystemML** [Data Eng. Bull. '14], **RIOT** (including I/O costs), **SpMachO** (including sparsity for intermediates) [EDBT'15],
  - Best known algorithm: O(n log n)

Matrix Multiplication Chain Optimization

M1	M2	M3	M4	M5
10x7	7x5	5x1	1x3	3x9

Cost matrix m



m[1,3] = min(
m[1,1] + m[2,3] + p1p2p4,
m[1,2] + m[3,3] + p1p3p4)

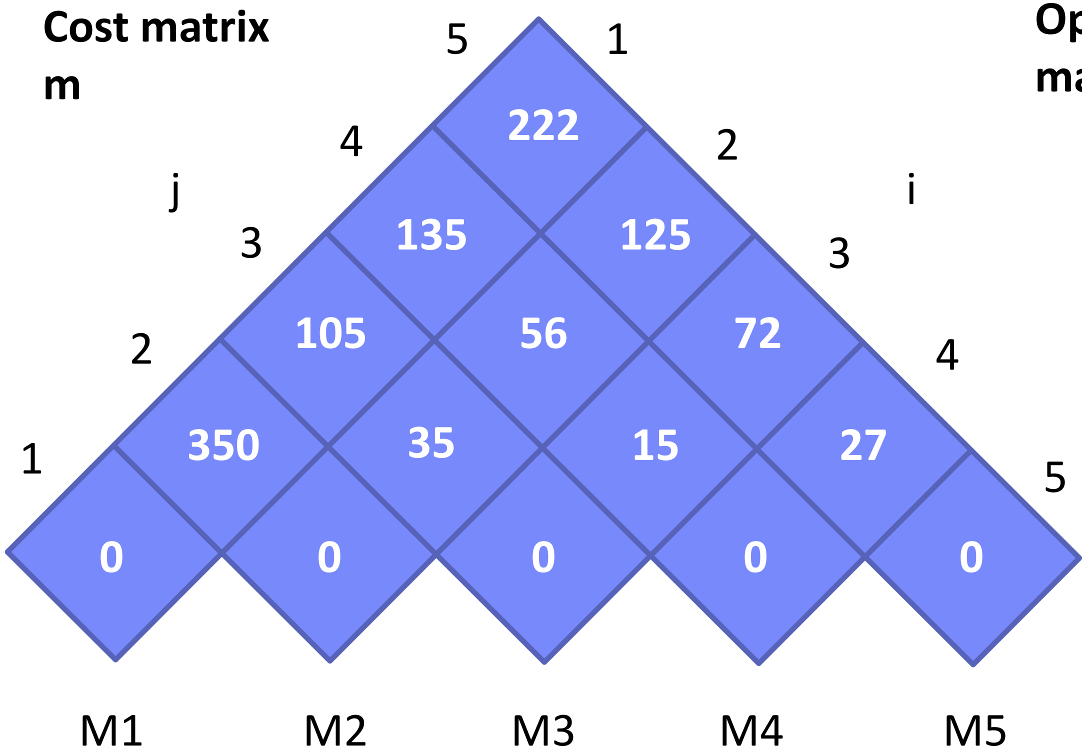
= min(
0 + 35 + 10*7*1,
350 + 0 + 10*5*1)

= min(
105,
400)

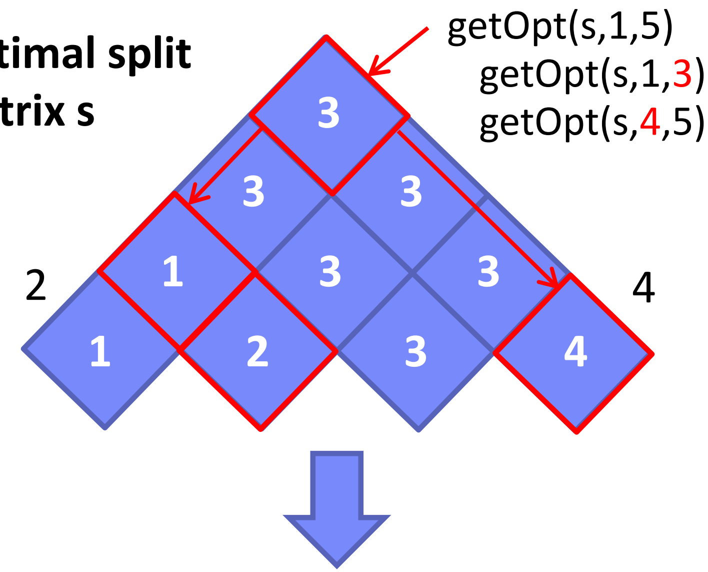
Matrix Multiplication Chain Optimization

M1	M2	M3	M4	M5
10x7	7x5	5x1	1x3	3x9

Cost matrix m



Optimal split matrix s



(M1 M2 M3 M4 M5)

((M1 M2 M3) (M4 M5))

((M1 (M2 M3)) (M4 M5))

→ ((M1 (M2 M3)) (M4 M5))

→ Open questions: DAGs; other operations, joint opt w/ rewrites, CSE, fusion, and physical operators

Physical Rewrites and Optimizations

- **Distributed Caching**
  - Redundant compute vs. memory consumption and I/O
  - **#1 Cache intermediates w/ multiple refs** (Emma)
  - **#2 Cache initial read and read-only loop vars** (SystemML)
- **Partitioning**
  - Many frameworks exploit co-partitioning for efficient joins
  - **#1 Partitioning-exploiting operators** (SystemML, Emma, Samsara)
  - **#2 Inject partitioning to avoid shuffle per iteration** (SystemML)
  - **#3 Plan-specific data partitioning** (SystemML, Dmac [SIGMOD'15], Kasen [PVLDB'16])
- **Other Data Flow Optimizations** (Emma)
  - **#1 Exists unnesting** (e.g., filter w/ broadcast → join)
  - **#2 Fold-group fusion** (e.g., groupByKey → reduceByKey)
- **Physical Operator Selection**

Physical Operator Selection

- **Common Selection Criteria**
  - **Data and cluster characteristics** (e.g., data size/shape, memory, parallelism)
  - **Matrix/operation properties** (e.g., diagonal/symmetric, sparse-safe ops)
  - **Data flow properties** (e.g., co-partitioning, co-location, data locality)
- **#0 Local Operators**
  - SystemML mm, tsmm, mmchain; Samsara/Mllib local linalg
- **#1 Special Operators** (often fused operators)
  - Special patterns (SystemML **tsmm**, tsmm2, mapmmchain, pmm; Samsara AtA
  - Sparsity exploiting (SystemML wdivmm, **wsloss**, wcemm; Cumulon maskMult)
- **#2 Broadcast-Based Operators** (aka broadcast join)
  - SystemML **mapmm, mapmmchain**
- **#3 Co-Partitioning-Based Operators** (aka improved repartition join)
  - SystemML zipmm; Emma, Samsara OpAtB
- **#4 Shuffle-Based Operators** (aka repartition join)
  - SystemML cpmm, rmm; Samsara OpAB

