SCIENCE
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LIMA: Fine-grained Lineage Tracing and Reuse in Machine Learning Systems

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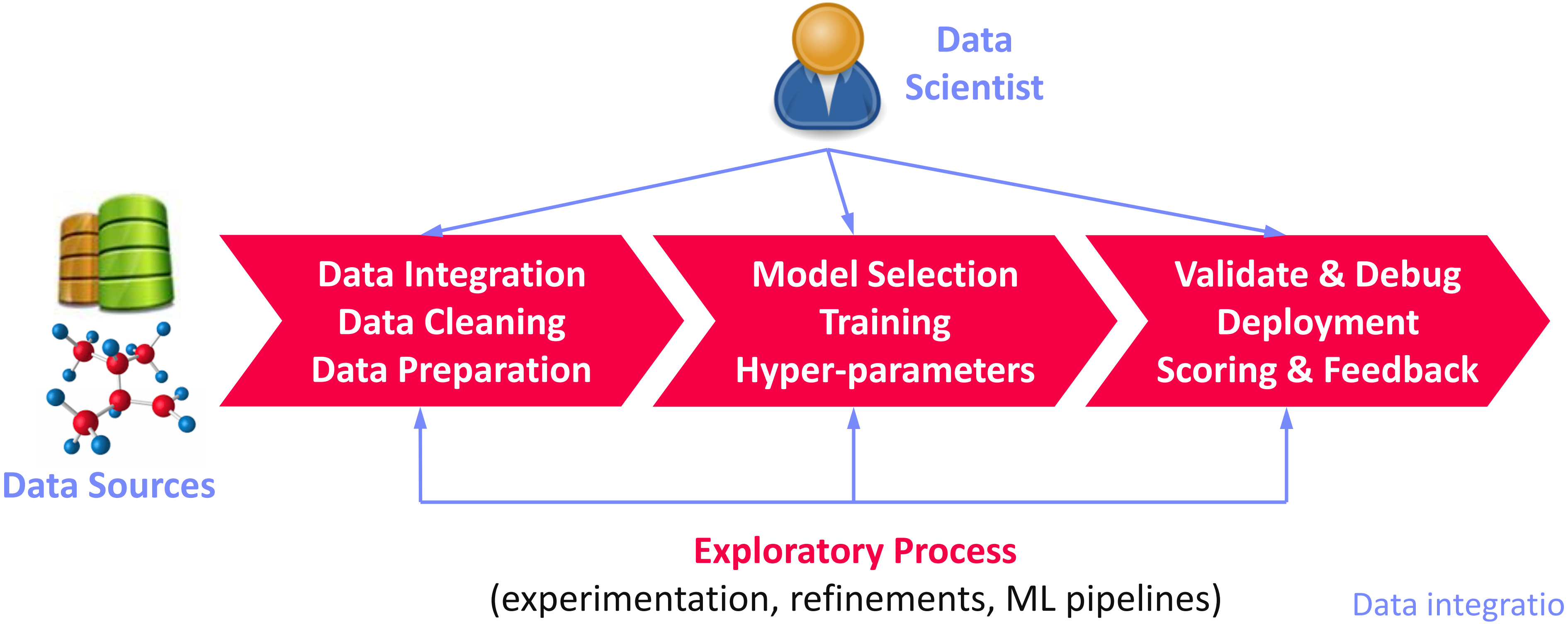
Exploratory Data Science



Data integration, cleaning and preparation techniques are themselves based on ML.

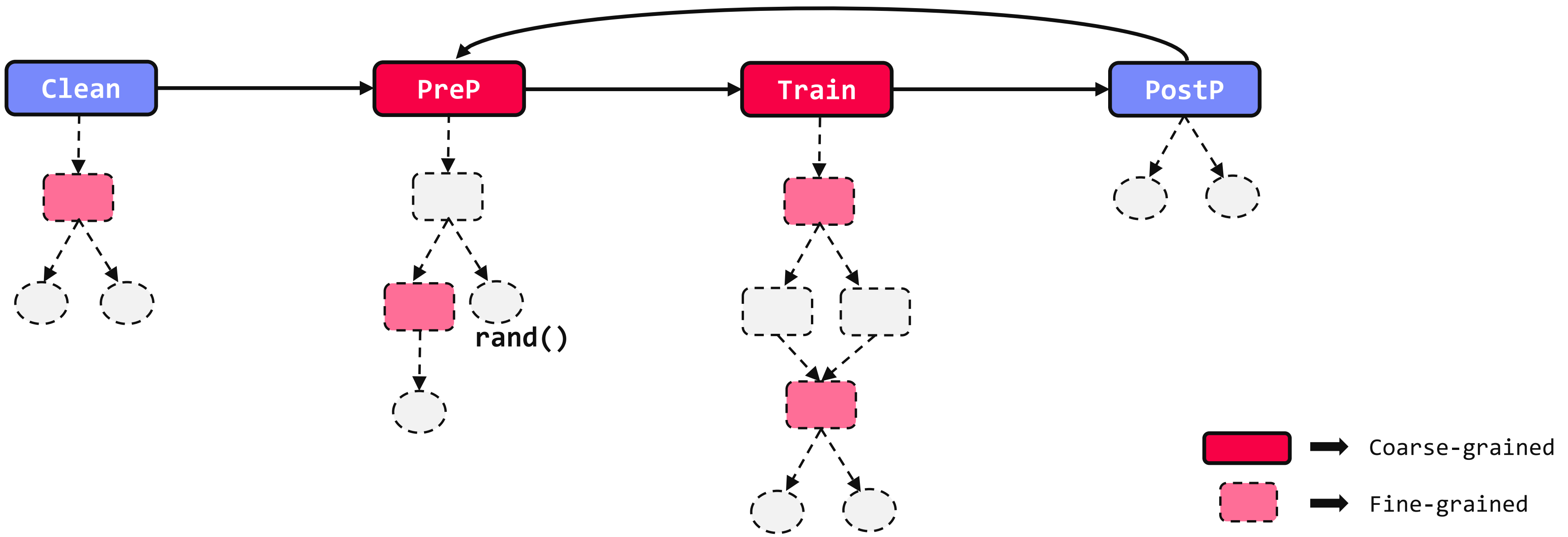
- **Problem**
  - High **computational redundancy** in ML pipelines
  - **Reproducibility** and **explainability** of trained models (data, parameters, prep)

Coarse-grained Reuse

- **Existing Approaches**
  - **Coarse-grained** lineage tracing of top-level tasks
  - **Black-box view** of individual steps (hidden substeps)
  - Cannot eliminate **fine-grained redundancy**
  - Fail to detect internal **non-determinism** (`rand()`, random reshuffling and initialization, drop-out layers)

[Doris Xin et al: Helix: Holistic Optimization for Accelerating Iterative Machine Learning. **PVLDB 12, 4 (2018)**]

[Behrouz Derakhshan et al: Optimizing Machine Learning Workloads in Collaborative Environments. **SIGMOD 2020**]



