SCIENCE
PASSION
TECHNOLOGY

Architecture of ML Systems
03 Size Inference, Rewrites, and Operator Selection

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Announcements/Org

- **#1 Modified Course Logistics**
  - **5 ECTS** (lectures+exam, and project),
    ➔ pick a **(1) programming project**, or
    (2) survey / experimental analysis project

- **#2 Programming/Analysis Projects**
  - **Apr 05:** Project selection
  - Discussion individual projects (first come, first served)

Agenda

- **Compilation Overview**
- **Size Inference and Cost Estimation**
- **Rewrites and Operator Selection**

Compilation Overview

Recap: Linear Algebra Systems

- **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

DB

PL **HPC**

Compilers for Large-scale ML

- **#1 Interpretation** (operation at-a-time)
  - Examples: **R**, **PyTorch**, **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], **Julia**, **Cumulon** [SIGMOD'13], **Tupleware** [PVLDB'15]

Optimization Scope

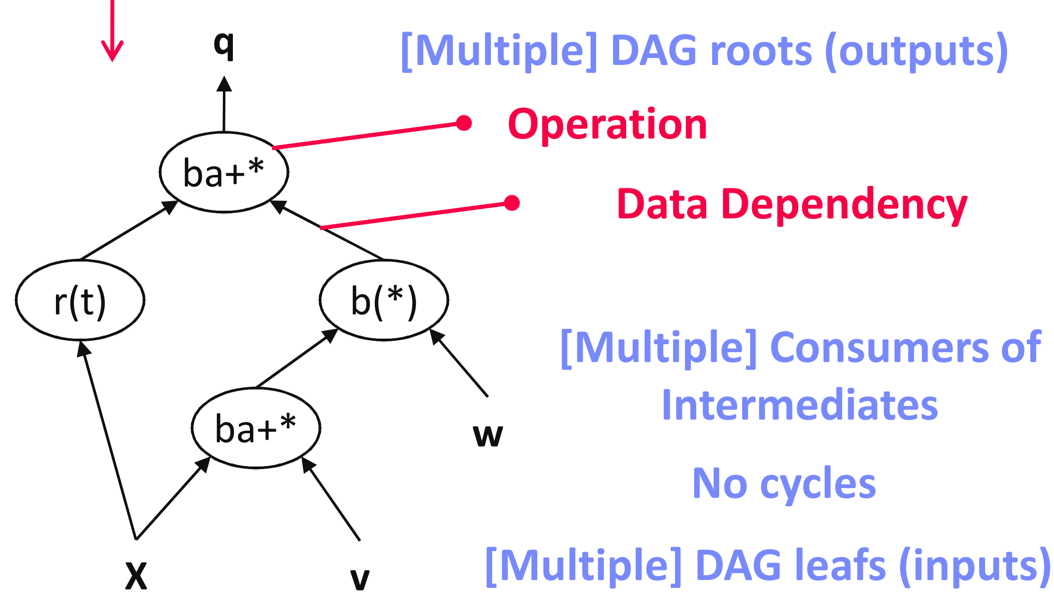
```
X = read($1); # n x m matrix
y = read($2); # n x 1 vector
maxi = 50; lambda = 0.001;
intercept = $3;
...
r = -(t(X) %*% y);
norm_r2 = sum(r * r); p = -r;
w = matrix(0, ncol(X), 1); i = 0;
while(i<maxi & norm_r2>norm_r2_trgt)
{
   q = (t(X) %*% X %*% p)+lambda*p;
   alpha = norm_r2 / sum(p * q);
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

ML Program Compilation

- **Script:**

```
while(...) {
   q = t(X) %*% (w * (X %*% v)) ...
}
```

- **Operator DAG**
  - a.k.a. “graph”
  - a.k.a. intermediate representation (IR)

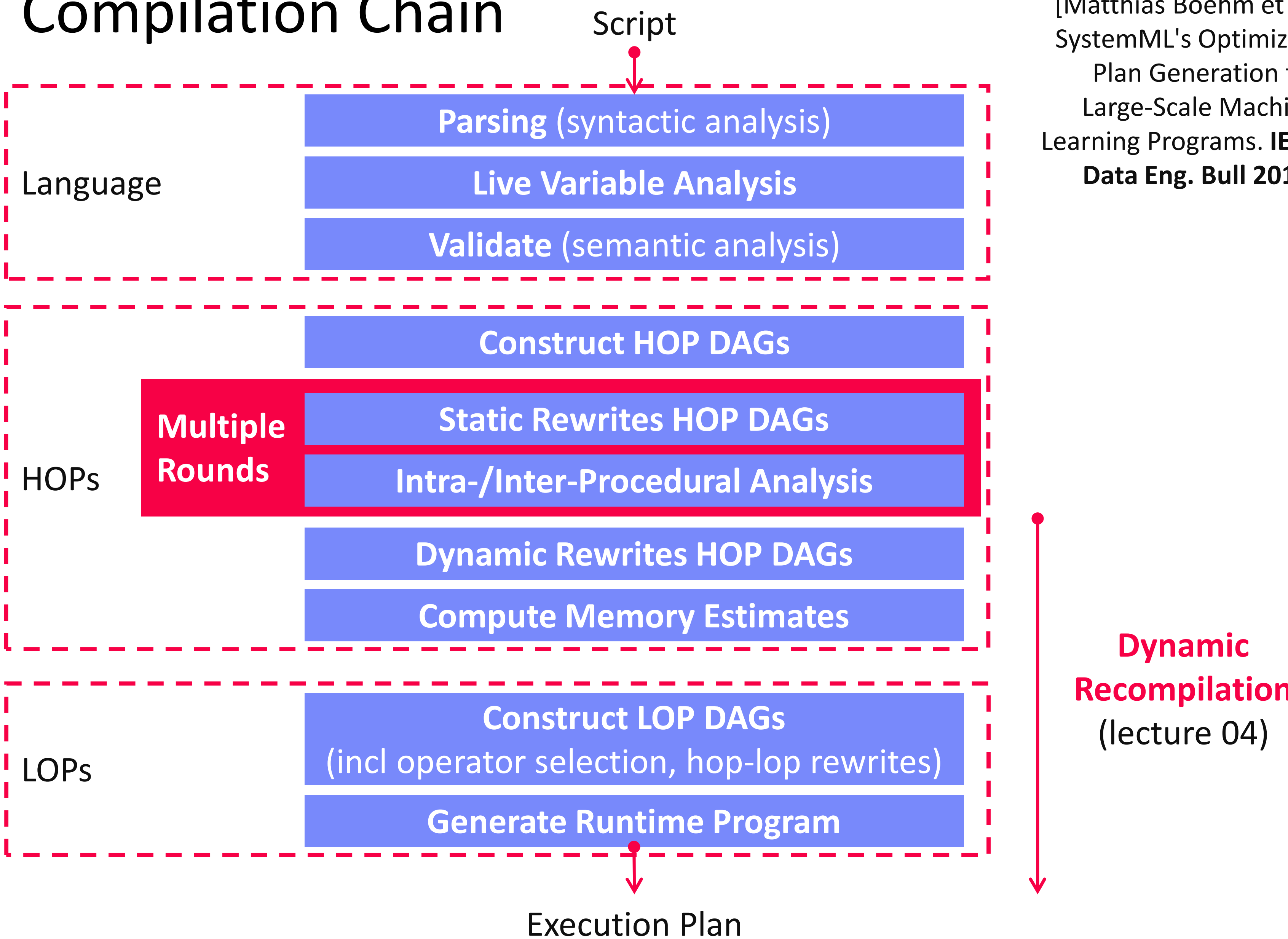


- **Runtime Plan**
  - Compiled runtime plans Interpreted plans