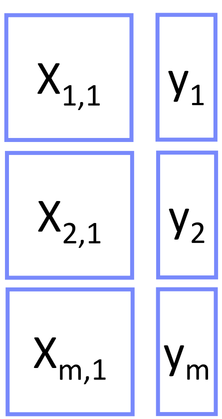
Selection Preference

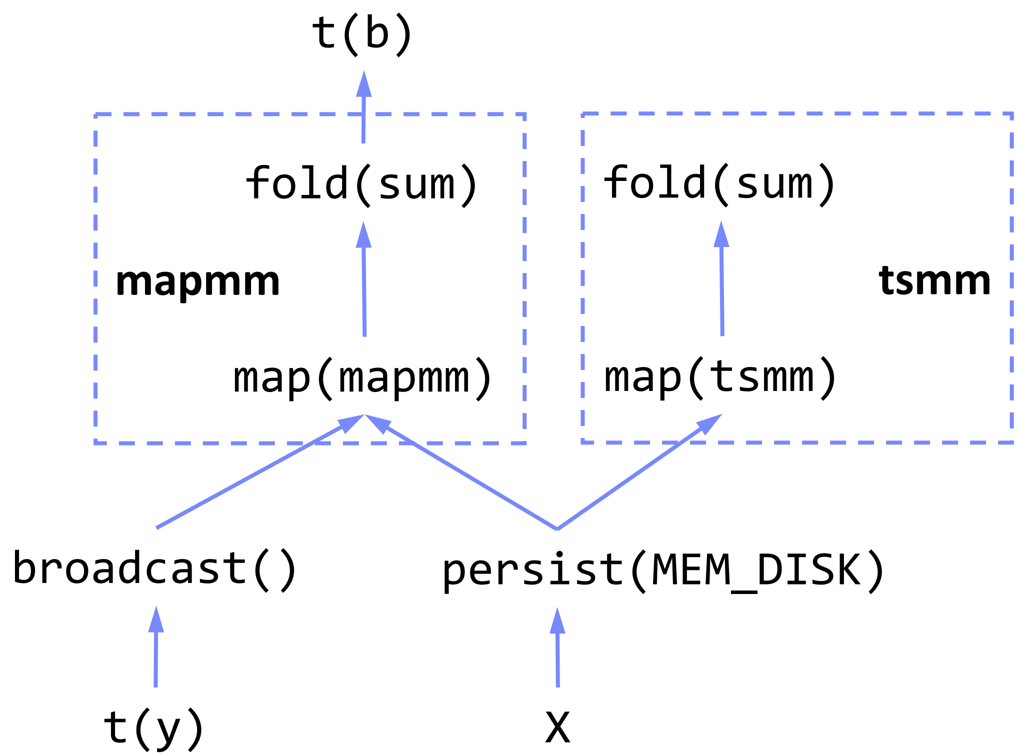
Example Physical Operators

- **Example Linear Regression Direct Solve**
  - Transpose-self for t(X)%*%X
  - Broadcast-based for t(X) %*% y
  - Logical and physical rewrites
  - E.g., Samsara, SystemML

```
A = t(X) %*% X
b = t(X) %*% y
w = solve(A, b)
```

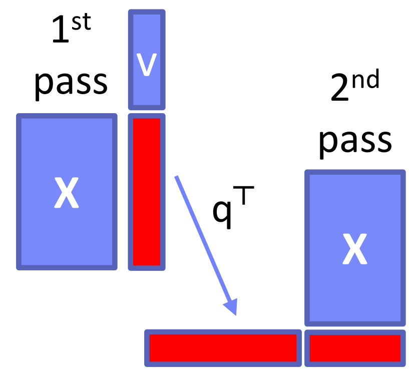
Input Matrices



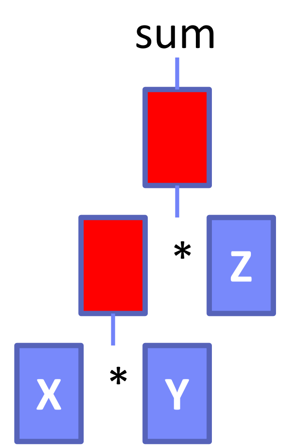


Fused Operators

- **Motivation**
  - Problem: **Memory-bandwidth-bound operations** (I/O)
  - Goal: Reduce number of **scans and intermediates**
- **Matrix-Vector Chains:** `t(X) %*% (X%*%v)`
  - Fused single-pass operator: **mmchain** [PPoPP'15]
  - Row-aligned creation/consumption



- **Ternary Aggregates:** `sum(X*Y*Z)`
  - Fused aggregation operator
  - Avoid materialized intermediates



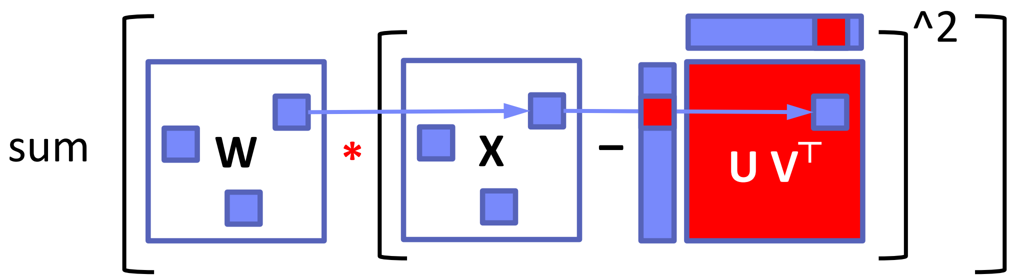
- **Other ML-Specific Operators**
  - Sample proportion: `X * (1-X)`
  - Sigmoid: `1 / (1 + exp(-X))`
  - Axpy: `X + s*Y, X - s*Y`

Sparsity-Exploiting Fused Operators

- **Goal:** Avoid dense intermediates and unnecessary computation

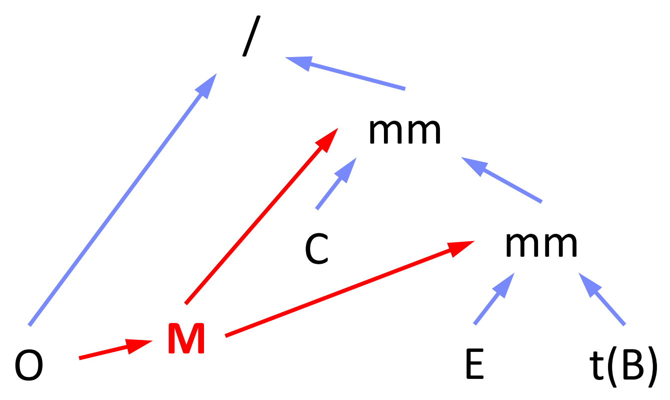
- **#1 Fused Physical Operators**
  - E.g., SystemML [PVLDB'16] wsloss, wcemm, wdivmm
  - Selective computation over non-zeros of **"sparse driver"**

`sum(W * (X – U %*% t(V))^2)`



- **#2 Masked Physical Operators**
  - E.g., Cumulon MaskMult [SIGMOD'13]
  - Create mask of **"sparse driver"**
  - Pass mask to single masked matrix multiply operator

`O / (C %*% E %*% t(B))`



➔ **Open questions: NaN handling, automatic operator fusion (codegen)**

Automatic Operator Fusion

- **Motivation**
  - Large development effort for hand-coded fused operators
  - UDF-centric systems w/o pre-defined operators
- **General Approach: Fuse by Access Pattern**
  - **#1 Loop fusion** (OptiML, Tupleware, Weld, TensorFlow XLA [github'17])
  - **#2 Templates** (Kasen, SPOOF [CIDR'17])
  - Scope: expression or program compilation

```
R = (A + s*B) * C

for( i in 1:n )
   tmp[i] = s*B[i]
for( i in 1:n )
   tmp[i] = A[i]+tmp[i]
for( i in 1:n)
   tmp[i] = tmp[i]*C[i]
```

$\downarrow$

```
for( i in 1:n )
   tmp[i] = (A[i]+s*B[i]) * C[i]
```

- **Additional Techniques**
  - Tupleware: **Micro optimizations** (tile-at-a-time, predicates, result allocation)
  - Weld: **Cross-library optimizations** (via common IR of basic operations)
  - SystemML-SPOOF: **sparsity-exploiting fused operators**

➔ Open question: Optimization of fusion plans for DAGs (redundant compute vs materialization, access patterns)

Runtime Adaptation (see AQP)

- **Problem of Unknown/Changing Size Information**
  - Dimensions/sparsity required for **cost comparisons/valid plans**
  - Unknowns → **conservative fallback plans**
- **Challenges**
  - Conditional control flow, function call graphs, UDFs
  - Data-dependent ops (e.g., sampling, group by classes, output sparsity)
  - Computed size expressions, changing dimensions/sparsity
- **Approaches**
  - **#1 Lazy expression optimization** (RIOT, OptiML, Emma, Weld, Samsara)
    - Optimize on triggering actions (unconditional scope)
  - **#2 Dynamic inter-DAG recompilation** (SystemML)
    - Split/mark DAGs, recompile DAGs/functions w/ exact stats

➔ **Open questions:**

- **Estimating the size and sparsity of intermediates**
- **Adaptive query processing and storage**

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Part 5: Compression, Scan Sharing, and Index Structures

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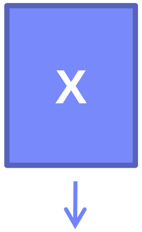
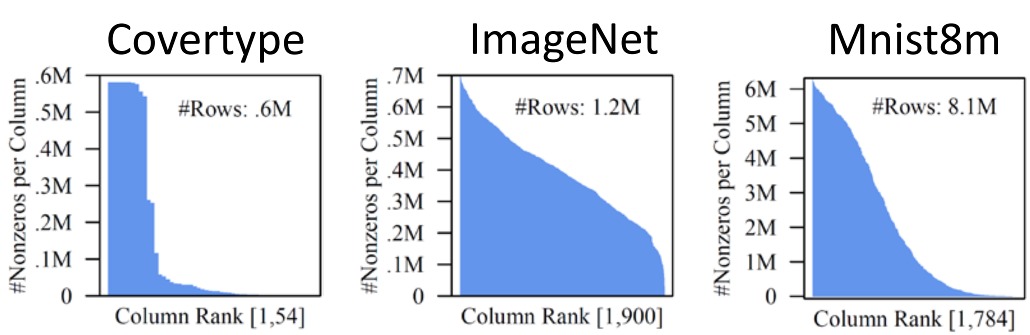
Motivation: Workload Characteristics