Sources of Redundancy

- **Running Example: Grid Search Hyper-parameter Tuning for LM**

User Script

```
X = read('data/X.csv')
y = read('data/y.csv')
for(i in 1:10) {
  s = sample(15, ncol(X));
  [loss, B] = gridSearch('lm',
   'l2norm',...,
   list('reg','icpt','tol')
  print(loss+ "for feature set s");
}
```

Internal Built-in Functions

```
lm = function(...) {
  if (ncol(X) <= 1024)
    B = lmDS(X,y,icpt,reg)
  else
    B = lmCG(X,y,icpt,
             reg,tol)
}
```

```
lmDS = function(...) {
  if (icpt > 0) {
    X = cbind(X, Ones);
    if (icpt == 2)
      X = scaleAndShift(X)
  } ...
  l = matrix(reg,ncol(X),1)
  A = t(X) %*% X + diag(l)
  b = t(X) %*% y
  beta = solve(A, b) ...}
```

```
lmCG = function(...) {
  if (icpt > 0) {
    X = cbind(X, Ones);
    if (icpt == 2)
      X = scaleAndShift(X);
  } ...
  while (i<maxi & nr2>tgt) {
    q = (t(X) %*% (X%*%ssX_p))
    p = -r + (nr2/old_nr2)*p;
}
```

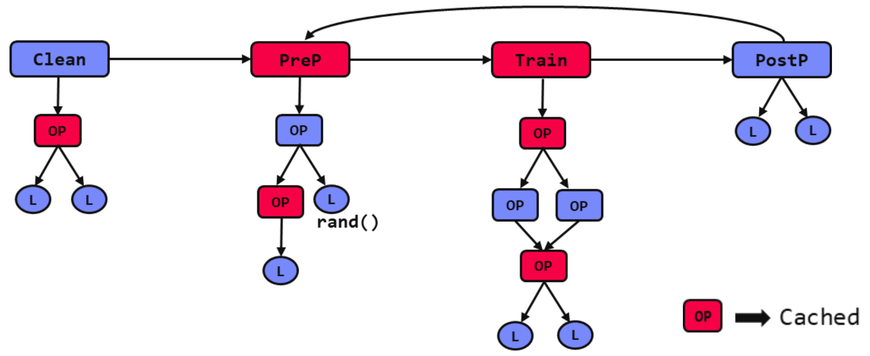
- #1 Redundant `lmDS` calls for tuning `'tol'`
- #2 $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}^T\mathbf{y}$ in `lmDS` are independent of `'reg'`
- #3 Same pre-processing block for `lmDS` and `lmCG`
- #4 Same `cbind` calls for `'icpt'` = 1 and 2
- #5 Partially overlapping $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}^T\mathbf{y}$ with `cbind` of Ones
- #6 Random feature sets exhibit overlapping features

Redundancy across data science lifecycle tasks

Introducing LIMA

- **Lineage/Provenance as Key Enabling Technique**
  - Model versioning, **reuse of intermediates**, incremental maintenance, auto differentiation, and **debugging** (results and intermediates, convergence behavior via query processing over lineage traces)

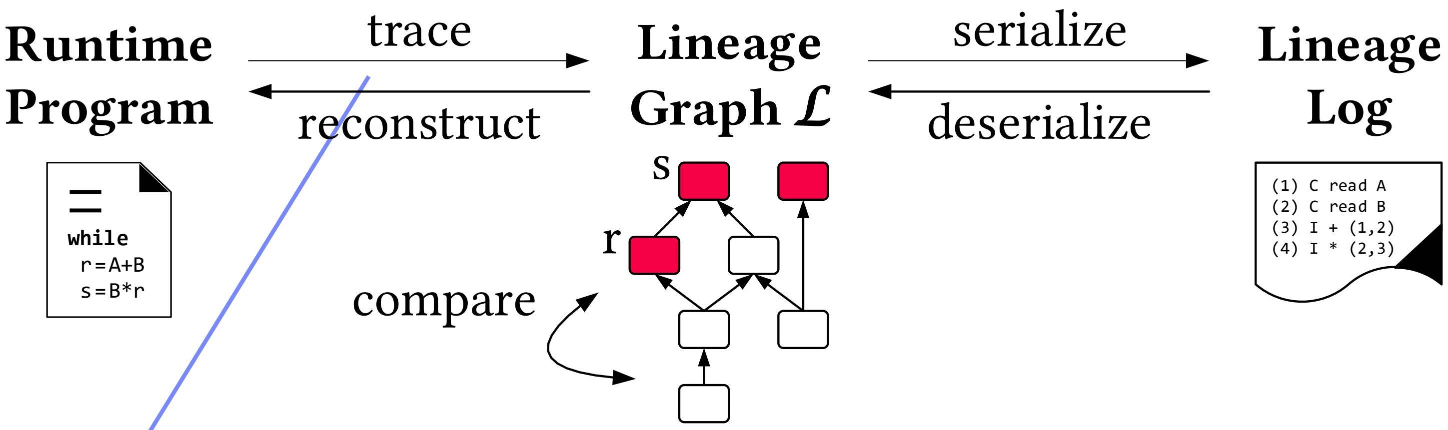
- **LIMA**
  - A framework for **fine-grained** lineage tracing and reuse **inside ML systems**
  - Efficient, **low-overhead** lineage tracing of individual operations
  - **Full and partial reuse** across the program hierarchy



Lineage Tracing

(Key Operations and Lineage Deduplicaton)

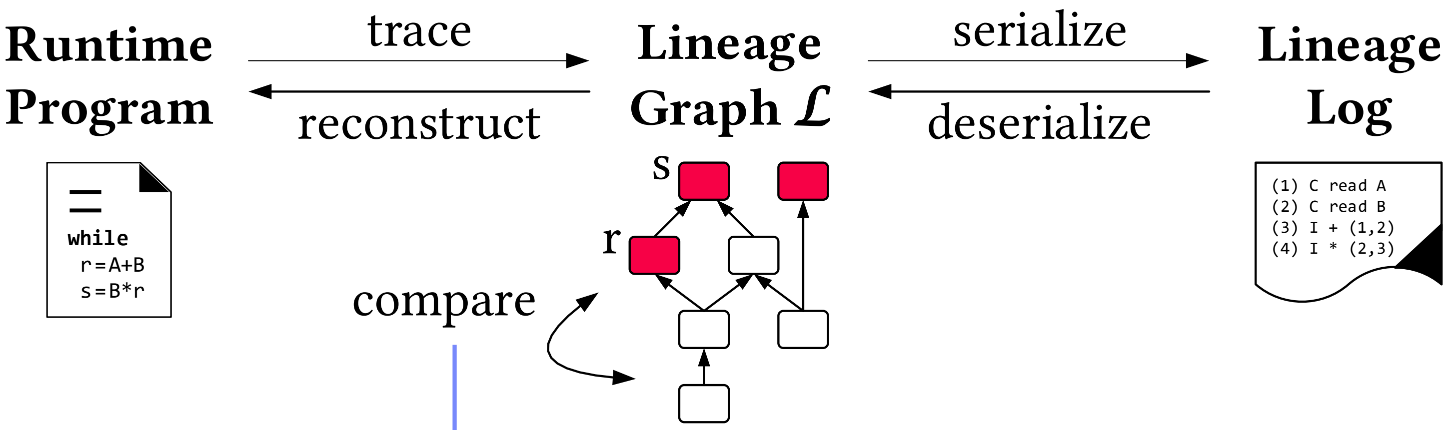
Basic Lineage Tracing



Lineage Tracing Lifecycle

- a) **Efficient Lineage Tracing**
  - Trace lineage of logical operations for **all live variables**
  - Tracing of inputs, literals, and **non-determinism**
  - **Immutable** lineage DAG
  - Execution context maintains `LineageMap` that **maps live variable names to lineage items**