```
SPARK mapmmchain X.MATRIX.DOUBLE w.MATRIX.DOUBLE
v.MATRIX.DOUBLE _mVar4.MATRIX.DOUBLE XtwXv
```

Compilation Chain

[Matthias Boehm et al: SystemML's Optimizer: Plan Generation for Large-Scale Machine Learning Programs. **IEEE Data Eng. Bull 2014**]



Recap: Basic HOP and LOP DAG Compilation

LinregDS (Direct Solve)

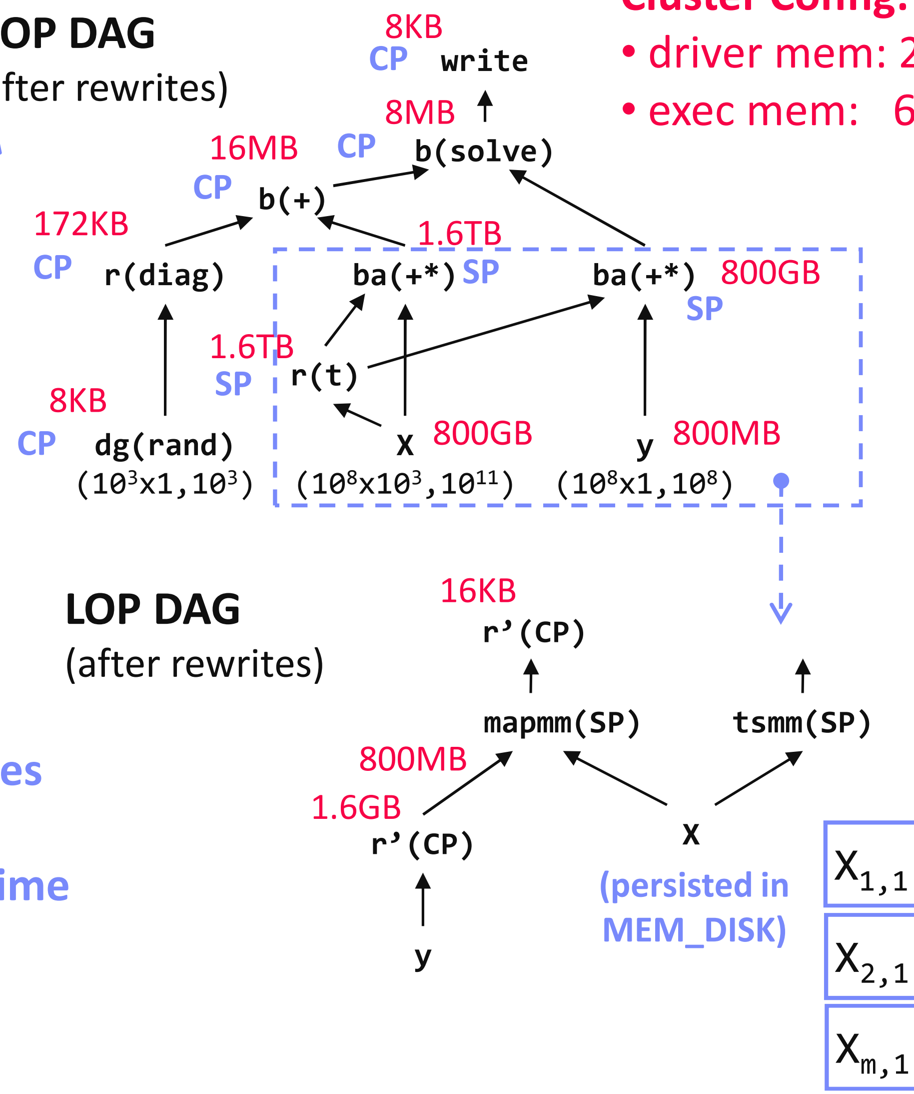
```
X = read($1);
y = read($2);
intercept = $3;
lambda = 0.001;
...
if( intercept == 1 ) {
  ones = matrix(1, nrow(X), 1);
  X = append(X, ones);
}
I = matrix(1, ncol(X), 1);
A = t(X) %*% X + diag(I)*lambda;
b = t(X) %*% y;
beta = solve(A, b);
...
write(beta, $4);
```

Scenario:
X: $10^8 \times 10^3$, 10^{11}
y: $10^8 \times 1$, 10^8

Cluster Config:
- driver mem: 20 GB
- exec mem: 60 GB

HOP DAG (after rewrites)

LOP DAG (after rewrites)



➔ **Hybrid Runtime Plans:**
- **Size propagation / memory estimates**
- **Integrated CP / Spark runtime**
- **Dynamic recompilation during runtime**

➔ **Distributed Matrices**
- **Fixed-size (squared) matrix blocks**
- **Data-parallel operations**

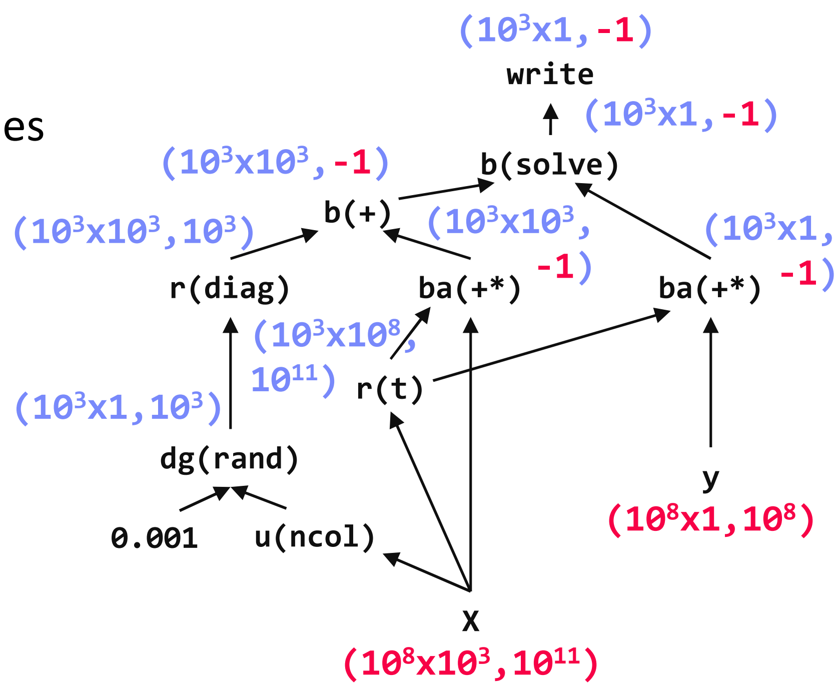
Size Inference and Cost Estimation

Constant and Size Propagation

- **Size Information**
  - Dimensions (#rows, #columns)
  - Sparsity (#nnz/(#rows * #columns))
  - ➔ **memory estimates and costs**

```
X = read($1);
y = read($2);
I = matrix(0.001, ncol(X), 1);
A = t(X) %*% X + diag(I);
b = t(X) %*% y;
beta = solve(A, b);
```

- **DAG-level Size Propagation**
  - **Input:** Size information for leaf nodes
  - **Output:** size information for all operators, -1 if still unknown
  - **Propagation based on operation semantics** (single bottom-up pass over DAG)



Constant and Size Propagation, cont.

- **Constant Propagation**
  - Relies on live variable analysis
  - Propagate constant literals into read-only statement blocks

- **Program-level Size Propagation**
  - Relies on **constant propagation** and **DAG-level size propagation**
  - **Propagate size information across conditional control flow:** size in leafs, DAG-level prop, extract roots
  - **if:** reconcile if and else branch outputs
  - **while/for:** reconcile pre and post loop, reset if pre/post different

```
X = read($1); # n x m matrix
y = read($2); # n x 1 vector
maxi = 50; lambda = 0.001;
if(...){ }
r = -(t(X) %*% y);
r2 = sum(r * r);
p = -r;                          # m x 1
w = matrix(0, ncol(X), 1);       # m x 1
i = 0;
while(i<maxi & r2>r2_trgt) {
   q = (t(X) %*% X %*% p)+lambda*p;
   alpha = norm_r2 / sum(p * q);
   w = w + alpha * p;            # m x 1
   old_norm_r2 = norm_r2;
   r = r + alpha * q;
   r2 = sum(r * r);
   beta = norm_r2 / old_norm_r2;
   p = -r + beta * p;            # m x 1
   i = i + 1;
}
write(w, $4, format="text");
```

Inter-Procedural Analysis

- **Intra/Inter-Procedural Analysis (IPA)**
  - Integrates all size propagation techniques (**DAG+program**, **size+constants**)
  - Intra-function and inter-function size propagation (**called once**, **consistent sizes**, **consistent literals**)