- **Memory-Bandwidth-Bound Operations**
  - Iterative ML algorithms w/ read-only data access
  - **#1:** I/O-bound matrix vector products
    ➔ **Crucial to fit matrix into memory**
    (single node, distributed, GPU)
    ➔ **Avoid unnecessary scans**
  - **#2:** Matrix and vector intermediates
    ➔ **Reduce number of reads and writes**



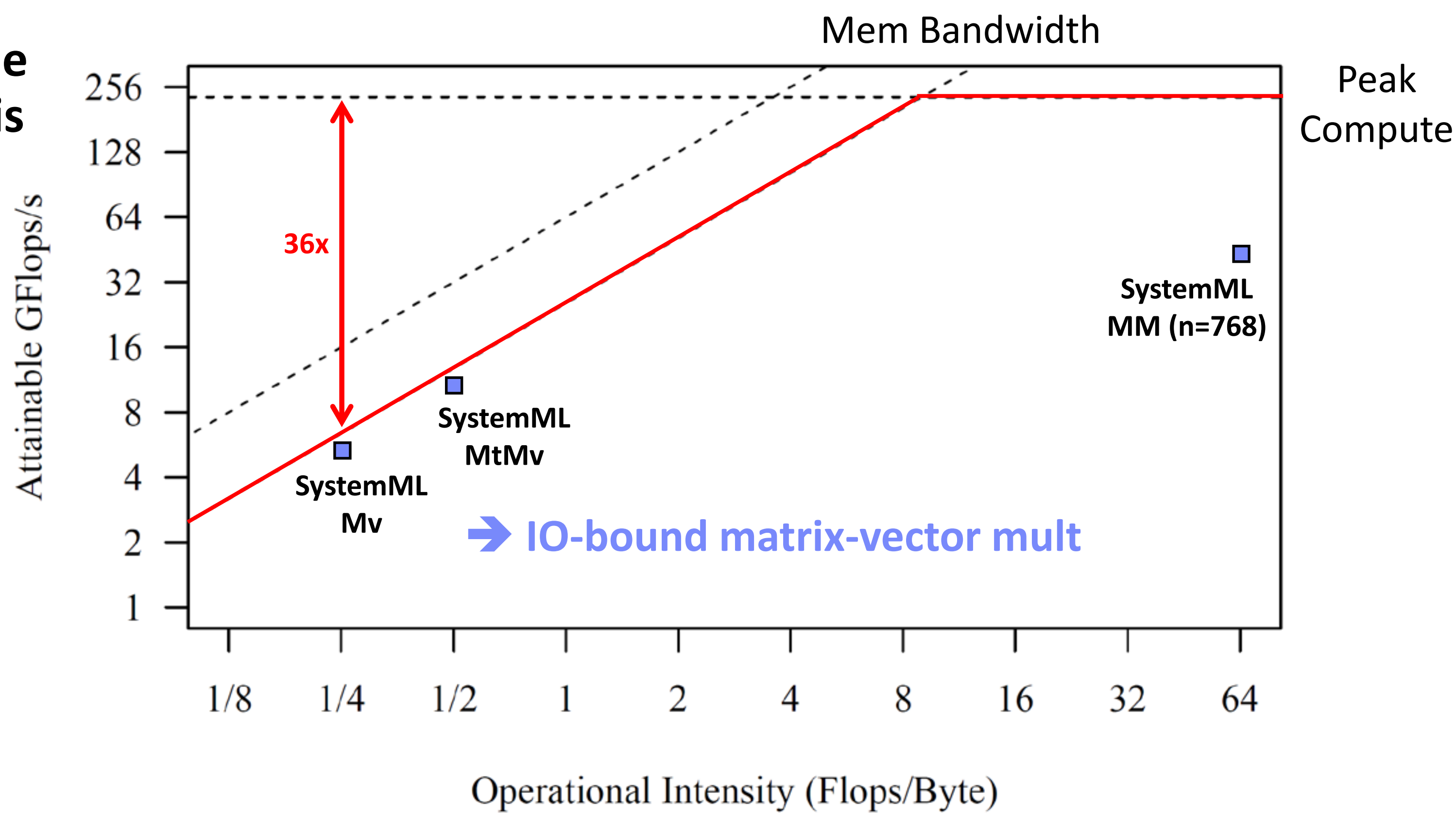

```
while(!converged) {
  … q = X %*% v …
}
```

- **Common Data Characteristics**
  - Tall & skinny matrices (#row >> #columns)
  - Non-uniform sparsity
  - Low column cardinality
  - Column correlations



Motivation: Workload Characteristics

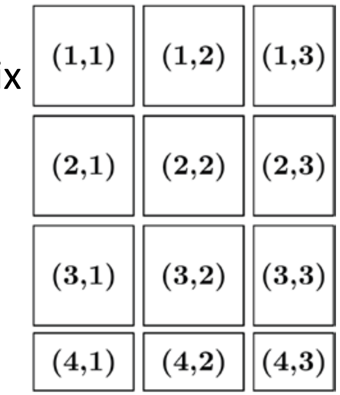
- **Single Node:** 2x6 E5-2440 @2.4GHz–2.9GHz, DDR3 RAM @1.3GHz (ECC)
  - Peak memory bandwidth: **2 x 32GB/s** (local), **2 x 12.8GB/s** (remote QPI)
  - Peak compute bandwidth: **2 x 115.2GFlops/s**
- **Roofline Analysis**



Background: Block Partitioning and Layouts

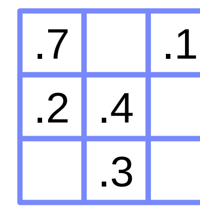
- **Blocked Matrix Representations**
  - Blocks, a.k.a. “tiles”, “chunks”, or “pages”
  - **#1 Logical (fixed-size) blocking** (→ var. physical size)
  - **#2 Physical blocking** (→ fixed physical size)
  - Blocks encoded independently (dense/sparse)
  - Local matrices → single block

Logical blocking
3,400x2,700 matrix
(w/ B_c=1,000)

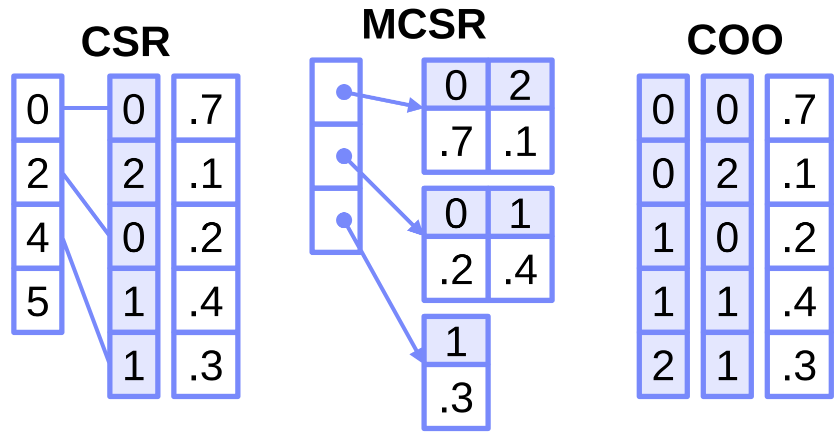


- **Common Block Representations**
  - **Dense** (linearized arrays)
  - **CSR** (compressed sparse rows)
  - **CSC** (compressed sparse columns)
  - MCSR (modified CSR)
  - **COO** (Coordinate matrix)
  - …

Example
3x3 Matrix

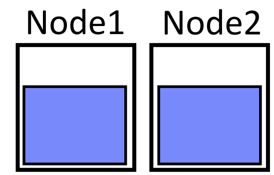


Dense (row-major)



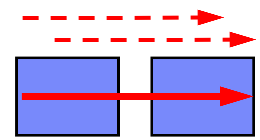
Overview Techniques for Data-Intensive Machine Learning

- **#1 (Distributed) Caching**
  - Keep read only feature matrix in (distributed) memory

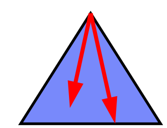


- **#2 Compression**
  - Fit larger datasets into available memory

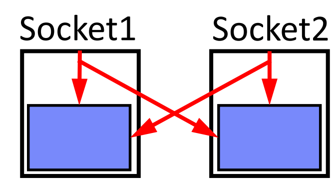
- **#3 Scan Sharing (and operator fusion)**
  - Reduce the number of scans as well as read/writes



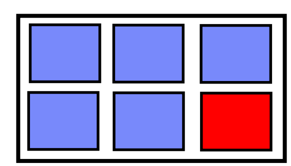
- **#4 Index Structures**
  - Out-of-core data, I/O-aware ops, updates



- **#5 NUMA-Aware Partitioning and Replication**
  - Matrix partitioning / replication → data locality