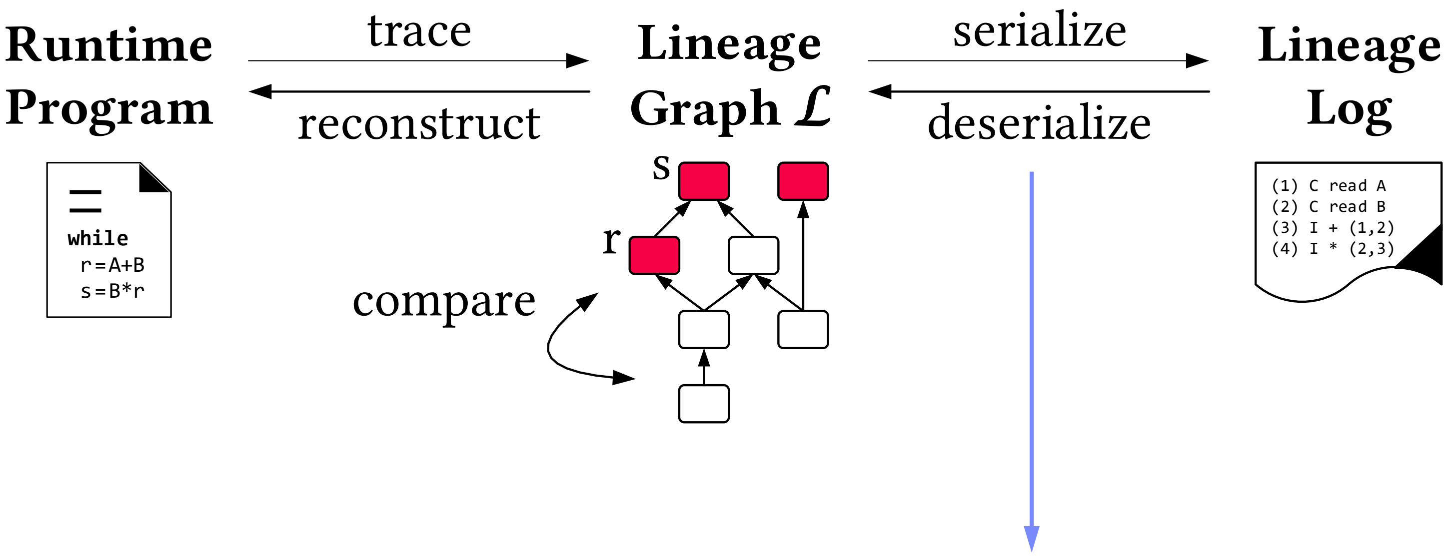
Basic Lineage Tracing



Lineage Tracing Lifecycle

- **b) Comparison of Lineage DAGs**
  - Lineage items implement **`hashCode()`** and **`equals()`**
  - Hash over the hashes of opcode, data item, and all inputs
  - **Non-recursive** equals; returns true if the opcode, data and all inputs are equivalent

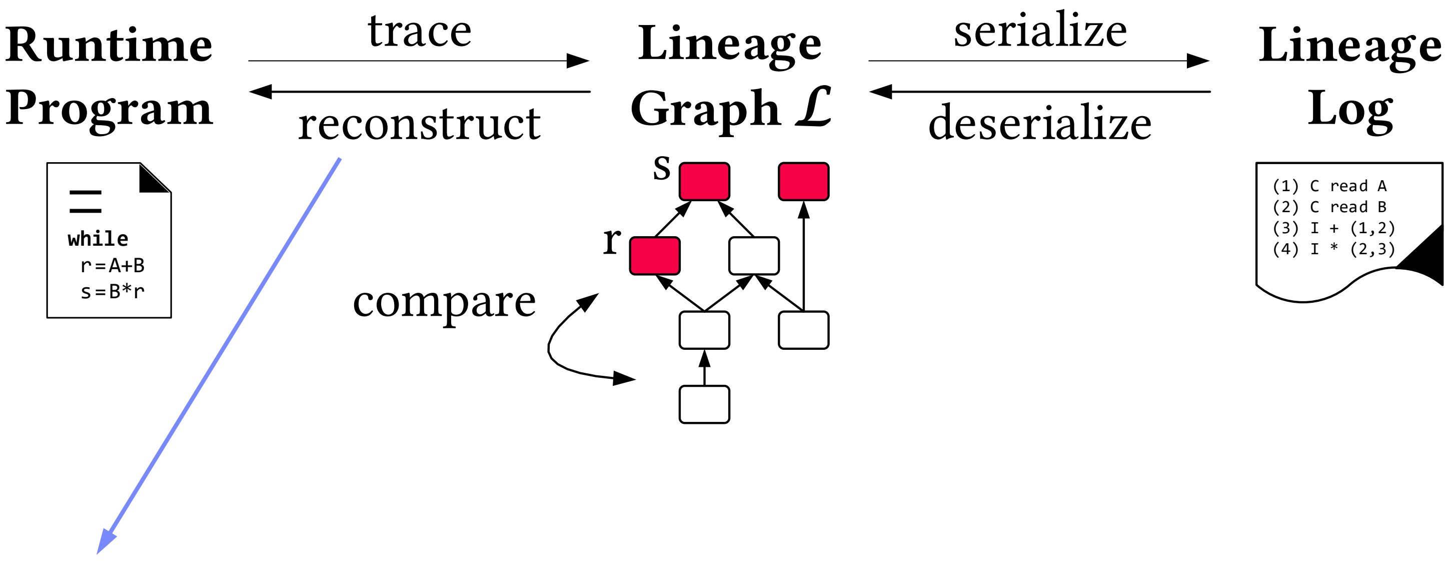
Basic Lineage Tracing



Lineage Tracing Lifecycle

- **c) Serialization and Deserialization of Lineage DAGs**
  - `lineage(X)`, and `write(X, 'f')` always generates `'f.lineage'`
  - Serialization unrolls the DAG in a depth-first manner
  - Deserialization converts lineage log into a lineage DAG