```
X = read($X1)
X = foo(X);
if( $X2 != “ ” ) {
  X2 = cbind(X,
    matrix(1,n,1));
  X2 = foo(X2);
}...
```

1M x 1

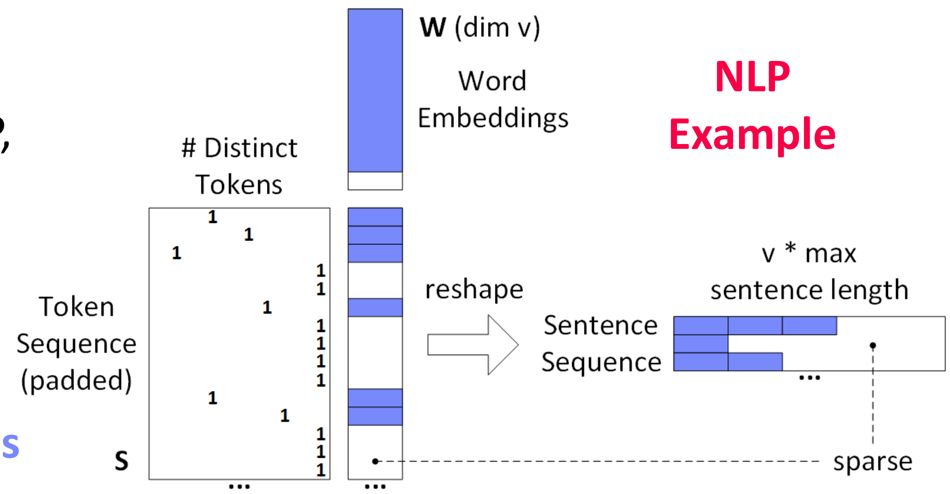
1M x 2