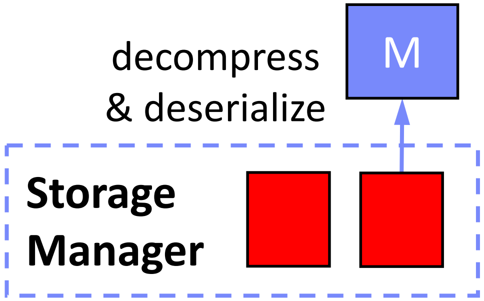


- **#6 Buffer Pool Management**
  - Graceful eviction of intermediates, out-of-core ops

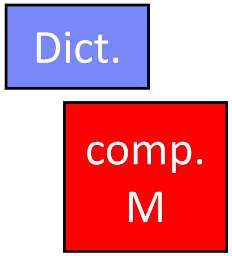


Compression Techniques

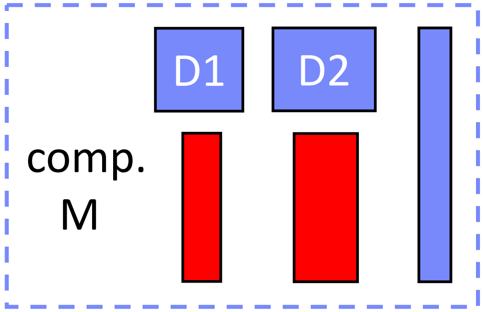
- **#1 Block-Level General-Purpose Compression**
  - Heavyweight or lightweight compression schemes
  - Decompress matrices block-wise for each operation
  - E.g.: Spark RDD compression (Snappy/LZ4), **SciDB** SM [SSDBM'11], **TileDB** SM [PVLDB'16]



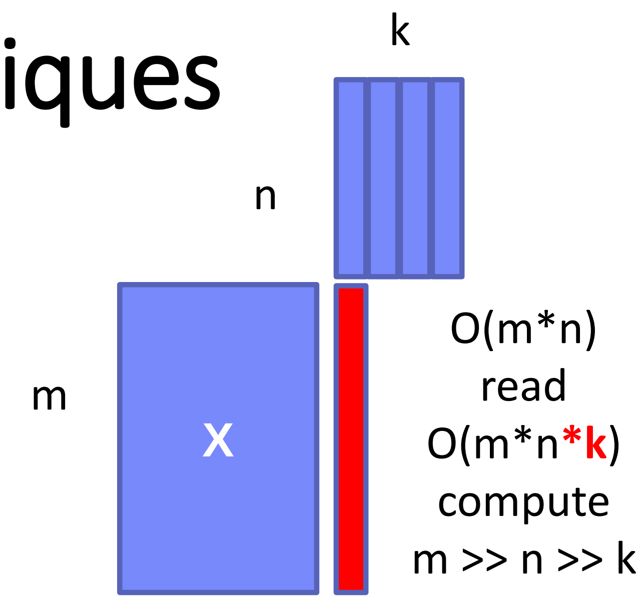
- **#2 Block-Level Matrix Compression**
  - Compress matrix block with common encoding scheme
  - Perform LA ops over compressed representation
  - E.g.: **CSR-VI** (dict) [CF'08], **cPLS** (grammar) [KDD'16], **TOC** (LZW w/ trie) [CoRR'17]



- **#3 Column-Group-Level Matrix Compression**
  - Compress column groups w/ heterogenous schemes
  - Perform LA ops over compressed representation
  - E.g.: **SystemML CLA** (RLE, OLE, DDC, UC) [PVLDB'16]



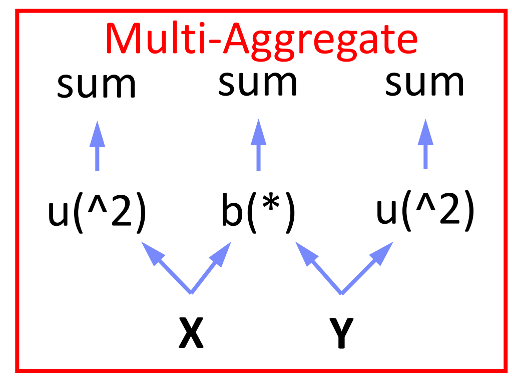
Scan Sharing Techniques



- **#1 Batching**
  - One-pass evaluation of multiple configurations
  - Use cases: EL, CV, feature selection, hyper parameter tuning
  - E.g.: **TUPAQ** [SoCC'16], **Columbus** [SIGMOD'14]

- **#2 Fused Operator DAGs**
  - Avoid unnecessary scans, (e.g., part 4 mmchain)
  - Avoid unnecessary writes / reads
  - Multi-aggregates, redundancy
  - E.g.: **SystemML codegen**

```
a = sum(X^2)
b = sum(X*Y)
c = sum(Y^2)
```



- **#3 Runtime Piggybacking**
  - Merge concurrent data-parallel jobs
  - "Wait-Merge-Submit-Return"-loop
  - E.g.: **SystemML parfor** [PVLDB'14]

```
parfor( i in 1:numModels )
  while( !converged )
    q = X %*% v; ...
```

Index Structures and NUMA Awareness

- **Goals:** Out-of-core operations and data placement

- **Index Structures**
  - Tree structures of blocks w/ user-defined/fixed linearization functions
  - **LAB-Tree** (Linearized Array B-tree, RIOT) [PVLDB'11]
    - Leaf-splitting strategies, and update batching via flushing policies
  - **TileDB Storage Manager** [PVLDB'16]
    - Two-level blocking and update batching via fragments
  - **AT MATRIX** (Adaptive Tile Matrix, SAP HANA) [ICDE'16]
    - Two-level blocking and NUMA-aware range partitioning

- **NUMA-Aware Model/Data Replication**
  - **DimmWitted:** HW vs statistical efficiency [PVLDB'14]
  - Model: PerCore, PerNode, PerMachine
  - Data: partitioning (sharding), full replication

➔ Open questions: Heterogenous hardware, cache coherence, etc

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Backup: Compressed Linear Algebra (CLA)

[PVLDB 2016]

- **Overview compression framework**
  - Column-wise matrix compression (values + offset lists / references)
  - Column co-coding (column groups encoded as single unit)
  - Heterogeneous column encoding formats (OLE, RLE, DDC, UC)

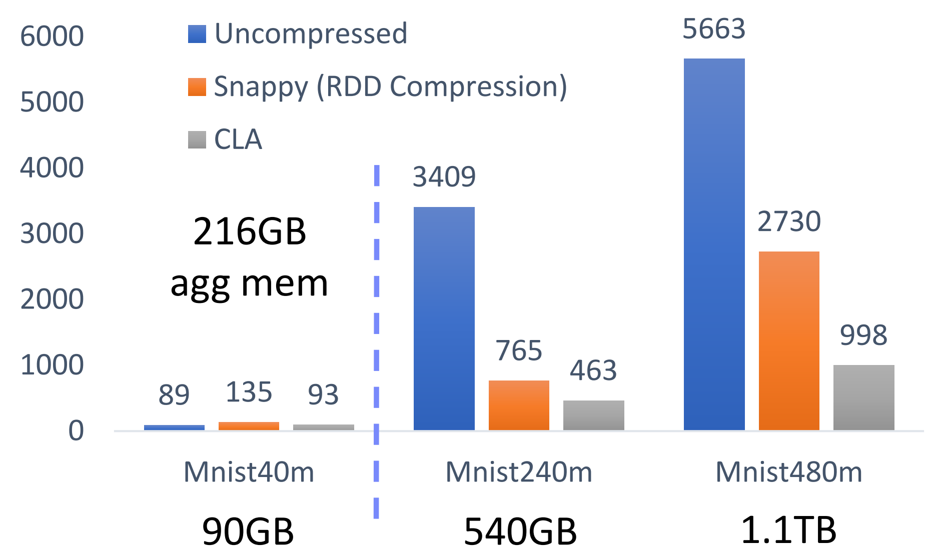
Automatic Planning

- **Experiments**
  - **LinregCG**, 10 iterations, SystemML 0.14
  - 1+6 node cluster, Spark 2.1

Compression Ratios

Dataset	Gzip	Snappy	CLA
Higgs	1.93	1.38	**2.17**
Census	17.11	6.04	**35.69**
Covtype	10.40	6.13	**18.19**
ImageNet	5.54	3.35	**7.34**
Mnist8m	4.12	2.60	**7.32**
Airline78	7.07	4.28	**7.44**

End-to-End Performance [sec]



Backup: Index Structures

- **Overview Common Indexing Techniques**
  - Physical blocking w/ leaf splitting strategies
  - Dense and sparse leaf blocks w/ contiguous ranges of cells
  - Batching of updates (deferred insertion)