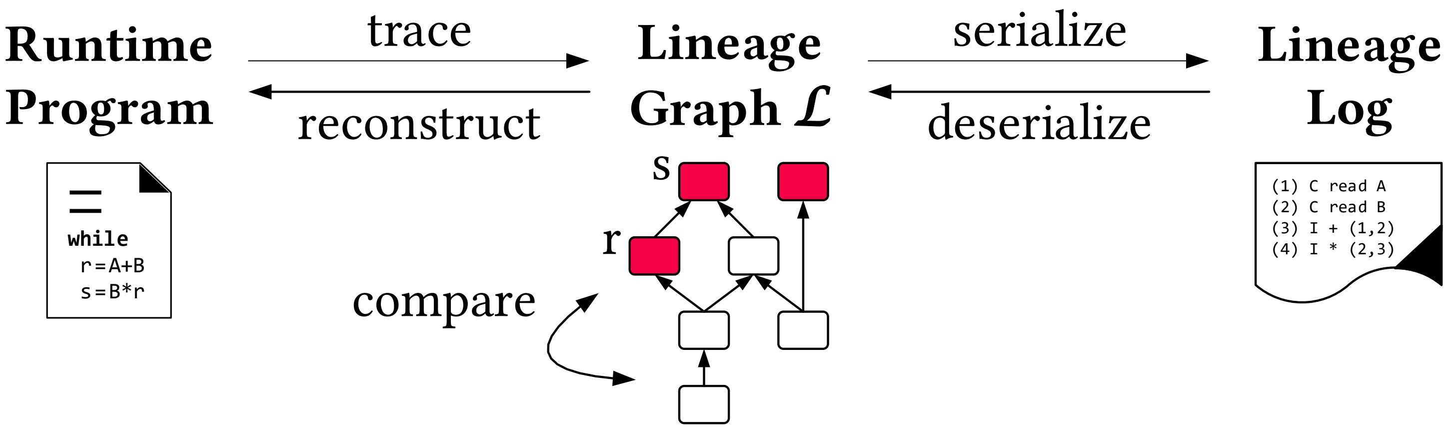
Basic Lineage Tracing



Lineage Tracing Lifecycle

- **d) Re-computation from Lineage**
  - Generate runtime program from a lineage DAG
  - Compute exactly the same intermediates
  - Does not contain control flow
  - `X = eval(deserialize(serialize(lineage(X))))`

Basic Lineage Tracing



Lineage Tracing Lifecycle

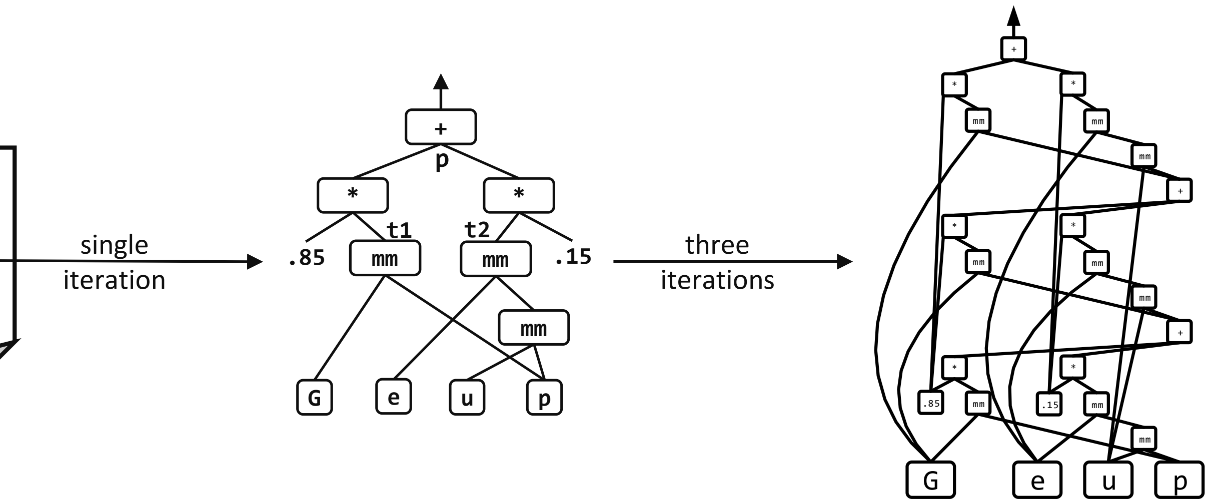
The entire lifecycle of lineage tracing with the key operations is very valuable as it **simplifies testing, debugging and reproducibility**.

Lineage Deduplication

- **Problem**
  - Very **large lineage DAGs** for mini-batch training (repeated execution of loop bodies)
  - NN training w/ 200 epochs, batch-size 32, 10M rows, 1K instructions → 4TB → **4GB w/ deduplication**

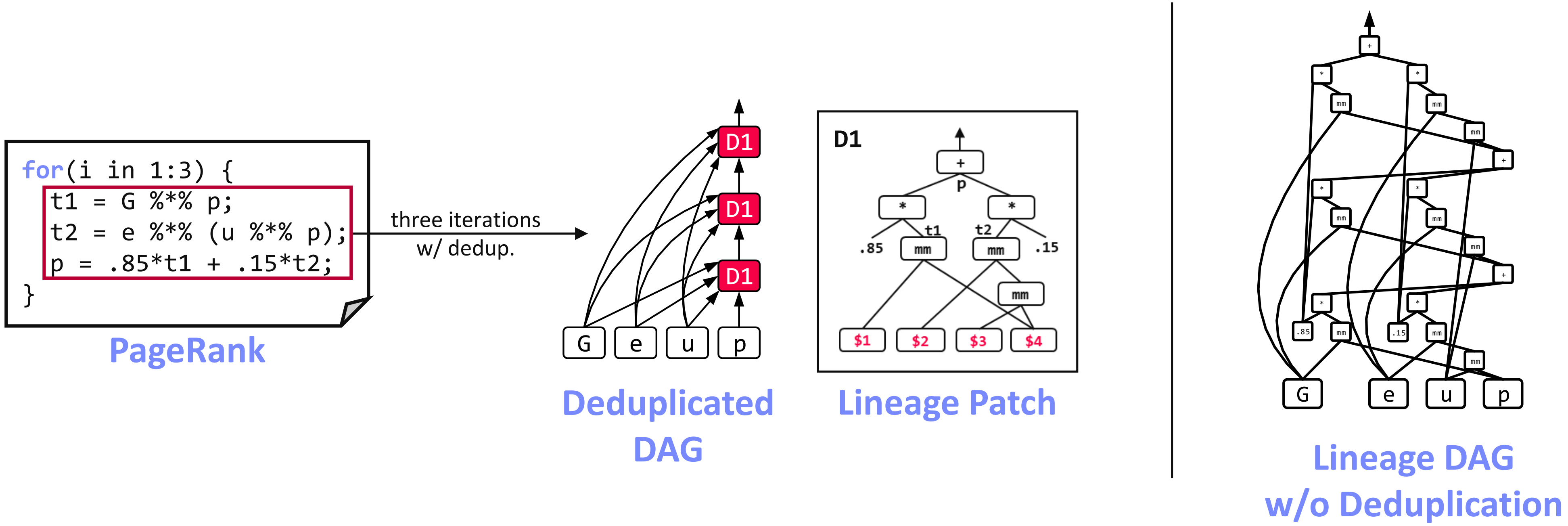
```
for(i in 1:3) {
  t1 = G %*% p;
  t2 = e %*% (u %*% p);
  p = .85*t1 + .15*t2;
}
```

