Architecture of ML Systems 03 Size Inference and Rewrites

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Announcements/Org

- **#1 Video Recording**
  - Link in **TeachCenter** & **TUbe** (lectures will be public)
  - https://tugraz.webex.com/meet/m.boehm

- **#2 AMLS Project Selections**
  - **Project selection** by **Mar 31** (see **Lecture 02** for four alternatives)
  - Discussion current status project selection (~6 students assigned)

https://issues.apache.org/jira/secure/Dashboard.jspa?selectPageId=12335852#Filter-Results/12365413
https://mboehm7.github.io/teaching/ss22_amls/AMLS_DAPHNE_projects.pdf
http://sigmod2022contest.eastus.cloudapp.azure.com/index.shtml
https://mboehm7.github.io/teaching/ss22_amls/AMLS_2022_Exercise.pdf

Agenda

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

SystemDS, and several other ML systems

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

PL → **DB** → **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], **TensorFlow** [OSDI'16] **Mahout Samsara** [MLSystems'16], **Dask**
  - Examples w/ control structures: **Weld** [CIDR'17], **OptiML** [ICML'11], **Emma** [SIGMOD'15]
- **#3 Program Compilation** (entire program)
  - Examples: **SystemML** [ICDE'11/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");
```

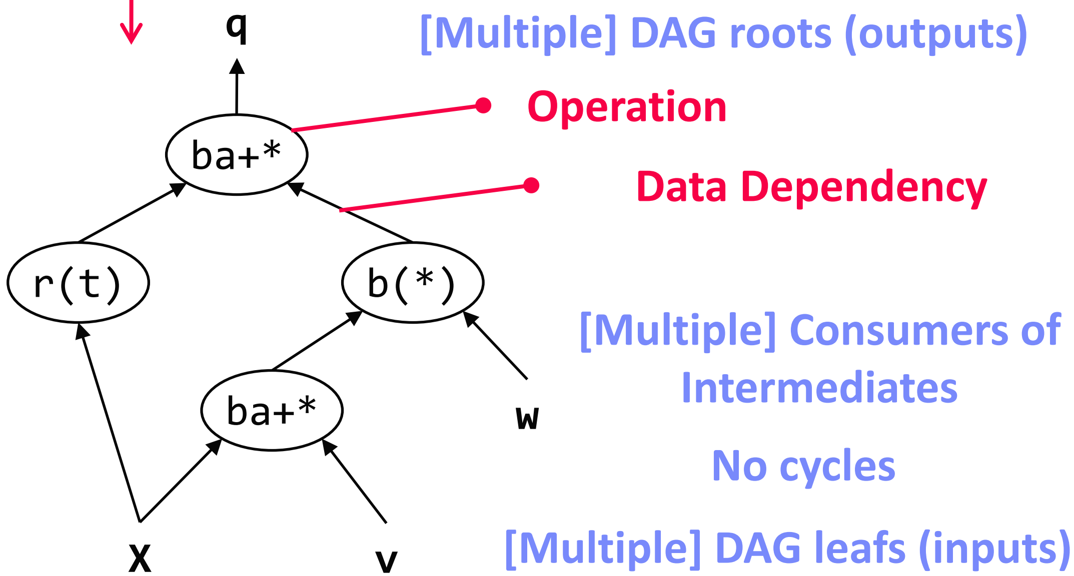
ML Program Compilation / Graphs

- **Script:**

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

Statement Block Hierarchy

- **Operator DAG** (today's lecture)
  - a.k.a. "graph" (data flow graph)
  - a.k.a. intermediate representation (IR)



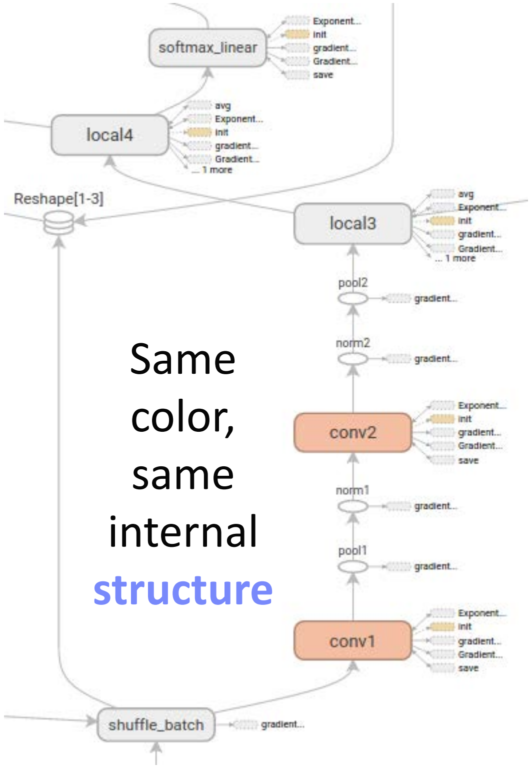
- **Runtime Plan**
  - Compiled runtime plans
    Interpreted plans

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

ML Program Compilation / Graphs, cont.

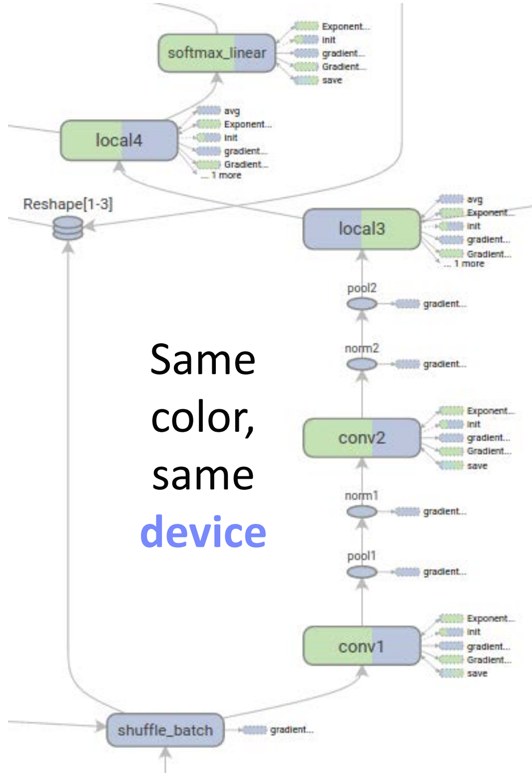
- **Example TF TensorBoard**

(Node) **Structure View**



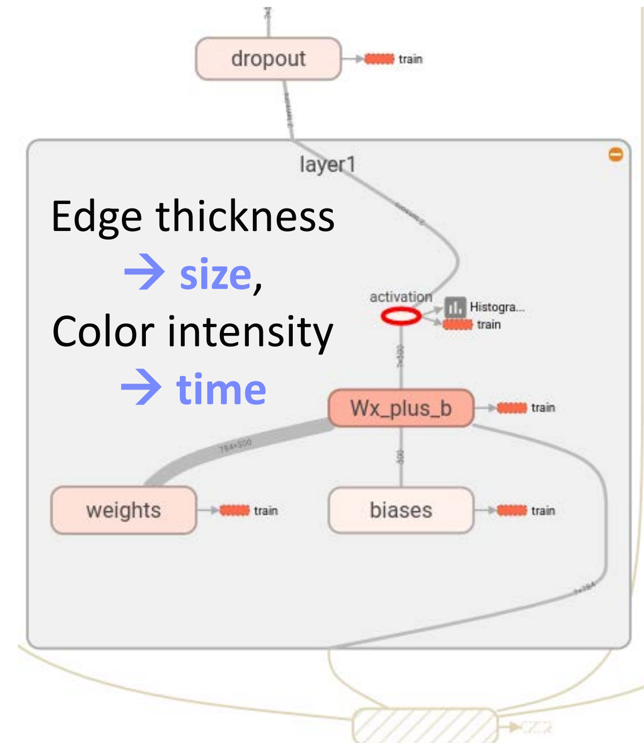
Same color, same internal **structure**

Device View (CPU, GPU)



Same color, same **device**

Tensor Shapes and **Runtime Statistics** (time, mem)



Edge thickness → **size**, Color intensity → **time**

[https://github.com/tensorflow/tensorboard/blob/master/docs/r1/graphs.md]