- **LAB-Tree (Linearized Array B-tree, RIOT)** [PVLDB 2011]
  - Operations: get, scan (iterator w/ given order), left/right indexing (on disk)
  - B-tree w/ physical blocking (sparse/dense), leaves have assigned ranges
  - Array linearization via UDFs (e.g., row/column major, Z-order, etc)
  - **Leaf splitting strategies:** split-in-middle, split-aligned, split-off-dense, split-defer-next, split-balanced-ratio
  - **Flushing policies for update batching:** flush-all, least-recently-used, smallest-page, largest-page, largest-page-probabilistically, largest-group

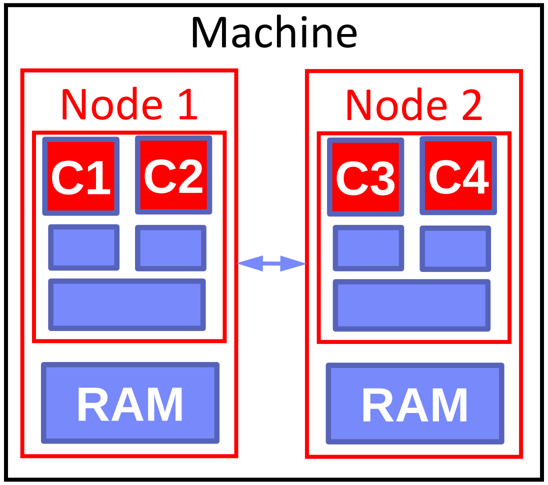
Backup: Index Structures, cont.

- **AT MATRIX (Adaptive Tile Matrix, SAP HANA)** [ICDE 2016]
  - Operations: matrix multiplication ATMult (in-memory)
  - Two-level blocking: **Adaptive variable-sized tiles** (dense or sparse w/ CSR), composed of atomic squared blocks
  - Two-dimensional quad-tree, w/ Z-order as linearization function
  - **Horizontal partitioning across NUMA nodes**

- **TileDB Storage Manager** [PVLDB 2016]
  - Operations: init, write, read, consolidate, finalize (on disk)
  - Two-level blocking: space tiles (fixed size), data tiles (variable size for sparse)
  - Two-level linearization: cell order and tile order (row/column major)
  - **Fragments for update batching**
    (“a timestamped snapshot of a batch of array updates”)

Backup: NUMA-Aware Partitioning and Replication

- **AT MATRIX (Adaptive Tile Matrix)**
  - Recursive NUMA-aware partitioning into dense/sparse tiles
  - Inter-tile (worker teams) and intra-tile (threads in team) parallelization
  - Job scheduling framework from SAP HANA (horizontal range partitioning, socket-local queues with task-stealing)



- **NUMA-Aware Model and Data Replication**
  - **DimmWitted: HW vs statistical efficiency**
  - Model Replication
    - PerCore, PerMachine
    - PerNode (hybrid)
  - Data Replication
    - Partitioning (sharding)
    - Full replication

→ Open questions: Heterogenous hardware, cache coherence, etc.

Backup: Buffer Pool Management

- **#1 Intermediates of LA Programs**
  - Hybrid runtime plans of in-memory and distributed operations
  - **Graceful eviction of intermediates at granularity of variables**
  - Example: SystemML
    - Soft references for in-memory matrices and broadcasts
    - LRU, FIFO buffer replacement strategies
- **#2 Operation/Algorithm-Specific Buffer Management**
  - Operations/algorithms over out-of-core matrices and factor graphs
  - **Page-level storage layout and buffer replacement policies**
  - Example #2a: RIOT
    - Chains of matrix multiplications
    - Operation-aware I/O schedules
  - Example #2b: Elementary
    - LR, CRF, LDA over out-of-core factor graphs
    - Materialization strategies and MRU/LFU buffer replacement

Part 6: Resource Elasticity

"Intelligence is the ability to adapt to change."

Stephen Hawking (?)

Jun Yang

Duke University
Durham, NC, USA

SIGMOD 2017

http://picshype.com/rubber-band-ball/amazon.com-:-acco-rubber-band/37225

Rise of Cloud

- **Cluster computing for big data is easier than ever**
  - Clouds allow you to get a cluster on demand, and pay as you go
  - There is a growing ecosystem of platforms and tools for data analysis

Challenges

- **Maddening array of “knobs”**
  - Hardware provisioning, software configuration, program tuning
- **“Elastic” environment**
  - Multi-tenant clusters, fluctuating markets, failures
  - Particularly hard for large-scale, long-running ML workloads

Roadmap

- **Provisioning (& scheduling): what do I need (& when)?**
- **Recovery: what do I do when what I need fails?**
- **Working with markets**

☞**These problems are not limited to DB & ML workloads, but we shall see how DB & ML add twists**

Provisioning: Example Decisions

- **Given an ML program, what types of machines to acquire, and how many** *Cumulon* [SIGMOD'13+follow-up]
  - A bigger cluster may get results faster, but cost more
  - No perfect speedup, so big clusters may not give good cost/time trade-off
- **Given a cluster, how to configure the execution of an ML program**
  - What's the appropriate degree of parallelism for an execution step? *SystemML* [DEBull'14,PVLDB'16] *ScalOps* [DeBull'12]
    - Overhead of parallelism isn't always justified
  - How much memory do we allocate to master and work processes? *SystemML* [SIGMOD'15]
    - Optimal allocation depends on computation and data access patterns

☞**Decisions interact with optimizations discussed earlier**

- Cluster configuration affects degree of parallelism and memory allocation, as well as optimal execution strategies

Provisioning/Scheduling: Techniques

Depend on the level of abstraction:

- **Program is a black box**
  - First observe, and then decide; can leverage past execution profiles
- **Program is broken down into a workflow with clear input/output for each unit, e.g., *MapReduce*, *Spark***
  - More effective profiling and optimization on a per-unit basis
- **Program is specified declaratively, DB-style**
  - Reusable and composable cost models
  - Bigger search space through rewrites
  - Cost-based what-if analysis

SystemML [ICDE'11+follow-up]
Cumulon [SIGMOD'13+follow-up]

- **Program follows a specific template**
  - Even more opportunities arise; e.g., scheduling parameter updates/synchronization in ***parameter servers*** [VLDB'10,OSDI'14] + resource provisioning in ***Dolphin*** [MLSys'16] + adapting learning rate by update staleness in ***DynSGD*** [SIGMOD'17]

☞**Adaptation is always key, regardless of abstraction level**

Recovery: General Techniques

Depend on the level of abstraction:

- **Program is a black box**
  - Checkpointing VM state in reliable/redundant storage
- **Program is a workflow with clear input/output for each unit**
  - Write input/output to reliable storage + rerun failed units, e.g., ***Hadoop/MapReduce***
  - Intermediate results can be in memory and lost + recover using lineage ***Spark RDD* [NSDI'12]**
- **Program is specified declaratively, DB-style**
  - Finer-grained lineage-based recovery using knowledge of operators + intelligent selective checkpointing ***Cümülön* [PVLDB'15]**

Recovery: Algorithm-Specific

- **Many ML algorithms can tolerate missing input or errors by design**
  - Instead of recovering to a state where as if failures never occurred, convert failures into “soft” ones that algorithms can handle themselves
- **Example: distributed batch gradient descent**

Narayanamurthy+ (*REEF*) [BigLearn'13]

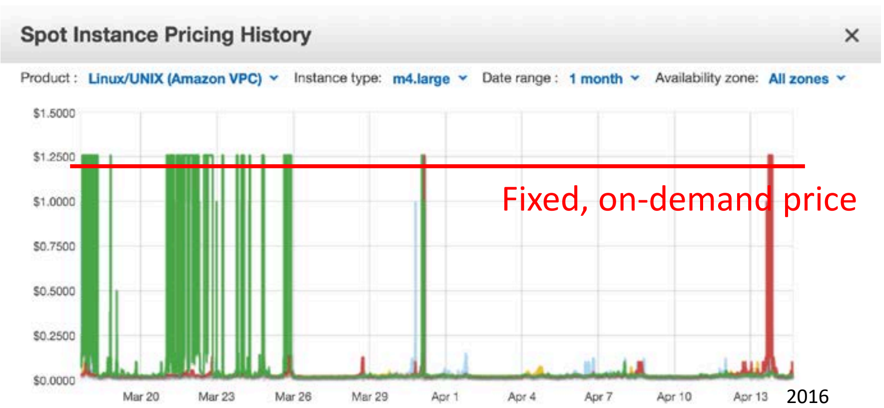
  - In an iteration, if a task fails to calculate the contribution from one partition of data, simply use an approximation (from the previous iteration)
  - Algorithm still converges

☞**Generalized to user-defined, algorithm-specific “compensations”**

Schelter+ [CIKM'13]