PageRank



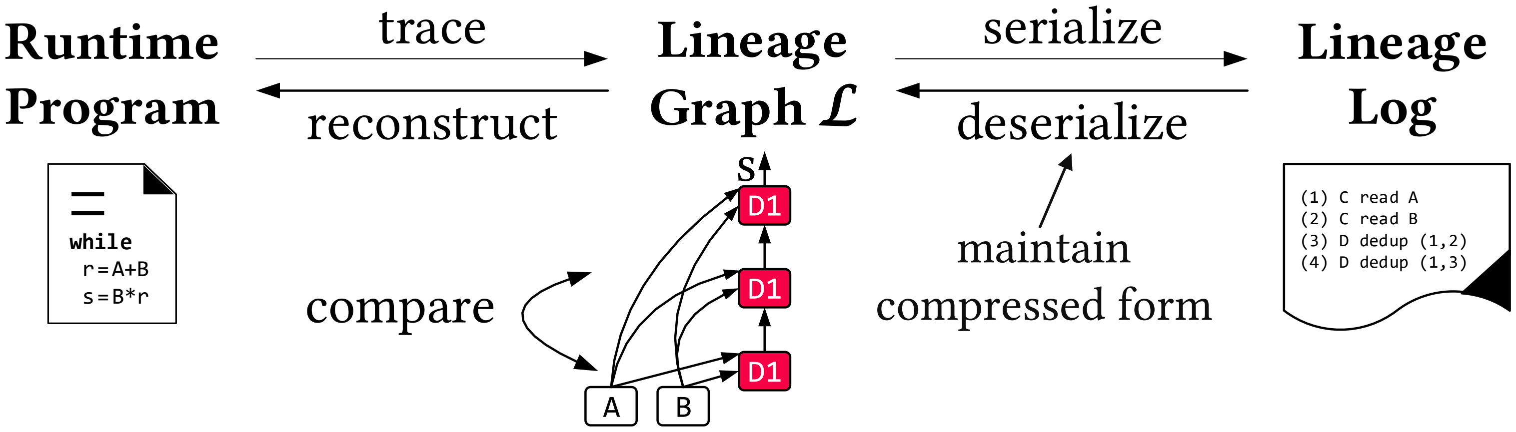
Lineage DAG

Lineage Deduplication



- **Solution**
  - Trace **each independent path once**; store as patches
  - Refer to the patches via **single lineage items**
- **Implementation**
  - Proactive setup: **count** distinct control paths
  - Runtime of iterations: trace lineage, **track taken path**
  - Post-iteration: save the patch, add a **single dedup lineage item** to the global DAG

Operations on Deduplicated Graphs



- **Integration**
  - Last-level `for`, `parfor`, `while` loops and functions
  - **Non-determinism**: add seeds (e.g. dropout layers) as input placeholders
  - **Compare** regular and deduplicated DAGs
  - Serialize, deserialize, re-compute **w/o causing expansion**

Lineage-based Reuse

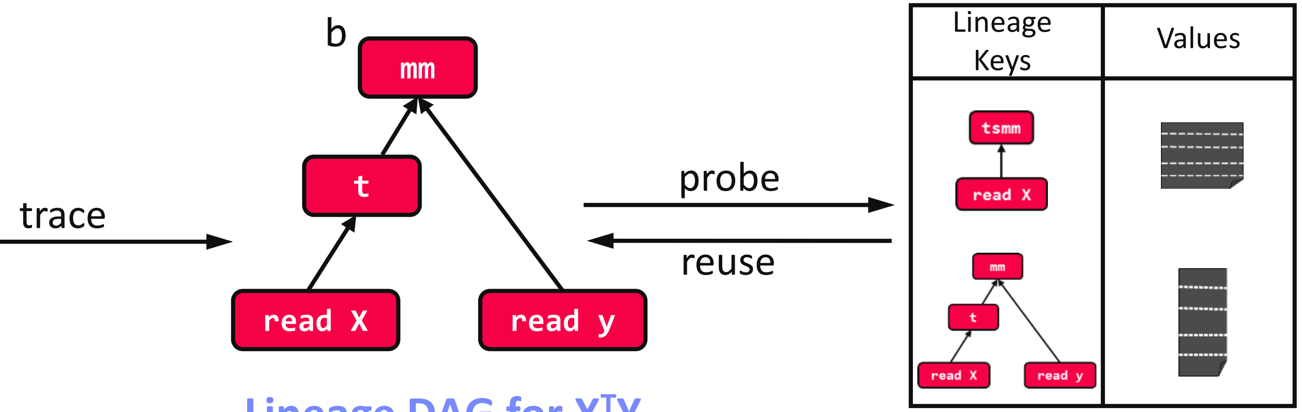
(Lineage Cache, Multi-level Reuse, Partial Reuse and Eviction Policies)

Lineage-based Reuse

- **Operation-Level Full Reuse**
  - Lineage cache comprises a hash map, **`Map<Lineage, Intermediate>`**
  - Before executing instruction, **probe lineage cache** for outputs
  - Leverage compare functionality via efficient `hashCode()` and `equals()`

```
lmDS = function(...) {
  [...]
  A = t(X) %*% X + diag(l)
  b = t(X) %*% y
  beta = solve(A, b) ...}
```

Closed-Form Linear Regression



Lineage DAG for X^TY

Lineage Cache

Multi-Level Full Reuse

- **Limitations of Operation-level Reuse**
  - Fails to remove **coarse-grained redundancy**, e.g., entire function
  - Cache pollution and interpretation overhead

```
X = read('data/X.csv')
y = read('data/y.csv')
[loss, B] = gridSearch('lm', 'l2norm',
   ,..,list('reg','icpt','tol')
 print(loss+ "for feature set s");
}
```

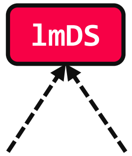
```
lm = function(...) {
  if (ncol(X) <= 1024)
    B = lmDS(X,y,icpt,reg)
  else
    B = lmCG(X,y,icpt,
             reg,tol)
}
```

```
lmDS = function(...) {
 if (icpt > 0) {
   X = cbind(X, Ones);
   if (icpt == 2)
     X = scaleAndShift(X)
 } ...
 l = matrix(reg,ncol(X),1)
 A = t(X) %*% X + diag(l)
 b = t(X) %*% y
 beta = solve(A, b) ...}
```