```
foo = function (Matrix[Double] A)
    return (Matrix[Double] B)
{
  B = A - colSums(A);
  if( sum(B!=B)>0 )
    print(“NaNs encountered.”);
}
```

- **Additional IPA Passes (selection)**
  - **Inline functions** (single statement block, small)
  - **Dead code elimination** and simplification rewrites
  - Remove unused functions & flag functions for recompile-once

Sparsity Estimation Overview

- **Motivation**
  - Sparse input matrices from NLP, graph analytics, recommender systems, scientific computing
  - Sparse intermediates (selections, dropout)
  - Selection/permutation matrices

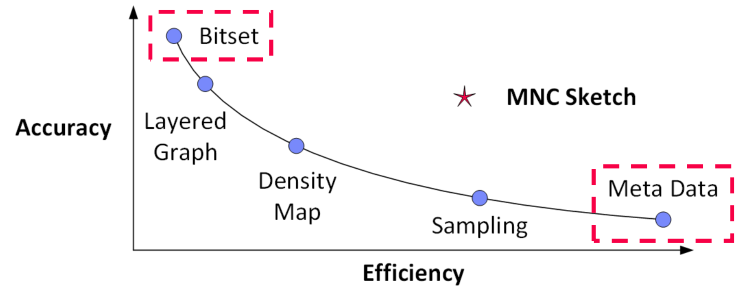


- **Problem Definition**
  - Sparsity estimates used for **format decisions**, **output allocation**, **cost estimates**
  - Matrix A with sparsity s_A = nnz(A)/(mn) and matrix B with s_B = nnz(B)/(nl)
  - Estimate sparsity s_C of matrix product C = A B; d=max(m,n,l)
  - Assumptions (Boolean matrix product)
    - **A1:** No cancellation errors (round of errors)
    - **A2:** No not-a-number (NaN)

Sparsity Estimation – Naïve Estimators

- **Average-case Estimator (meta data)**
  - Computes output sparsity based on s_A and s_B (e.g., SystemML, SpMachO)
  - Assumes uniform nnz distribution
  - $\hat{s}_C = 1 - (1 - s_A \cdot s_B)^n$,

O(1)
O(1)



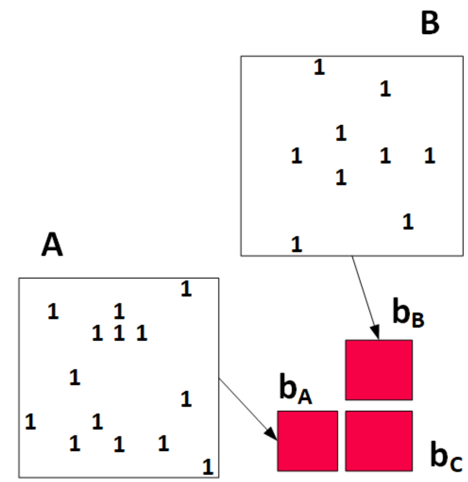
- **Worst-case Estimator (meta data)**
  - Computes output sparsity based on sA and sB (e.g., SystemML)
  - Assumes worst-case scenario (upper bound)

O(1)
O(1)

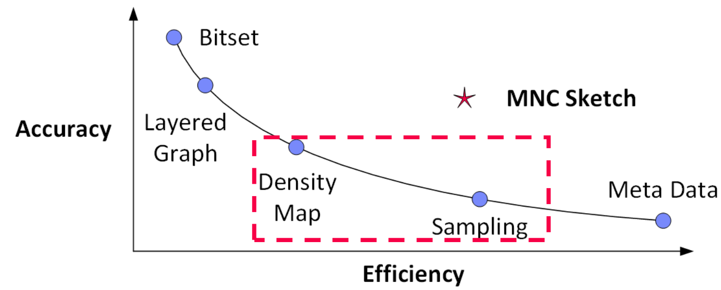
$$\hat{s}_C = \min(1, \text{nnz}(\mathbf{A})/m) \cdot \min(1, \text{nnz}(\mathbf{B})/l)$$
$$= \min(1, s_A \cdot n) \cdot \min(1, s_B \cdot n),$$

- **Bitset Estimator**
  - Constructs Boolean matrices and performs an exact Boolean matrix multiply (e.g., cuSPARSE, MKL, SciDB)
  - $s_C = \hat{s}_C = \text{bitcount}(\mathbf{b}_C)/(ml)$,

O(mn+nl +ml)
O(mnl)

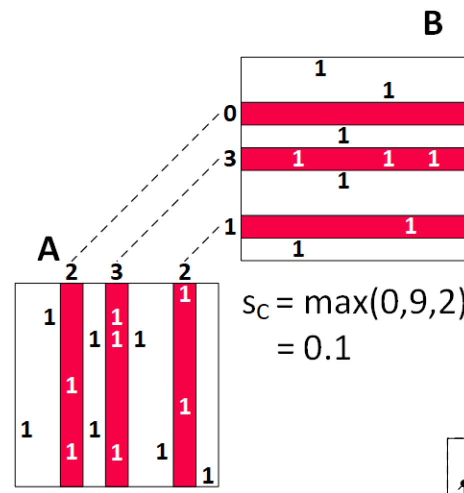


Sparsity Estimation – Sampling and Density Map



- **Sampling-based Estimator**
  - Takes a sample S of aligned columns in A and rows in B (e.g., MatFast)
  - Estimates single matrix product via no-collisions assumption (lower bound)
  - Biased: $\hat{s}_C = \max_{k \in \mathcal{S}} (\text{nnz}(\mathbf{A}_{:k}) \cdot \text{nnz}(\mathbf{B}_{k:}))/(ml).$
  - (Unbiased: $\hat{s}_C = 1 - (1 - \overline{v})^q \prod_{k \in \mathcal{S}} (1 - v_k),$)

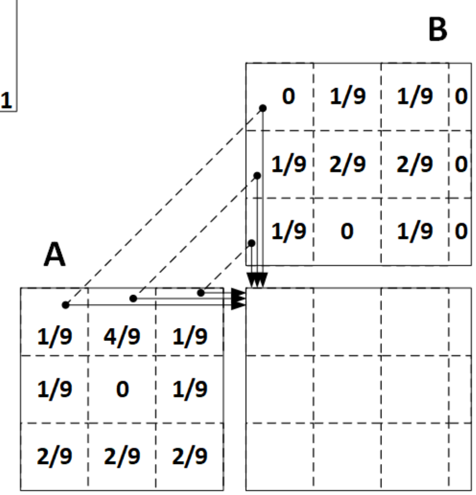
O(|S|)
O(|S|(m+l))



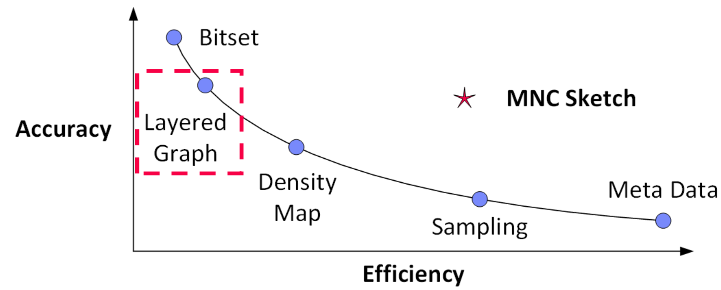