Compilation Chain

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

Script

Language
- **Parsing** (syntactic analysis)
- **Live Variable Analysis**
- **Validate** (semantic analysis)

HOPs
- **Construct HOP DAGs**
- **Multiple Rounds**
  - **Static/Dynamic Rewrites**
  - **Intra-/Inter-Procedural Analysis**
- **Static/Dynamic Rewrites**
- **Compute Memory Estimates**

LOPs
- **Construct LOP DAGs** (incl operator selection, hop-lop rewrites)
- **Generate Runtime Program**

Execution Plan

Dynamic Recompilation (lecture 04)

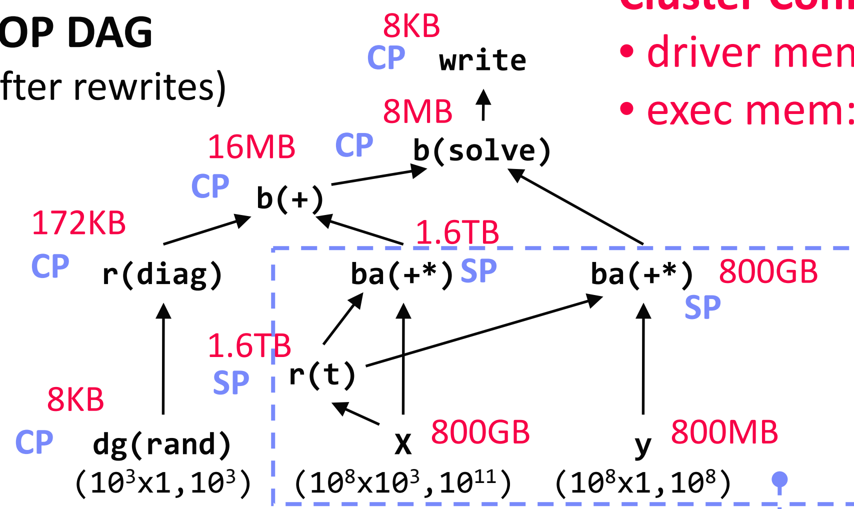
Recap: Basic HOP and LOP DAG Compilation

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: $10^8 \times 1, 10^8$

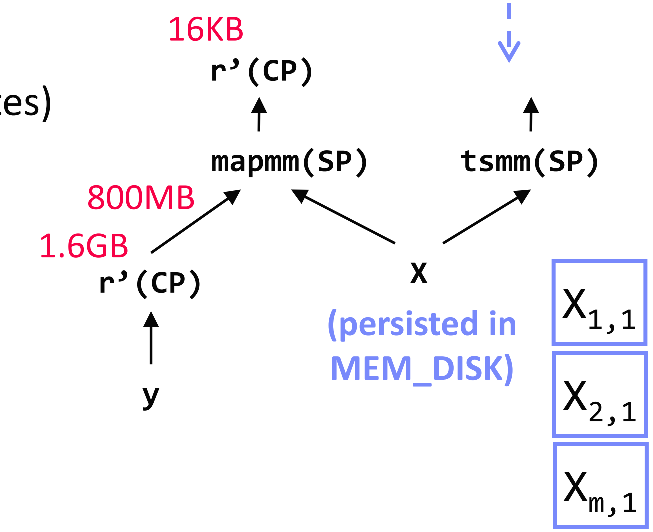
HOP DAG
(after rewrites)



Cluster Config:

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

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

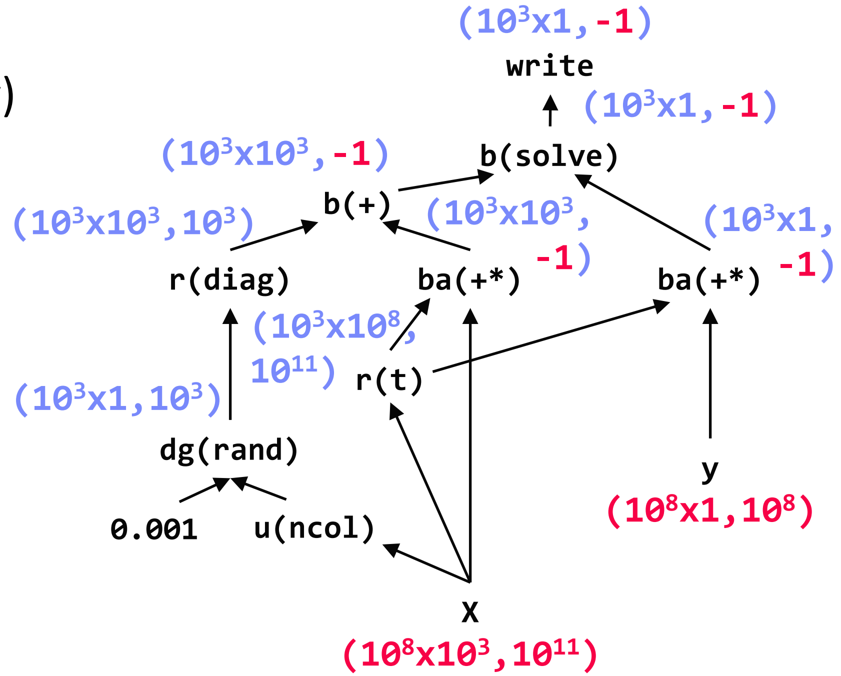
Crucial for Generating Valid Execution Plans
& Cost-based Optimization

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);
```