→ **Redundant lmDS calls**

→ **Redundant preprocessing block for `icpt` = 1, 2**

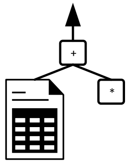
- **Solution: Multi-level Reuse**
  - **Hierarchical** program structure as reuse points
  - Mark if deterministic during compilation
  - **Special lineage item** to represent a function call
  - Avoid cache pollution and interpretation overhead
  - Similar to function, reuse **code blocks**

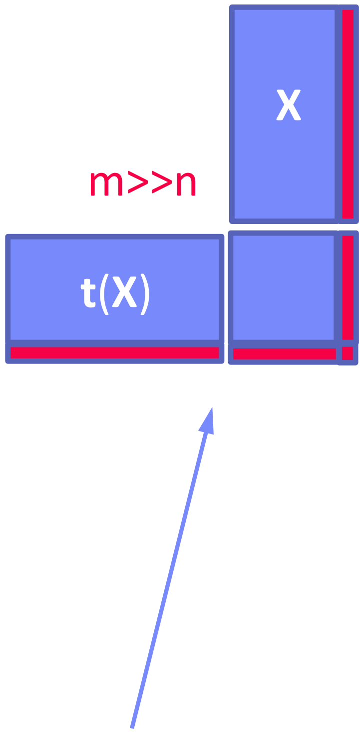


Partial Operation Reuse

- **Limitations of Full Reuse**
  - Often partial results overlap. Example: stepLM
- **Solution: Partial Reuse**
  - **Reuse partial results** via dedicated rewrites (compensation plans)
  - Probe ordered-list of rewrites of **source-target patterns**
  - Construct **compensation plan**, compile and execute
  - Based on real use cases
- **Example Rewrites**
  - #1 `rbind(X, ΔX)Y → rbind(XY, ΔXY);`
  - #2 `Xcbind(Y, ΔY) → cbind(XY, XΔY)`
  - #3 `dsyrk(cbind(X, ΔX)) → rbind(cbind(dsyrk(X), XᵀΔX), cbind(ΔXᵀX, dsyrk(ΔX)))`
  - ...

`where, dsyrk(X) = XᵀX`






```
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)
} }
```

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

$O(n^2(mn^2+n^3)) \rightarrow O(n^2(mn+n^3))$

Cache Eviction

- **Delete or spill.** Spill to disk if re-computation time > estimated I/O time

- **Statistics and Cost**
  - Static: operation execution time, distance from leaves, in-memory and in-disk sizes
  - Dynamic: last access timestamp, #accesses
  - Estimate: disk I/O

- **Eviction Policies**
  - Determine **order of eviction**
  - **LRU**: orders by normalized last access time
    → Pipelines with temporal reuse locality
  - **DAG-Height**: orders by depth of DAG (deep lineage traces have less reuse potential)
    → Mini-batch scenario. Reuse across epochs
  - **Cost&Size**: orders by cost, size ratio (preserve objects with high cost to size ratio) scaled by #accesses
    → Global reuse utility. Performs well in a wide variety of scenarios

Default Policy

Eviction Policies & Eviction Orders

Policy	Orders Objects by
LRU	normalized last access timestamp
Dag-Height	height of operation-DAG, descending
Cost&Size	cost/size * #accesses

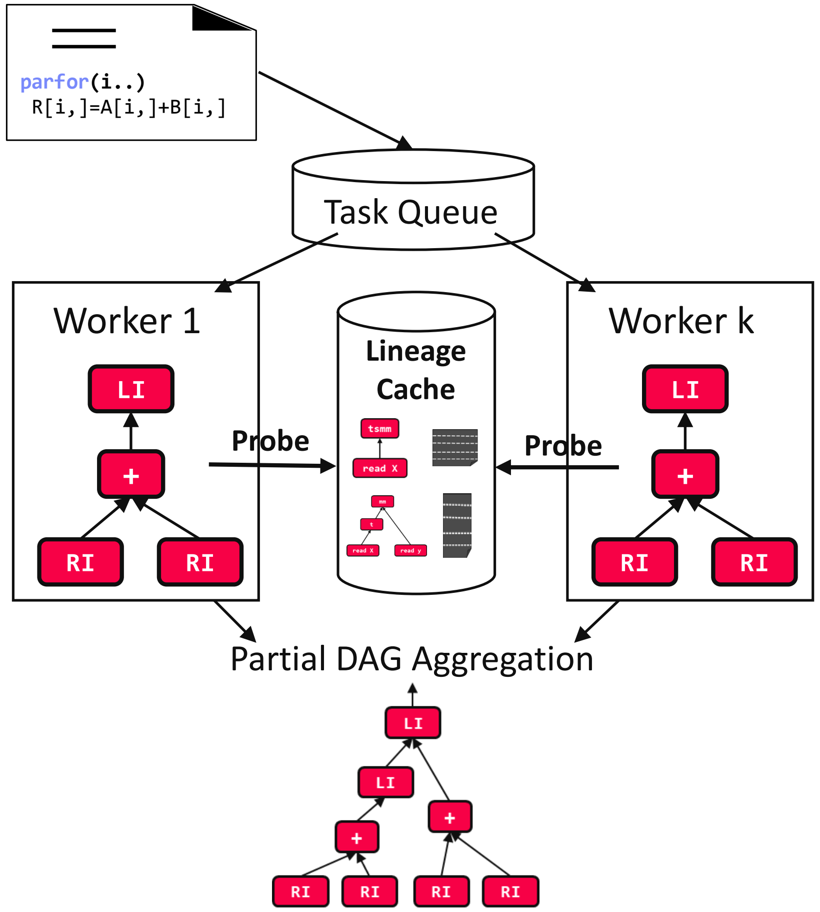
[Behrouz Derakhshan et al: Optimizing Machine Learning Workloads in Collaborative Environments. **SIGMOD 2020**]

Integration with ML Systems

- **#1 Task-parallel Loops**
  - **Worker-local** tracing. Merge in a linearized manner
  - Tasks share lineage cache in a **thread-safe** manner
  - Lineage cache "placeholders" to avoid redundant computation in parallel tasks

- **#2 Operator Fusion**
  - Fusion loses operator semantics
  - Construct lineage patches **during compilation**, and add those to the global DAG during runtime

- **#3 Compiler Assistance**
  - **Unmark** not reusable operations for caching to avoid cache pollution and probing
  - **Reuse-aware rewrites** during compilation to create additional reuse opportunities
  - Reuse-aware rewrites during runtime **recompilation**



Lineage Tracing and Task Parallelism

Experiments

(End-to-end ML Pipelines, ML Systems Comparison)

Experimental Setting

- **Baselines**

Apache SystemDS ™

TensorFlow

Helix

scikit learn

- **Datasets**

Dataset	nrow(X_0)	ncol(X_0)	nrow(X)	ncol(X)	ML Alg.
APS	60,000	170	70,000	170	2-Class
KDD 98	95,412	469	95,412	7,909	Reg.