s_C = max(0,9,2)/90
= 0.1

- **DensityMap Estimator**
  - Creates density map of squared block size b=256 (e.g., SPMachO)
  - Estimate chains via average-case estimates
  - $\text{dm}_{C_{ij}} = \oplus_{k=1}^{n/b} \text{E}_{\text{ac}}(\text{dm}_{A_{ik}}, \text{dm}_{B_{kj}})$
    with $s_{A \oplus B} = s_A + s_B - s_A s_B,$

$O(mn/b^2 + nl/b^2 + ml/b^2)$
$O(mnl/b^3)$



Sparsity Estimation – Layered Graph



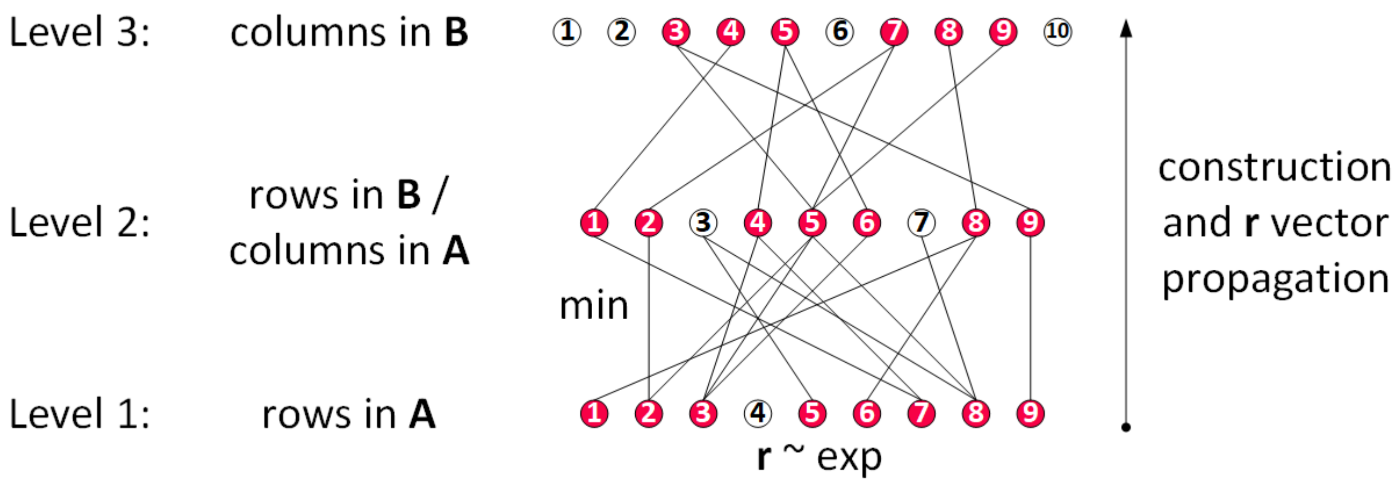
- **Layered Graph**

O(rd +nnz(A,B))

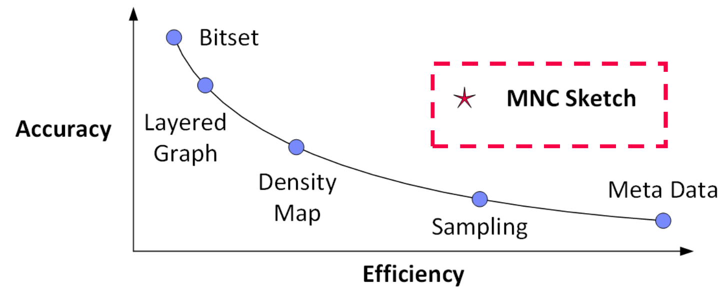
O(r(d +nnz(A,B)))

  - Construct layered graph for mm chain, where nodes represents rows/columns, and edges represent non-zeros
  - Assign vector r (variable size) to leafs, propagate via min(r1,…,rn), and estimate column counts as

$$\hat{s}_C = \left(\sum_{v \in \text{roots}} \frac{|\mathbf{r}_v| - 1}{\text{sum}(\mathbf{r}_v)} \right) / (ml),$$



Sparsity Estimation – MNC (Matrix Non-zero Count)



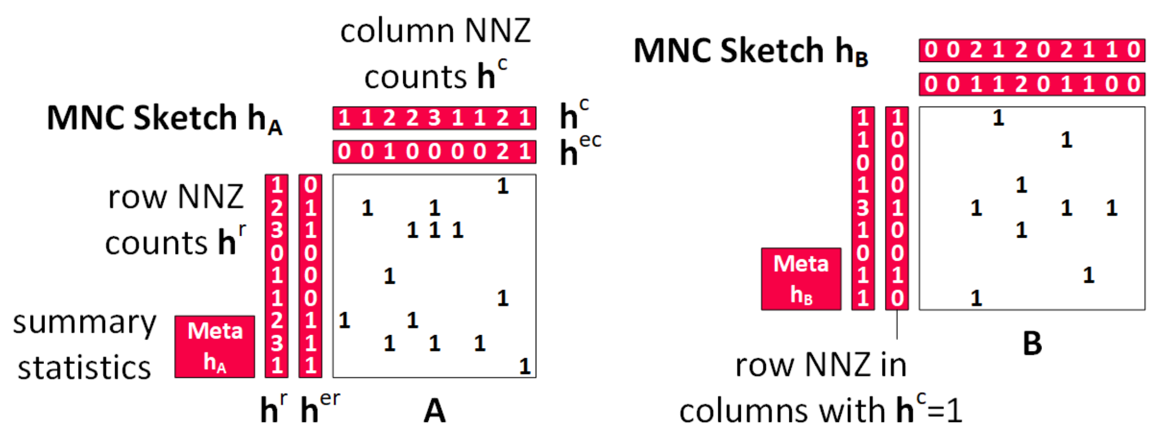
- **MNC Estimator (SystemML, SystemDS)**
  - Create MNC sketch for inputs A and B
  - Exact nnz estimates if structure

    $$s_C \equiv \hat{s}_C = \mathbf{h}^c_A \, \mathbf{h}^r_B / (ml) \; \textit{if} \; \max(\mathbf{h}^r_A) \leq 1 \vee \max(\mathbf{h}^c_B) \leq 1.$$
  - Partial exact/approximate nnz estimates, or fallbacks otherwise

O(d)

O(d +nnz(A,B))

[Johanna Sommer, Matthias Boehm, Alexandre V. Evfimievski, Berthold Reinwald, Peter J. Haas: MNC: Structure-Exploiting Sparsity Estimation for Matrix Expressions. **SIGMOD 2019**]



  - Support for other operations (reorganizations, elementwise ops)
  - Propagate sketches via sparsity estimation and scaling of input sketches

Memory Estimates and Costing

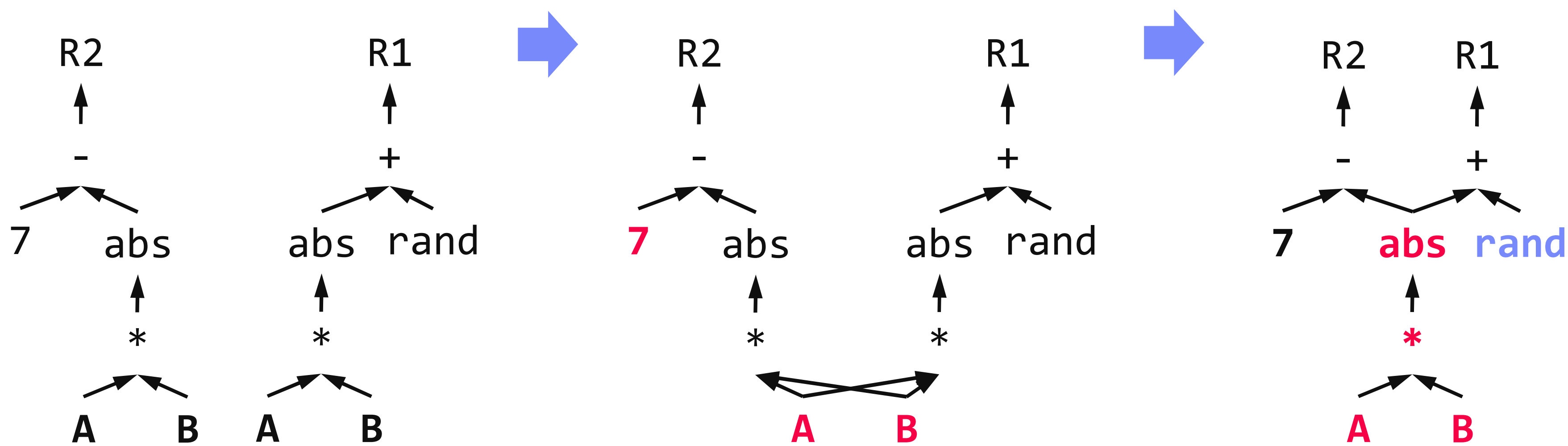
- **Memory Estimates**
  - **Matrix memory estimate :=** based on the dimensions and sparsity, decide the format (sparse, dense) and estimate the size in memory
  - **Operation memory estimate :=** input, intermediates, output
  - **Worst-case sparsity estimates** (**upper bound**)
- **Costing at Logical vs Physical Level**
  - Costing at physical level takes physical ops and rewrites into account but is much more costly
- **Costing Operators vs Plans**
  - Costing plans requires heuristics for **# iterations**, **branches** in general
- **Analytical vs Trained Cost Models**
  - Analytical: **estimate I/O and compute workload**
  - Training: **build regression models** for individual ops

Rewrites and Operator Selection

Traditional PL Rewrites