Working with Markets

- **“On-demand” (regular) instances: fixed price, guaranteed**
- **“Spot” instances: availability/price vary over time; e.g; on Amazon:**
  - You set a bid price, and get instances if bid price ≥ market price
  - You pay market price (@hour start), by hours
  - You lose the instances if market price rises above your bid, but your last hour will be free
- **Price can depend on machine type, region, and time**



☞**How do we leverage markets effectively?**

- Pop quiz: would you ever bid higher than the fixed price?
  - Yes! Less chance of losing them, yet still lower cost on average

Working with Markets: Techniques

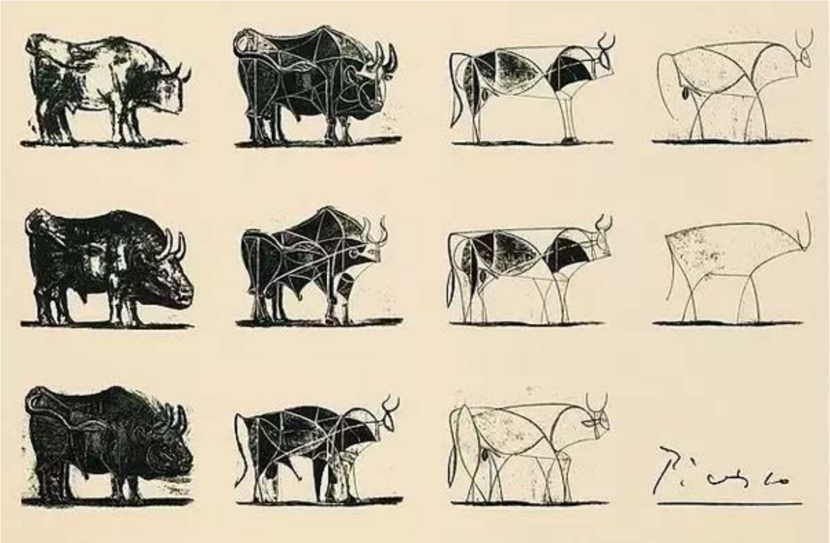
- **Diversify your portfolio: consider instances with different types, across regions**
  - If one market is too expensive, turn to others, e.g., ***Dyna* [TCC'16]**
  - A heterogeneous cluster may be best for mixed workloads, e.g., **Zhang+ [PER'15]**
- **Minimizing expected cost is often not enough; need to control risk**
  - Model the market to quantify uncertainty, e.g., ***Cümülön(-D)* [PVLDB'15,'17]**
- **Zafer+ [Cloud'12] squeezes entire execution on spots in an hour; retries with a higher bid price if you lose them**
  - Losing spots within an hour incurs no cost with Amazon
- ***Dyna* [TCC'16] tries faster spots before falling back to on-demand**
  - But only if doing so improves the execution time distribution
- ***Cümülön* [PVLDB'15] picks the optimal mix of spot/on-demand instances**
  - To minimize expected cost while meeting deadline/budget with high probability
  - Recovers and re-optimizes if spots are lost
- ***Cümülön-D* [PVLDB'17] adapts proactively dynamically and proactively**
  - Bids/terminates as needed, based on execution progress and market condition
  - Solves the optimization problem as a Markov Decision Process (MDP) and pre-compiles a "cookbook" to apply at run time

Summary

- **Large-scale ML is increasingly being done in a cloud**
- **Challenges of elasticity are not unique to DB & ML**

- **Lots of uncertainty, but adaption & stochastic modeling come to rescue**

- **Different levels of abstraction lead to different opportunities—declarative (DB-style) ML enables smarter, more effective solutions**



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Part 7: ML Lifecycle Systems

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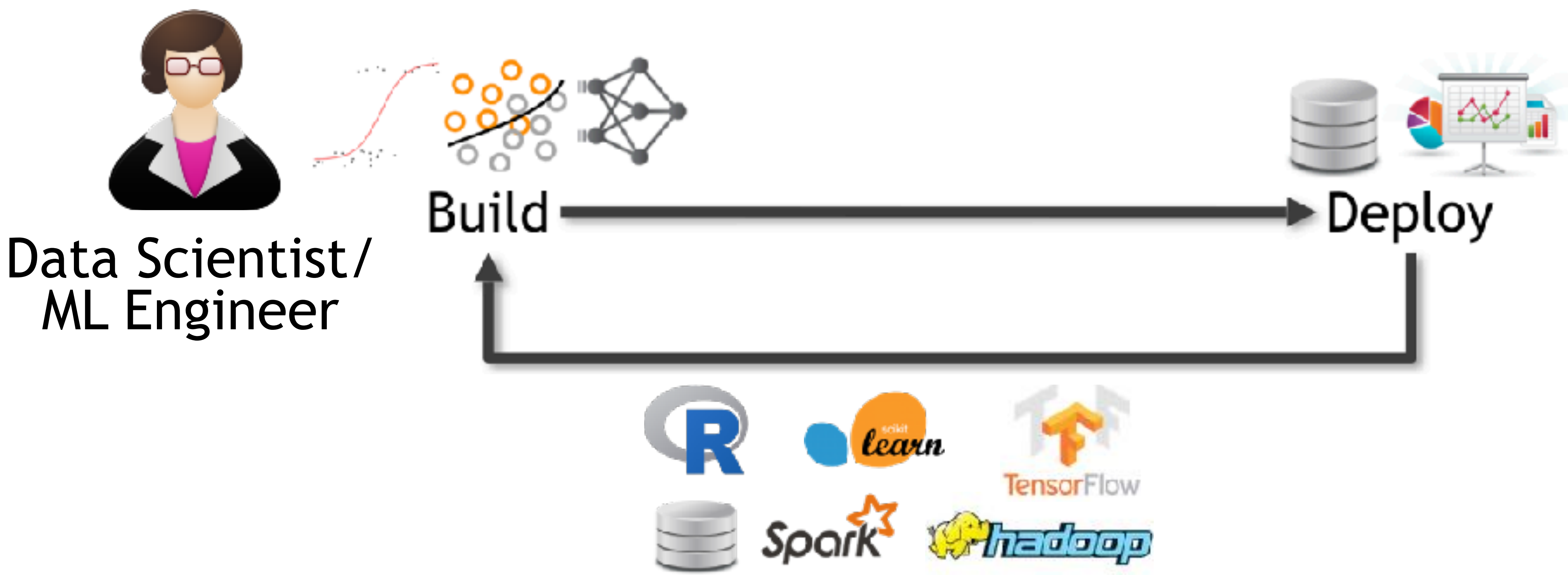
SIGMOD 2017

Overview: ML Lifecycle Issues



Data sourcing
Feature engineering
and model selection

Model serving
Tighter loop between
inference and learning

Model management

Feature Engineering

Q: *What is feature engineering (FE)?*

The process of obtaining a formal representation of the data-generating process as structured signals (features) for an ML model

Q: *Why is it important from a data management perspective?*

High-quality features are the "secret sauce" of applied ML

FE operations are basically data transformations!

Often "brushed under the carpet" by ML community

Q: *What sort of operations constitute feature engineering?*

Depends on the data type!

Structured data: Whitening, feature selection/ranking, joins, PCA, etc.

Text: Bag-of-words, Parsing-based, Domain-specific, Word2Vec, etc.

Deep CNNs and RNNs for images, audio, video, time series, etc.

Feature Engineering Systems

Feature selection:

Obtain a subset of features to improve accuracy and/or interpretability

Columbus [SIGMOD'14]:

Often not a single algorithm but a human-in-the-loop dialogue process

Data scientist explores multiple subsets based on domain insights

Understanding customer churn

CustID	Churn?	Age	Income	Gender	City	...
...	...	...	...	...	...	...