Lineage-based reuse is largely independent of data skew.

- **Workloads**

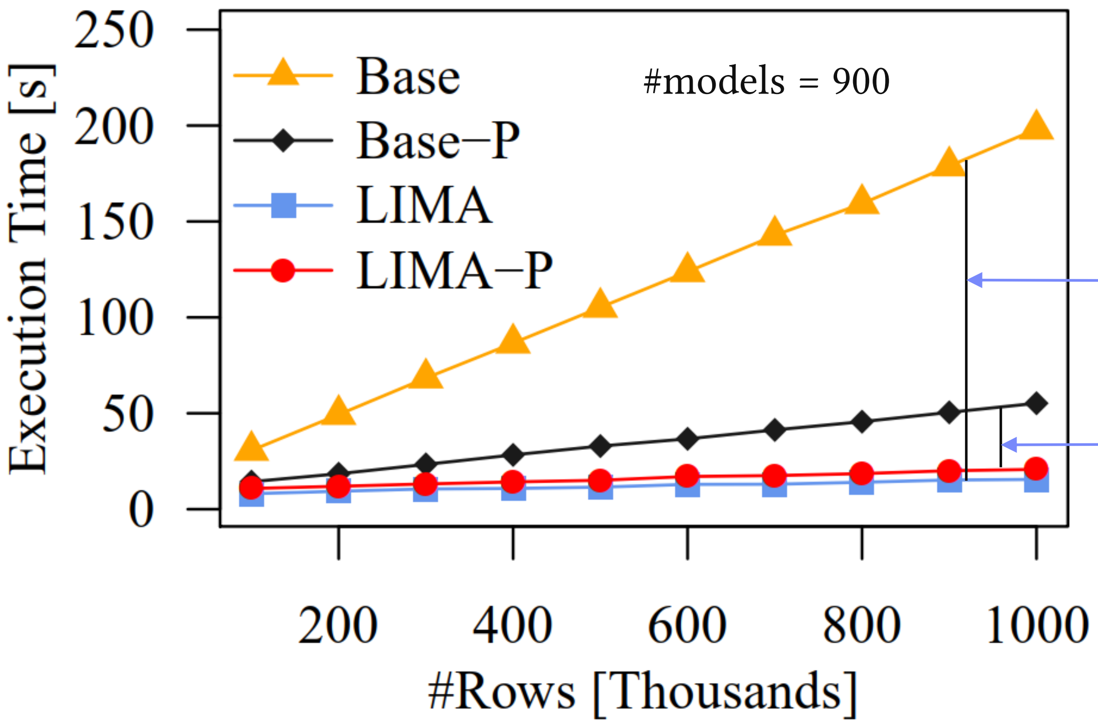
Variety of end-to-end ML pipelines incl. data prep., feature engineering, traditional ML training (regression, classification) and NN training.

Experiments

- **End-to-end ML Pipelines**

Baselines:
#1 Base = **SystemDS** default config.
#2 Base-P = Base **w/ task parallel** execution
#3 LIMA = Lineage tracing and reuse
#4 LIMA-P = LIMA **w/ task parallel** execution

Grid Search LR (w/ & w/o Task Parallelism)



12.4x w/o task parallelism

2.6x w/ task parallelism

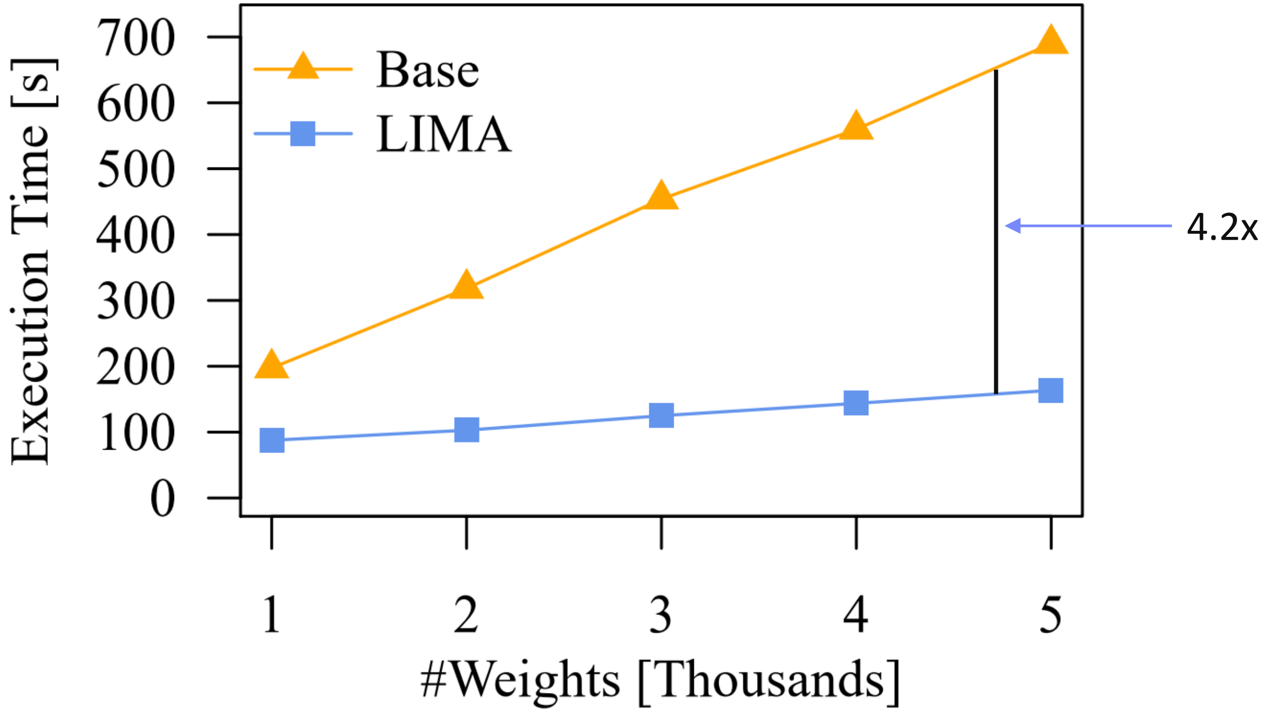
Setup: Hadoop cluster with each node having a single AMD EPYC 7302 CPUs (16/32 cores) and 128 GB DDR4 RAM

Experiments

- **End-to-end ML Pipelines**

Baselines:
#1 Base = **SystemDS** default config.
#2 LIMA = Lineage tracing and reuse

Weighted Ensemble (SVM, Log-Reg)