```
R1 = 7 – abs(A * B)
R2 = abs(A * B) + rand()
```

- **#1 Common Subexpression Elimination (CSE)**
  - **Step 1:** Collect and **replace leaf nodes** (variable reads and literals)
  - **Step 2:** recursively **remove CSEs bottom-up** starting at the leafs by merging nodes with same inputs (**beware non-determinism**)



Topic #10 Common Subexpression Elimination & Constant Folding

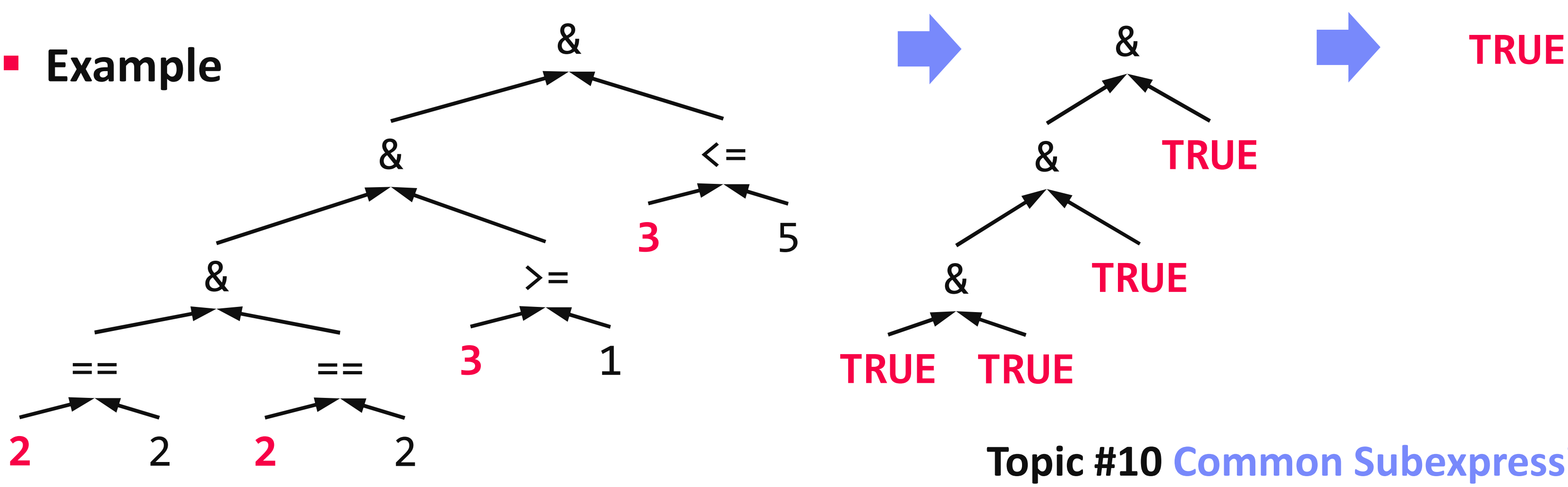
Traditional PL Rewrites, cont.

- **#2 Constant Folding**
  - Applied **after constant propagation**
  - Fold sub-DAGs over literals into a single literal
  - Handling of one-side constants
  - Approach: **recursively** compile and **execute runtime instructions**

```
ncol_y == 2 & dist_type == 2
  & link_type >= 1 & link_type <= 5
```

```
2 == 2 & 2 == 2 & 3 >= 1 & 3 <= 5
```

- **Example**



Topic #10 Common Subexpression Elimination & Constant Folding

Traditional PL Rewrites, cont.

- **#3 Branch Removal**
  - Applied after **constant propagation** and **constant folding**
  - **True predicate:** replace if statement block with if-body blocks
  - **False predicate:** replace if statement block with else-body block, or remove

- **#4 Merge of Statement Blocks**
  - **Merge sequences of unconditional blocks** (s1,s2) into a single block
  - Connect matching DAG roots of s1 with DAG inputs of s2

LinregDS (Direct Solve)

```
X = read($1);
y = read($2);
intercept = 0;
lambda = 0.001;
...        FALSE
if( intercept == 1 ) {
  ones = matrix(1, nrow(X), 1);
  X = cbind(X, ones);
}
I = matrix(1, ncol(X), 1);
A = t(X) %*% X + diag(I)*lambda;
b = t(X) %*% y;
beta = solve(A, b);
...
write(beta, $4);
```

Vectorization and Incremental Computation

- **Loop Transformations** (e.g., OptiML, SystemML)
  - **Loop vectorization**
  - Loop hoisting

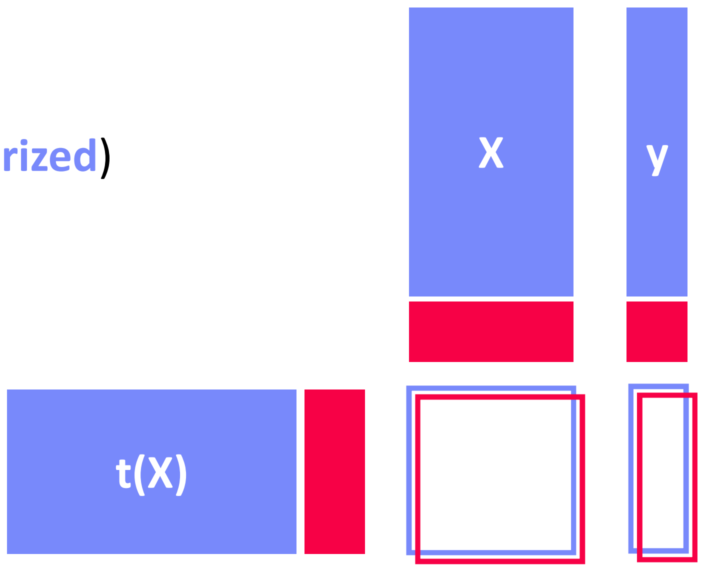
```
for(i in a:b)
   X[i,1] = Y[i,2] + Z[i,1]
```

→