Evaluate error with all features in chosen set

Drop demographic features and re-evaluate

Add Gender back in and so on …

A few such common steps encoded as "declarative" ops in DSL

Impl. on top of R/Python; optimizing code-gen middleware

Batching/materialization; QR decomposition; coresets; warm start

Feature Engineering Systems

Treating FE as a dataflow-oriented process; DB-style optimizations:

Brainwash [CIDR'13] / **DeepDive** [DataEng'14]

Workflows of UDFs; feature recommendations

KeystoneML [ICDE'17]

Alternative phy. impl. of solvers; cost-based op. selection

Reducing amount of work for feature coding/evaluation:

Zombie [ICDE'16]

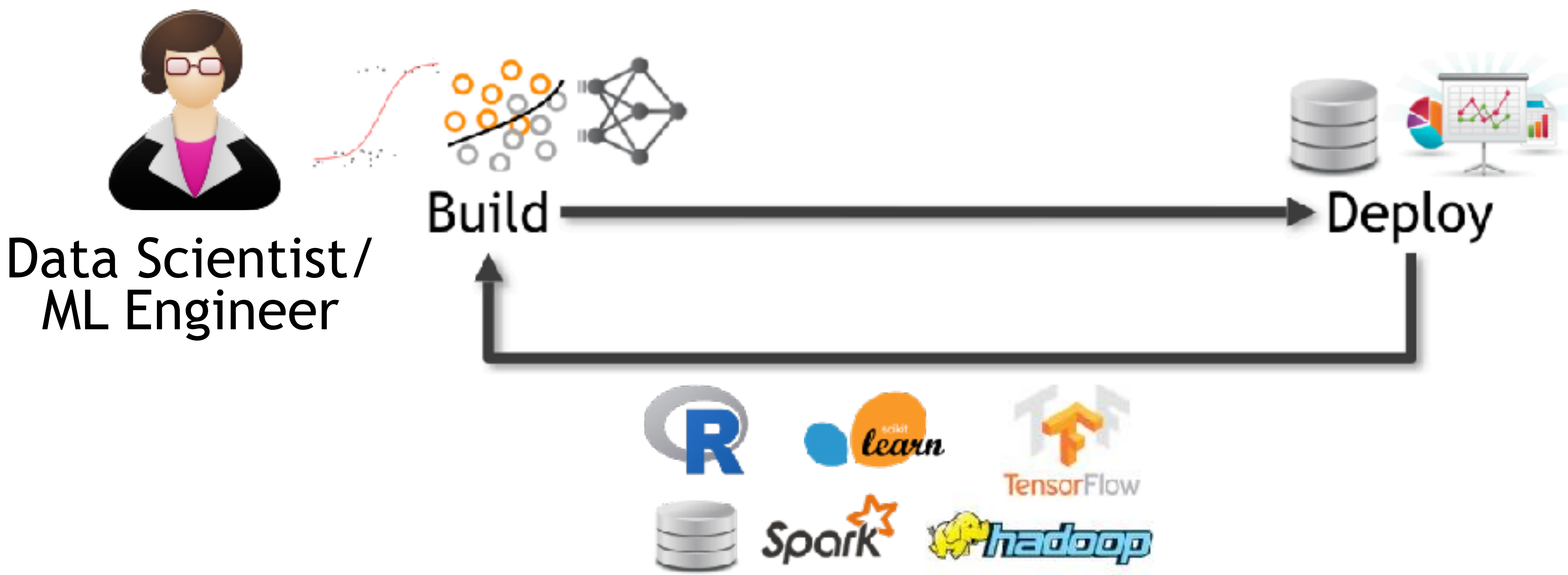
Index structure to sub select relevant data; bandit techniques

Applying learning theory to skip features and help with sourcing tables:

Hamlet [SIGMOD'16]

More open questions remain in *systematizing* feature engineering

Overview: ML Lifecycle Issues



Data sourcing
Feature engineering
and $\boxed{\text{model selection}}$

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Model Selection

Q: *What is model selection (MS)?*

The process of obtaining a prediction function to capture a data-generating process using data generated by that process

MSMS [SIGMODRec'15]

Model Selection Triple (MST)

(FE, AS, PT)

FE: Feature Engineering

AS: Algorithm Selection

PT: (Hyper-)Parameter Tuning

Q: *Why is it important from a data management perspective?*

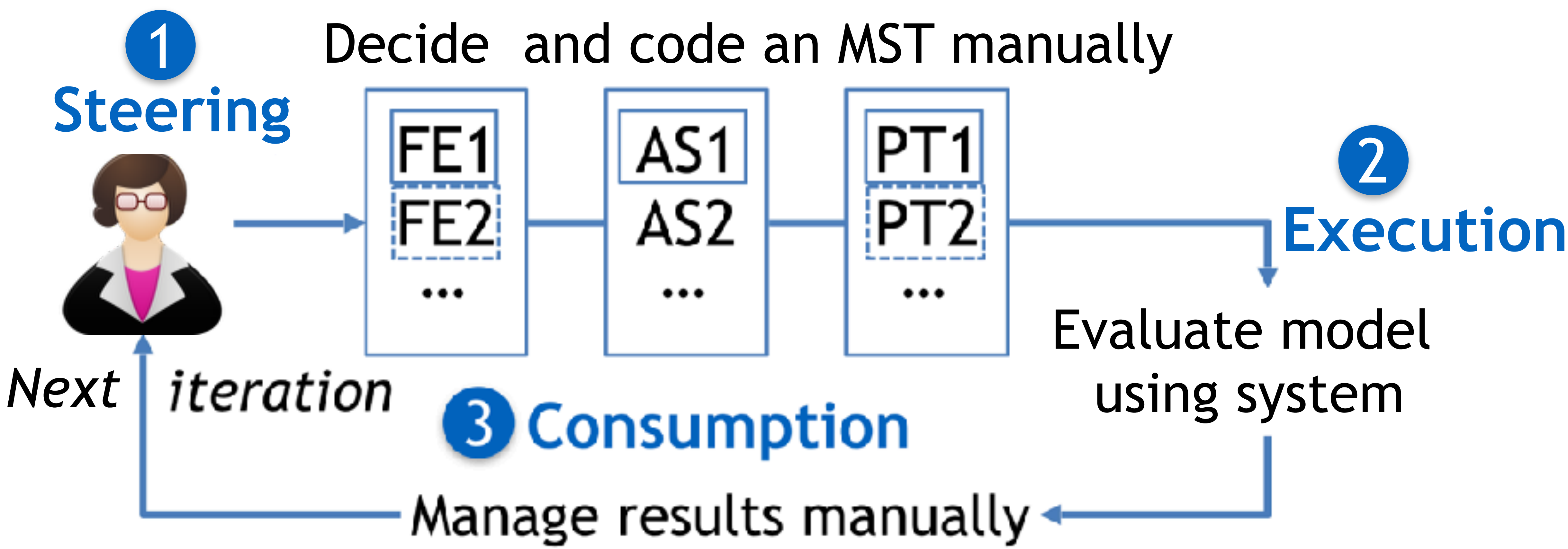
FE, AS, and PT often access the dataset (or subsets) repeatedly

A lot of opportunities to improve efficiency with DB-style opt.

FE, AS, and PT are *inter-dependent* and together constitute MS

Model Selection Process

MSMS [SIGMODRec'15] Model Selection Triple (MST): (FE, AS, PT)



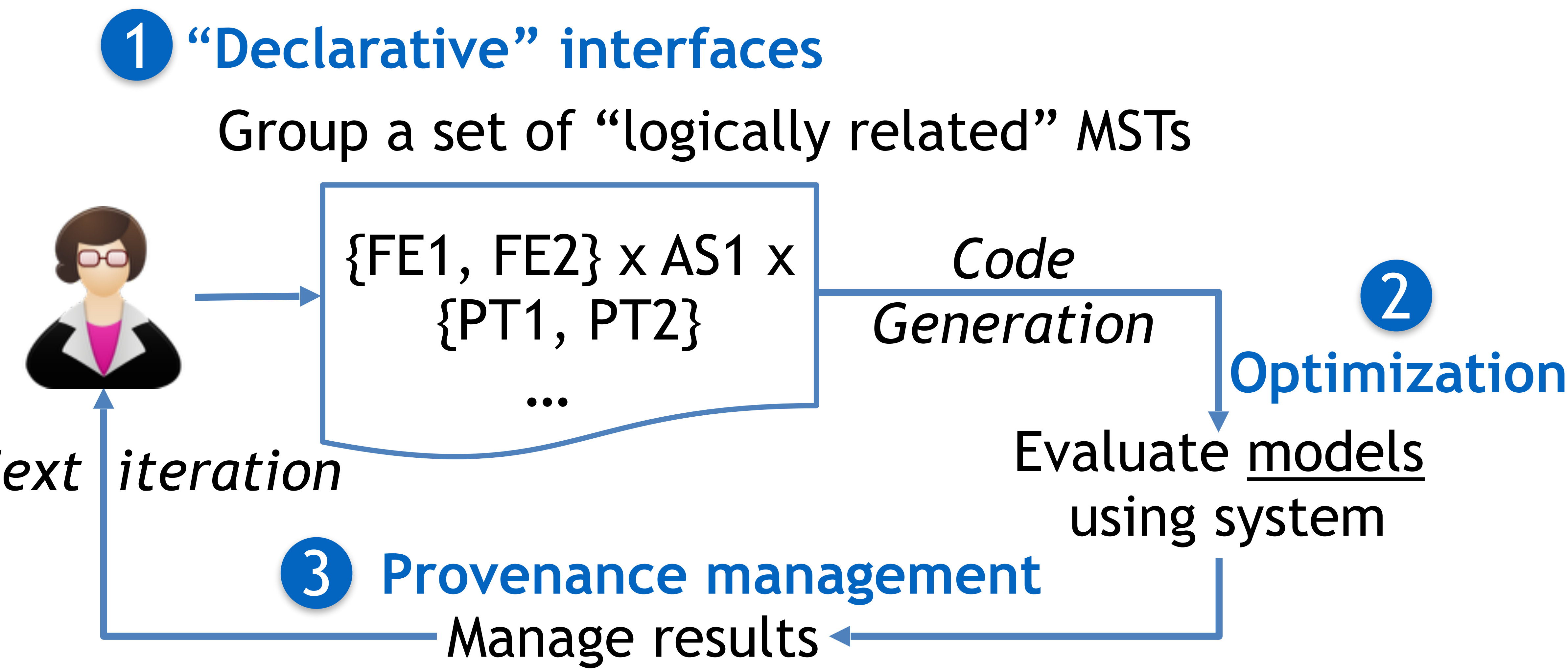
Data scientists typically think at a higher level of abstraction

Automation essentially groups MSTs en masse

MS abstractions can help capture intermediate points

Model Selection Process

MSMS [SIGMODRec'15] Model Selection Triple (MST): (FE, AS, PT)



Many old and recent MS abstractions can be "retro-fitted"

Several new MS abstractions can be introduced to co-exist

Model Selection Management Systems (MSMS)

MSMS [SIGMODRec'15]

<u>The Higher Layers</u>: Declarative Interfaces (some in hindsight!)