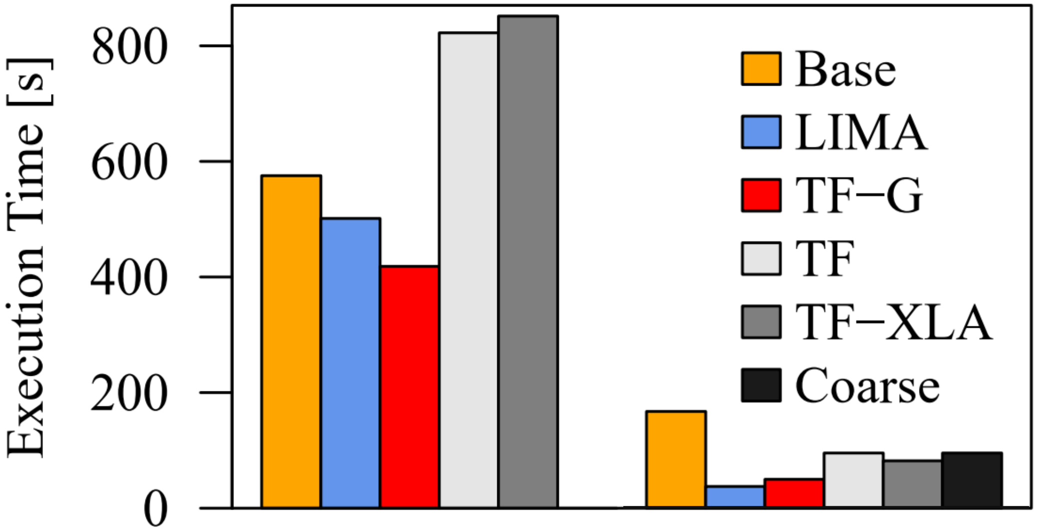
Large improvements due to **fine-grained redundancy elimination**

Setup: Hadoop cluster with each node having a single AMD EPYC 7302 CPUs (16/32 cores) and 128 GB DDR4 RAM

Experiments, cont.

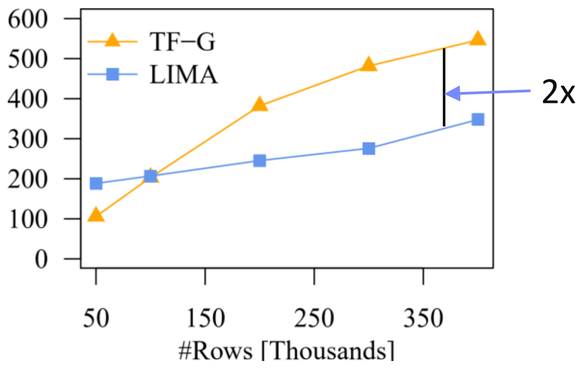
- **ML Systems Comparison**

LIMA vs. TF2.0 vs. Coarse-grained



Autoencoder w/ 2 Layers

PCA and Cross Validated LR



PCA and CV LR

Baselines:
#1 Base = **SystemDS** default config.
#2 LIMA = Lineage tracing and reuse
#3 TF-G = TensorFlow 2.3 **Graph mode**
#4 TF = TensorFlow 2.3 Eager mode
#5 TF-XLA = TF w/ XLA code gen. for CPU
#6 Coarse = **Coarse-grained** reuse (HELIX)

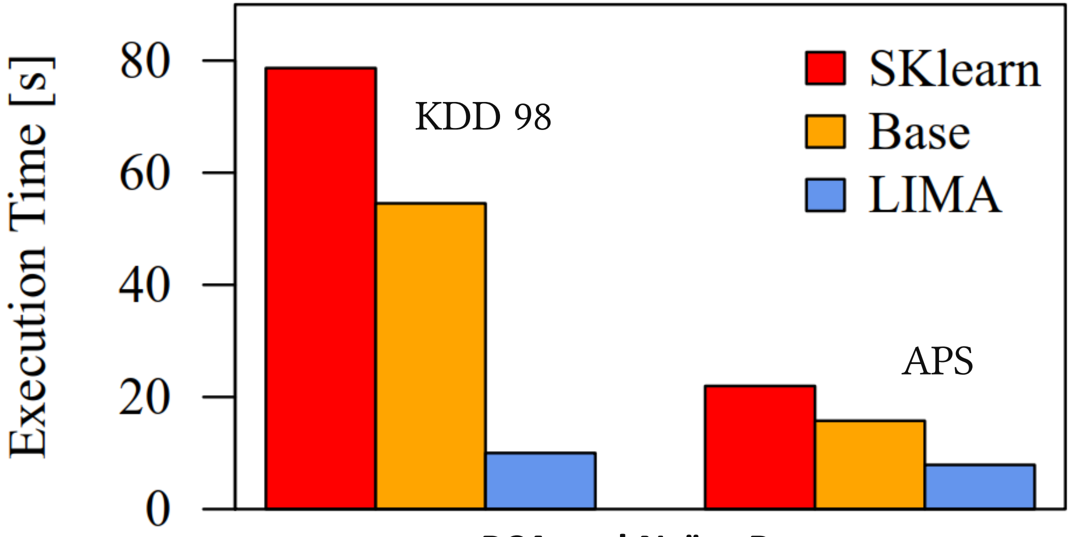
Setup: Hadoop cluster with each node having a single AMD EPYC 7302 CPUs (16/32 cores) and 128 GB DDR4 RAM

Experiments, cont.

- **ML Systems Comparison**

Baselines:
#1 SKlearn = Scikit-learn
#2 Base = **SystemDS** default config.
#3 LIMA = Lineage tracing and reuse

LIMA vs. Scikit-learn



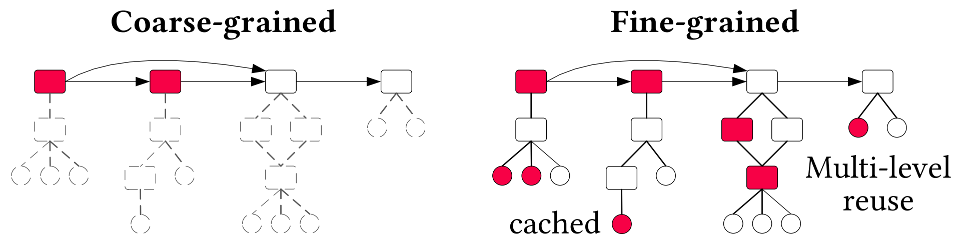
PCA and Naïve Bayes

Competitive baseline performance against state-of-the-art ML Systems

Setup: Hadoop cluster with each node having a single AMD EPYC 7302 CPUs (16/32 cores) and 128 GB DDR4 RAM

Conclusions

- **Summary**
  - **Fine-grained lineage tracing** in ML systems
  - **Deduplication** for loops to reduce overhead
  - Compiler-assisted **full, partial and multi-level reuse**
  - Support for **fused operators and task-parallelism**



- **Conclusion**
  - Increasing redundancy is inevitable and difficult to address by library developers
  - Compile time **CSE is only partially effective** due to conditional control flow
  - Compiler-assisted runtime-based lineage cache proved effective

- **Future Work**
  - Combine with persistent materialization of intermediates
  - Multi-location and multi-device caching
  - Extend lineage support for model debugging and fairness constraints