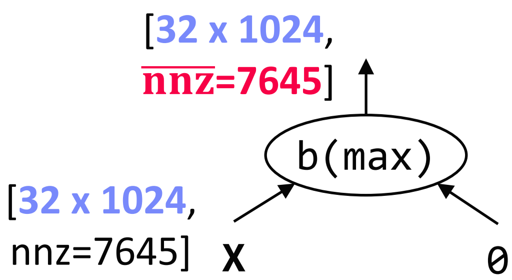
- **Principle: Worst-case Assumption**
  - Necessary for guarantees (memory)
- **DAG-level Size Propagation**
  - **Input:** Size information for leaves
  - **Output:** size information for all operators, -1 if still unknown
  - **Propagation based on operation semantics** (single bottom-up pass over DAG)



Constant and Size Propagation, cont.

- **Example SystemDS**
  - Hop `refreshSizeInformation()` (exact)
  - Hop `inferOutputCharacteristics()`
  - Compiler explicitly differentiates between exact and other size information
  - **Note:** ops like aggregate, ctable, rmEmpty challenging but w/ upper bounds

Example Relu
(rectified linear unit)



- **Example TensorFlow**
  - Operator registrations
  - Shape inference functions

```
REGISTER_OP("Relu")
    .Input("features: T")
    .Output("activations: T")
    .Attr("T: {realnumbertype, qint8}")
    .SetShapeFn(
      shape_inference::UnchangedShape)
```

[Alex Passos: Inside TensorFlow – Eager execution runtime, https://www.youtube.com/watch?v=qjx65mD6nrc, Dec 2019]

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);
}...
eval(“foo”, X)
```

1M x 1

1M x 2

? x ?

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

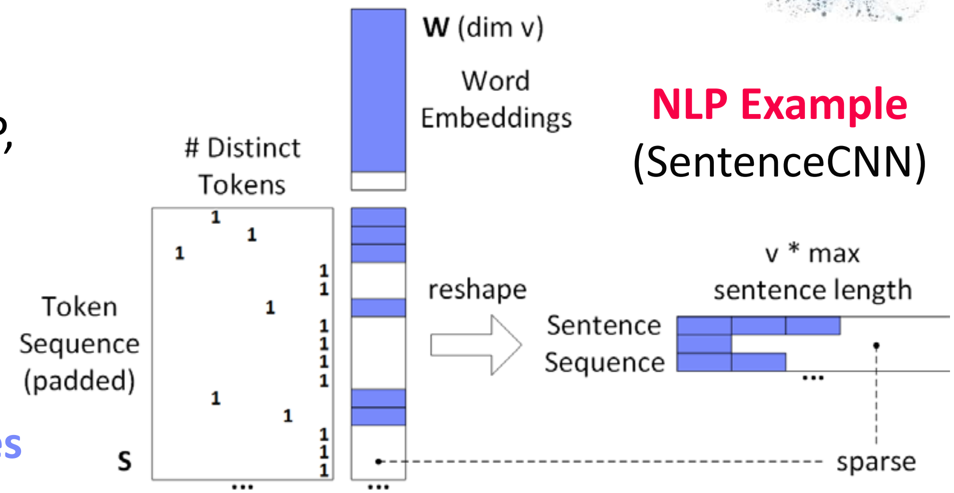
- **Additional IPA Passes (selection)**
  - **Inline functions** (single statement block, small)
  - **Dead code elimination** and simplification rewrites
  - Remove unused functions & flag recompile-once