```
X[a:b,1] = Y[a:b,2] + Z[a:b,1]
```

- **Incremental Computations**
  - **Delta update rules** (e.g., LINVIEW, factorized)
  - Incremental iterations (e.g., Flink)

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



Update-in-place

- **Example: Cumulative Aggregate via Strawman Scripts**
  - **But:** R, Julia, Matlab, SystemML, NumPy all provide cumsum(X), etc

```
cumsumN2 = function(Matrix[Double] A)
  return(Matrix[Double] B)
{
  B = A; csums = matrix(0,1,ncol(A));
  for( i in 1:nrow(A) ) {
    csums = csums + A[i,];
    B[i,] = csums;
  }
}
```

copy-on-write → O(n^2)

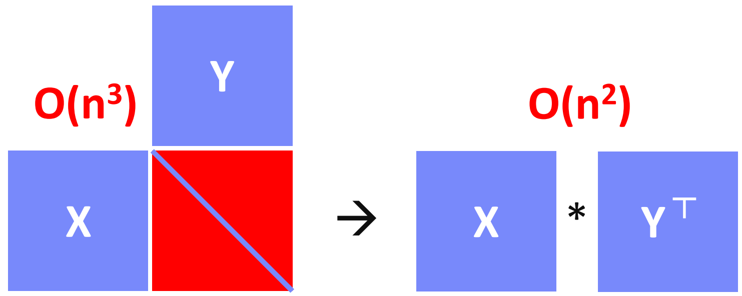
```
cumsumNlogN = function(Matrix[Double] A)
  return(Matrix[Double] B)
{
  B = A; m = nrow(A); k = 1;
  while( k < m ) {
    B[(k+1):m,] = B[(k+1):m,] + B[1:(m-k),];
    k = 2 * k;
  }
}
```

→ O(n log n)

- **Update in place** (w/ O(n))
  - **SystemML:** via rewrites (**why do the above scripts apply?**)
  - **R:** via reference counting
  - **Julia:** by default, otherwise explicit **B = copy(A)** necessary

Static and Dynamic Simplification Rewrites

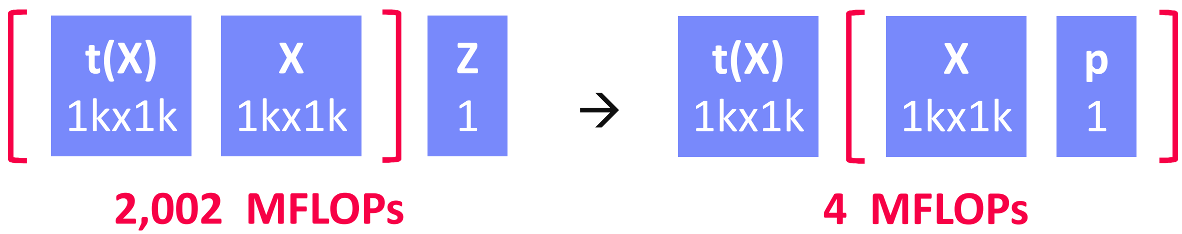
- **Examples of Static Rewrites**
  - `t(X) %*% y → t(t(y) %*% X)`
  - `trace(X%*%Y) → sum(X*t(Y))`
  - `sum(X+Y) → sum(X)+sum(Y)`
  - `(X%*%Y)[7,3] → X[7,]%*%Y[,3]`
  - `sum(t(X)) → sum(X)`
  - `rand()*7 → rand(,min=0,max=7)`
  - `sum(lambda*X) → lambda * sum(X);`



- **Examples of Dynamic Rewrites**
  - `X[a:b,c:d]=Y → X = Y iff dims(X)=dims(Y)`
  - `(...) * X → matrix(0, nrow(X), ncol(X)) iff nnz(X)=0`
  - `sum(X^2) → t(X)%*%X; rowSums(X) → X iff ncol(X)=1`
  - `sum(X%*%Y) → sum(t(colSums(X))*rowSums(Y)) iff ncol(X)>t`

Matrix Multiplication Chain Optimization

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



Size propagation and sparsity estimation

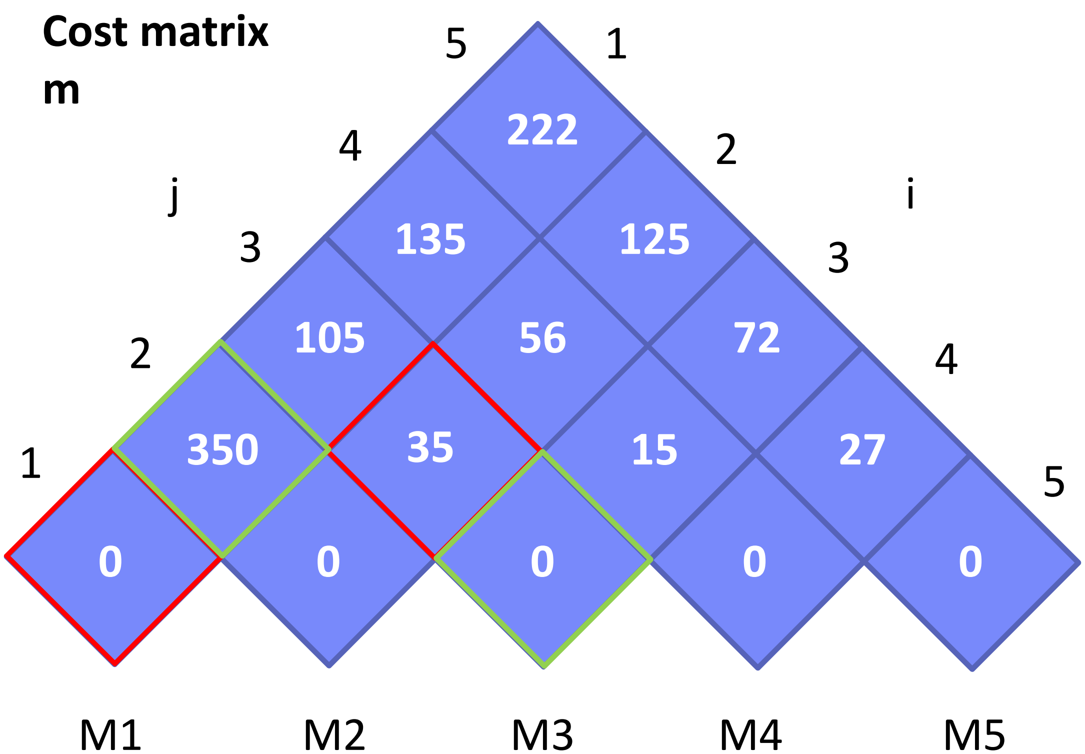
- **Search Space Characteristics**
  - Naïve exhaustive: Catalan numbers → $\Omega(4^n / n^{3/2})$)
  - DP applies: (1) optimal substructure, (2) overlapping subproblems
  - Textbook DP algorithm: $\Theta(n^3)$ time, $\Theta(n^2)$ space
    - Examples: SystemML '14, RIOT ('09 I/O costs), SpMachO ('15 sparsity)
  - Best known algorithm ('81): $O(n \log n)$

    [T. C. Hu, M. T. Shing: Computation of Matrix Chain Products. Part II. **SIAM J. Comput.** 13(2): 228-251, 1984]

n	C_{n-1}
5	14
10	4,862
15	2,674,440
20	1,767,263,190
25	1,289,904,147,324

Matrix Multiplication Chain Optimization, cont.

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



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)

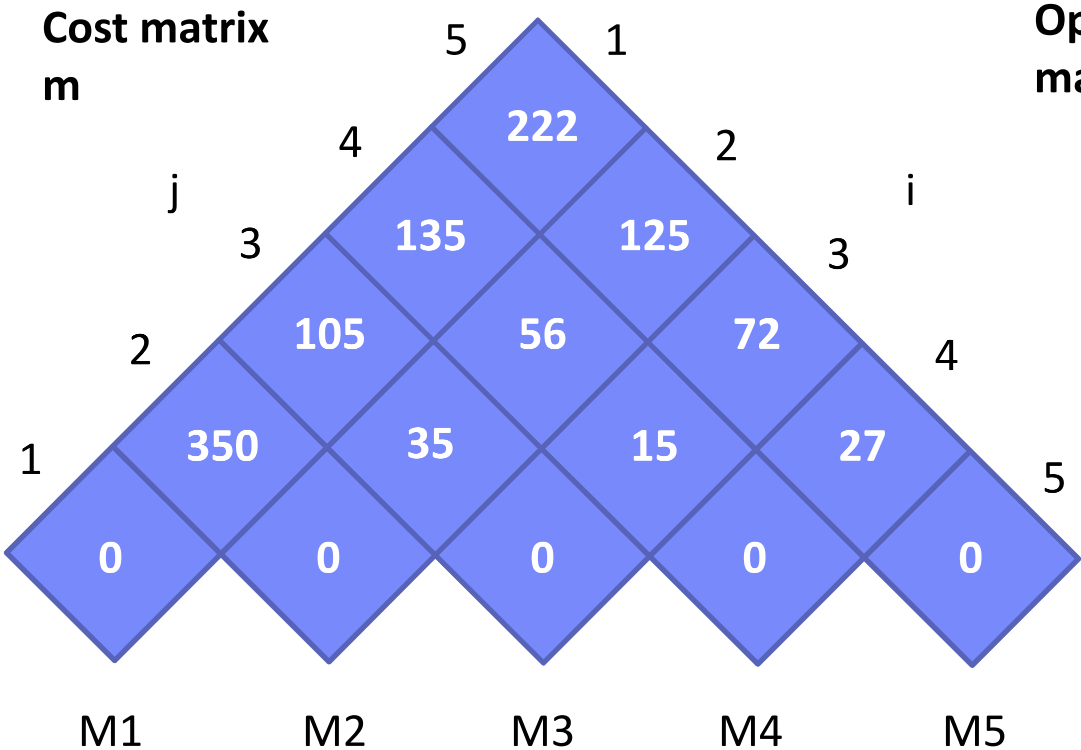
= min(
105,
400)

[T. H. Cormen, C. E. Leiserson, R. L. Rivest, C. Stein: Introduction to Algorithms, Third Edition, **The MIT Press**, pages 370-377, 2009]

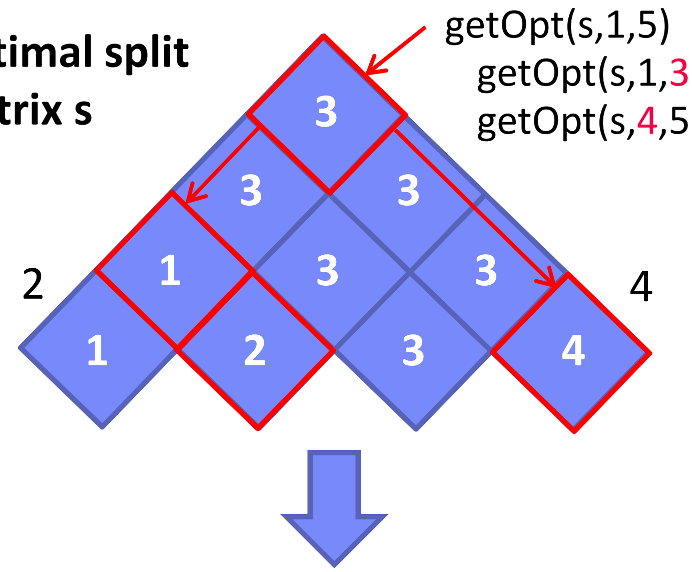
Matrix Multiplication Chain Optimization, cont.

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))

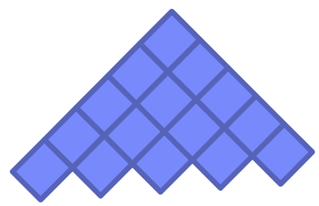
→ ((M1 (M2 M3)) (M4 M5))

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

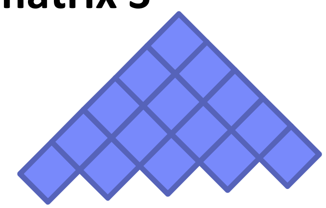
Matrix Multiplication Chain Optimization, cont.

- **Sparsity-aware mmchain Opt**
  - Additional n x n sketch matrix e

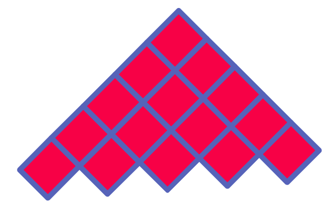
Cost matrix M



Optimal split matrix S

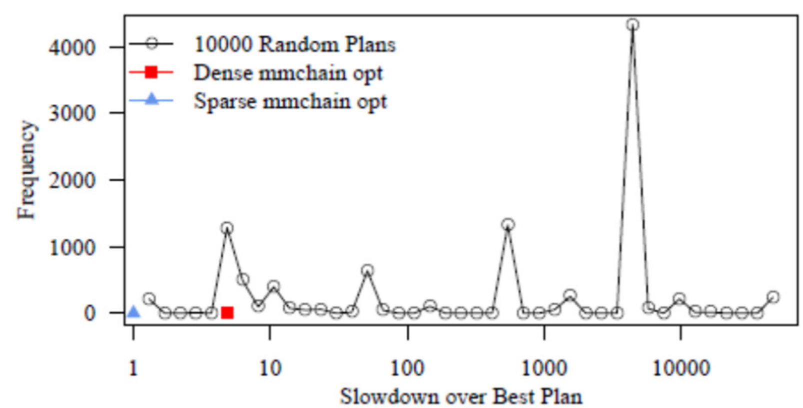


Sketch matrix E



  - Sketch propagation for optimal subchains (currently for all chains)
  - Modified cost computation via MNC sketches (**number FLOPs for sparse** instead of dense mm)

$$C_{i,j} = \min_{k\in[i,j-1]} \begin{pmatrix} C_{i,k} + C_{k+1,j} \\ + \mathbf{E_{i,k}.h^c E_{k+1,j}.h^r} \end{pmatrix}$$



Topic #2: Sparsity-Aware Optimization of Matrix Product Chains (incl DAGs)

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)

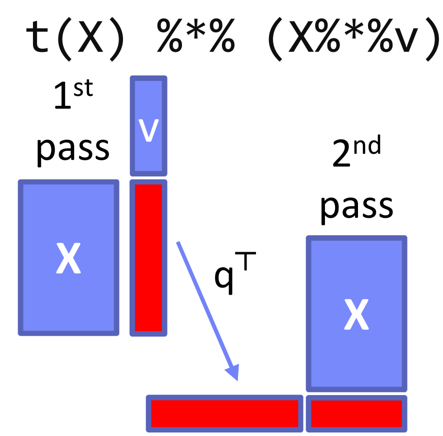
- **Partitioning**
  - Many frameworks exploit co-partitioning for efficient joins