Autotuned functions	Columbus	MLBase	*New Abstractions*
E.g., glmnet() in R	E.g., StepAdd()	E.g., doClassify()	…
FE x AS x {PT}	{FE} x AS x PT	FE x {AS1 x {PT}, AS2 x {PT}}	{FE} x {AS x PT}, …

{ {FE} x {AS} x {PT} }

<u>The Narrow Waist:</u>
A set of logically related Model Selection Triples (MST)

In-memory

In-RDBMS

Spark

Others

<u>The Lower Layers</u>: Optimized Implementations

Model Selection Systems

Automation of AS and PT search with pre-defined search space:

- **MLbase** [CIDR'13] / **TuPAQ** [SoCC'15]
  - Declarative ML tasks (e.g., "DoClassify"); fixed set of algorithms
  - Data batching; bandit techniques for explore-exploit search
- **Hemingway** [MLSys'16]
  - Joint AS and cluster sizing for optimization algorithms
  - Observe-and-adapt approach for convergence properties

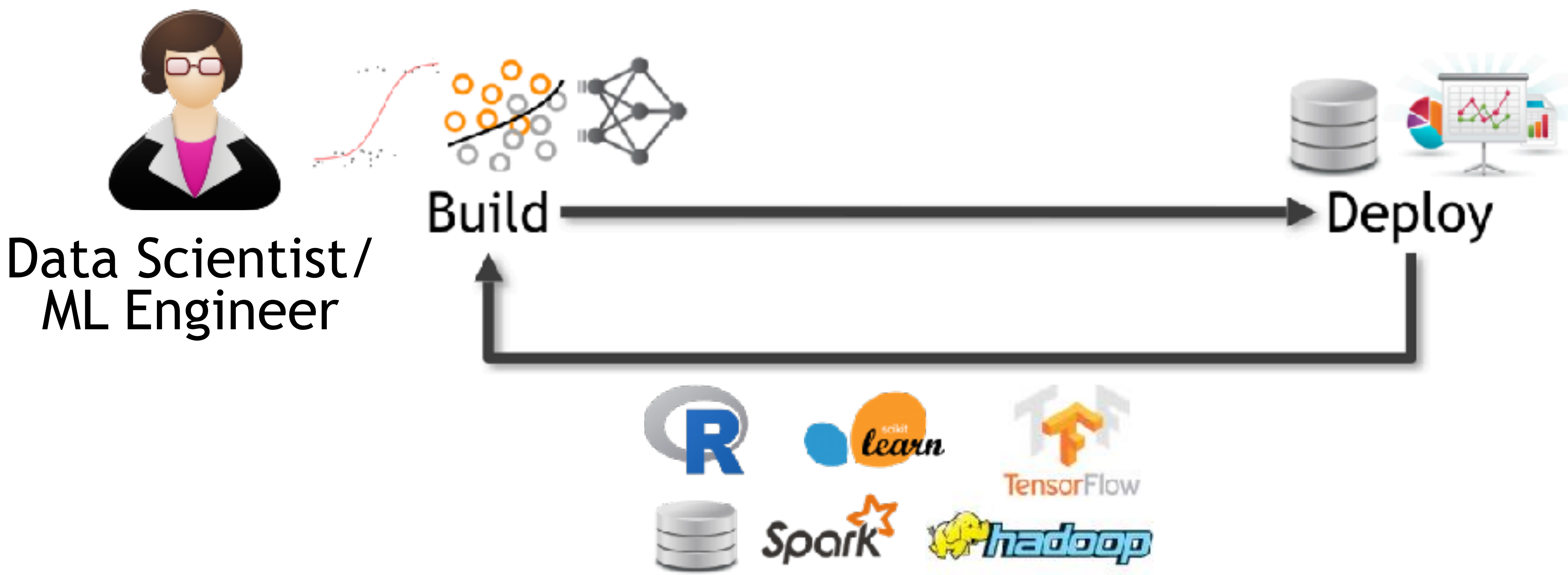
DB-style optimizations for PT and general meta-learning:

- **SystemML** [ICDE'15]; **GLADE** [DanaC'12]

Many open questions remain on optimizing/improving model selection

- Interactions of PT with AS and FE
- Exploiting redundancy across and within MSTs; cost models
- Incorporating constraint/approximations and visualizations, etc.

Overview: ML Lifecycle Issues



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Model Management Systems

***Q**: What is model management?*

Treating trained models as data themselves (store, query, debug, etc.)

Integrating ML models with SQL querying: **LongView** [CIDR'11]

Iterative ML debugging: **MindTagger** [VLDB'15], **PALM** [HILDA'17]

Specialized storage engines and custom optimizations:
- **ModelHub** [ICDE'17]
  - Versioned storage/retrieval of CNNs (sets of float matrices)
  - Optimizations for reducing storage footprint

Many open questions on managing large space of MSTs, especially for large models (DNNs/trees); ML provenance and debugging

Other ML Lifecycle Issues

Model Serving: High-throughput/low-latency inference/re-learning
- **MacroBase** [SIGMOD'17]
- **Clipper** [NSDI'17] / **Velox** [CIDR'15]
- Integrating data-driven applications with reinforcement learning

Data Sourcing: Modeling labeling process; ML+cleaning; ML+pricing
- **Snorkel** [NIPS'16]
- **ActiveClean** [VLDB'16]
- **Model-Based Pricing** [DEEM'17]

Interactive Model Building: Human-in-the-loop interfaces
- **Ava** [CIDR'17]
- **Vizdom** [VLDB'15]

References: Part 7

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Part 8: Open Problems and Conclusions

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Open Problems: Optimizer and Runtime

- **#1 Size and Sparsity Estimation**
  - Fundamental building block for cost comparisons / valid plan generation
  - Issues: function calls, UDFs, data-dependent operators, changing sizes
- **#2 Convergence Estimation**
  - Number of iterations until convergence unknown
  - Required for cost comparisons and progress estimation
- **#3 Adaptive Query Processing and Storage**
  - Unknown or changing workloads → adaptive query processing
  - Currently limited to inter-DAG recompilation and expression optimization
- **#4 Automatic Rewrites and Operator Fusion**
  - Huge potential for simplification rewrites and operator fusion
  - Challenging in presence of new access methods, compression, etc.
- **#5 Special Value Handling**
  - Special values such as NaN, INF, -0 ignored by most systems → **incorrect results**
  - Support these special values w/o sacrificing performance

Open Problems: End-to-End Lifecycle

- **#6 Integrating Relational and Linear Algebra**
  - Seamless optimizer / runtime integration in holistic framework
  - Including data transformations, training and prediction
- **#7 Seamless Feature Engineering and Model Selection**
  - (Semi-)automating feature engineering and model selection
  - Including abstractions, meta-algorithms, and system architectures
- **#8 ML System Benchmarks**
  - Existing benchmarks limited to ML tasks in terms of reference implementations of large-scale ML libraries or SQL-centric workloads
  - Broader range of benchmarks at various abstraction levels

Conclusions

- **Summary**
  - Compelling arguments for integrating **ML → DB** and **DB → ML**
  - ML in data systems, DB-inspired ML systems, ML lifecycle systems

- **#1 Existing Work to Build Upon**
  - Awareness of existing systems and techniques
  - Survey of effective optimization and runtime techniques

- **#2 Where the Data Management Community Can Help**
  - Integrating ML into existing data systems
  - Optimizer and runtime techniques for large-scale ML systems
  - Tools and systems to simplify/improve the end-to-end ML lifecycle

  ➔ **Many open technical problems**