  - **#1 Partitioning-exploiting operators** (SystemML, Emma, Samsara)
  - **#2 Inject partitioning to avoid shuffle per iteration** (SystemML)
  - **#3 Plan-specific data partitioning** (SystemML, Dmac, Kasen)

- **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

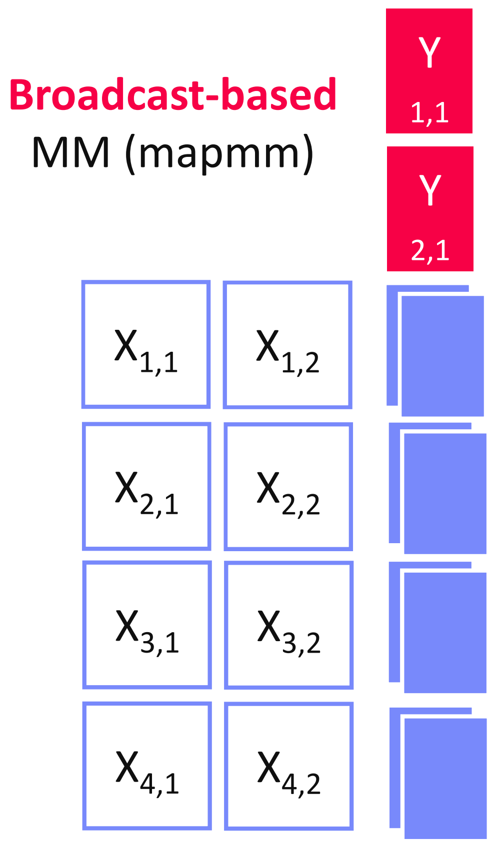
- **Common Selection Criteria**
  - **Data and cluster characteristics** (e.g., data size/shape, memory, parallelism)
  - **Matrix/operation properties** (e.g., diagonal/symmetric, sparse-safe ops)
  - **Data flow properties** (e.g., co-partitioning, co-location, data locality)
- **#0 Local Operators**
  - SystemML mm, tsmm, mmchain; Samsara/Mllib local
- **#1 Special Operators** (special patterns/sparsity)
  - SystemML **tsmm**, **mapmmchain**; Samsara AtA

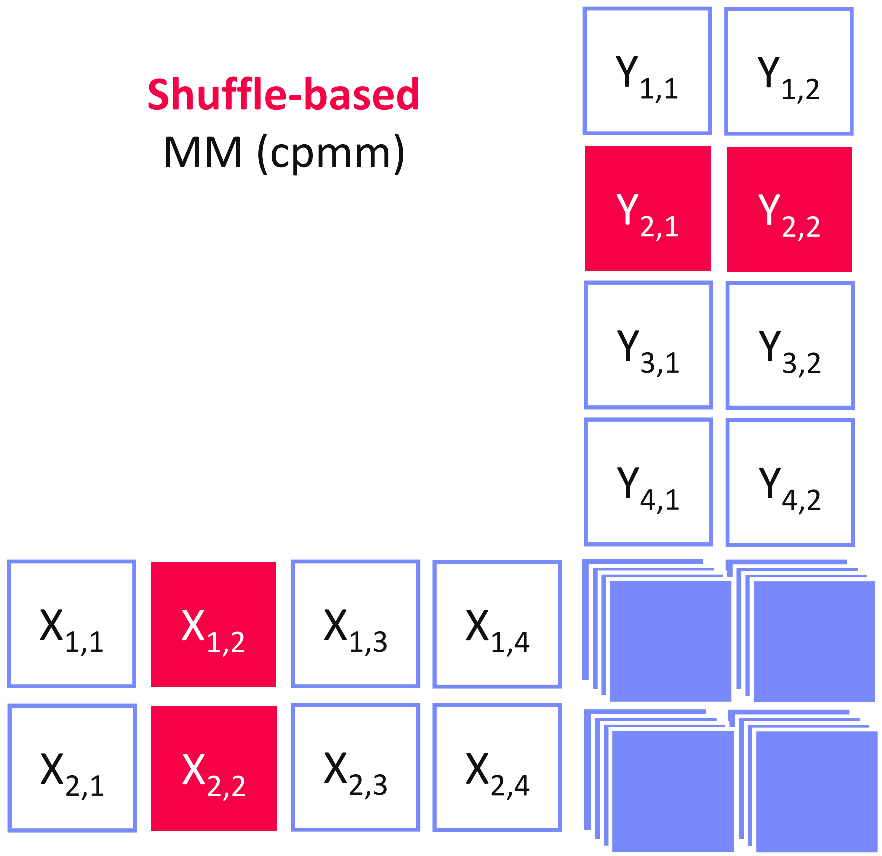


- **#2 Broadcast-Based Operators** (aka broadcast join)
  - SystemML **mapmm**, **mapmmchain**
- **#3 Co-Partitioning-Based Operators** (aka improved repartition join)
  - SystemML **zipmm**; Emma, Samsara OpAtB
- **#4 Shuffle-Based Operators** (aka repartition join)
  - SystemML **cpmm**, **rmm**; Samsara OpAB

Physical Operator Selection, cont.

- **Examples Distributed MM Operators**

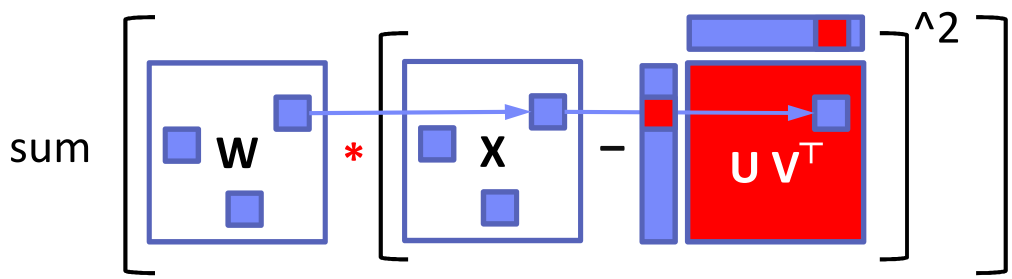




Sparsity-Exploiting Operators

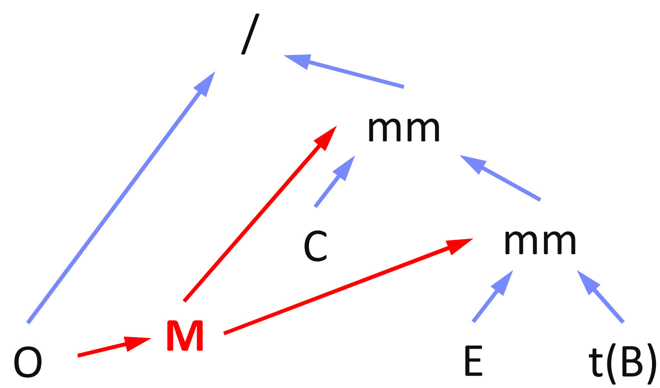
- **Goal:** Avoid dense intermediates and unnecessary computation
- **#1 Fused Physical Operators**
  - E.g., SystemML [PVLDB'16] wsloss, wcemm, wdivmm
  - Selective computation over non-zeros of "sparse driver"

`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))`



Conclusions

- **Summary**
  - Basic compilation overview
  - Size inference and cost estimation (**foundation for optimization**)
  - **Rewrites and operator selection**
- **Impact of Size Inference and Costs**
  - Advanced optimization of linear algebra programs requires size inference for cost estimation and validity constraints
- **Ubiquitous Rewrite Opportunities**
  - Linear algebra programs have plenty of room for optimization
  - Potential for changed asymptotic behavior
- **Next Lectures**
  - **04 Operator Fusion and Runtime Adaptation** [Apr 05] (advanced compilation)

Backup: Programming/Analysis Projects

Example Projects (to be refined by Mar 29)

- **#1 Auto Differentiation**
  - Implement auto differentiation for deep neural networks
  - Integrate auto differentiation framework in compiler or runtime
- **#2 Sparsity-Aware Optimization of Matrix Product Chains**
  - Extend DP algorithm for DAGs and other operations
- **#3 Parameter Server Update Schemes**
  - New PS update schemes: e.g., stale-synchronous, Hogwild!
  - Language and local/distributed runtime extensions
- **#4 Extended I/O Framework for Other Formats**
  - Implement local readers/writers for NetCDF, HDF5, libsvm, and/or Arrow
- **#5 LLVM Code Generator**
  - Extend codegen framework by LLVM code generator
  - Native vector library, native operator skeletons, JNI bridge
- **#6 Reproduce Automated Label Generation** (analysis)

Example Projects, cont.

- **#7 Data Validation Scripts**
  - Implement recently proposed integrity constraints
  - Write DML scripts to check a set of constraints on given dataset
- **#8 Data Cleaning Primitives**
  - Implement scripts or physical operators to perform data imputation and data cleaning (find and remove/fix incorrect values)
- **#9 Data Preparation Primitives**
  - Extend `transform` functionality for distributed binning
  - Needs to work in combination w/ dummy coding, recoding, etc
- **#10 Common Subexpression Elimination & Constant Folding**
  - Exploit commutative common subexpressions
  - One-shot constant folding (avoid compile overhead)
- **#11 Repartition joins and binary ops without replication**
  - Improve repartition mm and binary ops by avoiding unnecessary replication