```
//create ordered list of IPA passes
_passes = new ArrayList<>();
_passes.add(new IPAPassRemoveUnusedFunctions());
_passes.add(new IPAPassFlagFunctionsRecompileOnce());
_passes.add(new IPAPassRemoveUnnecessaryCheckpoints());
_passes.add(new IPAPassRemoveConstantBinaryOps());
_passes.add(new IPAPassPropagateReplaceLiterals());
_passes.add(new IPAPassInlineFunctions());
_passes.add(new IPAPassEliminateDeadCode());
_passes.add(new IPAPassFlagNonDeterminism());
//note: apply rewrites last because statement block rewrites
//might merge relevant statement blocks in special cases, which
//would require an update of the function call graph
_passes.add(new IPAPassForwardFunctionCalls());
_passes.add(new IPAPassApplyStaticAndDynamicHopRewrites());
```

Sparsity Estimation Overview

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

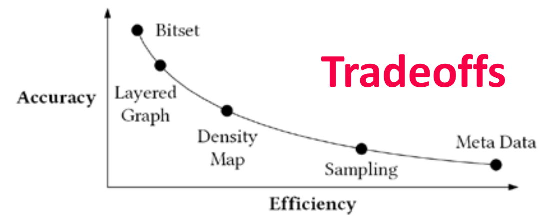
NLP Example (SentenceCNN)



- **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 = nnz(C)/(ml) of matrix product C = A B; d=max(m,n,l)
  - **Assumptions**
    - **A1:** No cancellation errors
    - **A2:** No not-a-number (NaN)

Common assumptions
➔ **Boolean matrix product**

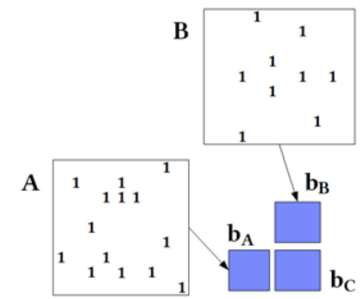
Sparsity Estimation – Estimators



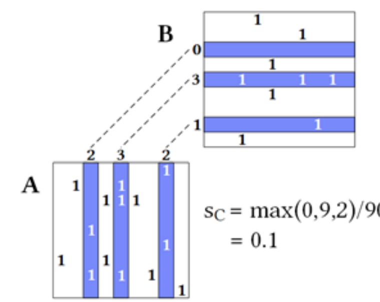
- **#1 Naïve Metadata Estimators**
  - Derive the output sparsity solely from the sparsity of inputs (e.g., SystemDS)

$$\hat{s}_C = 1 - (1 - s_A s_B)^n$$
$$\hat{s}_C = \min(1, s_A n) \cdot \min(1, s_B n)$$

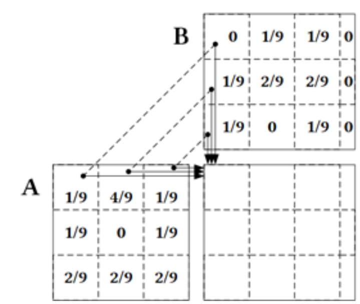
- **#2 Naïve Bitset Estimator**
  - Convert inputs to bitsets, perform Boolean mm (per row)
  - Examples: SciDB [SSDBM'11], NVIDIA cuSparse, Intel MKL



- **#3 Sampling**
  - Take a sample of aligned columns of A and rows of B
  - Sparsity estimated via max of count-products
  - Examples: MatFast [ICDE'17], improvements in paper

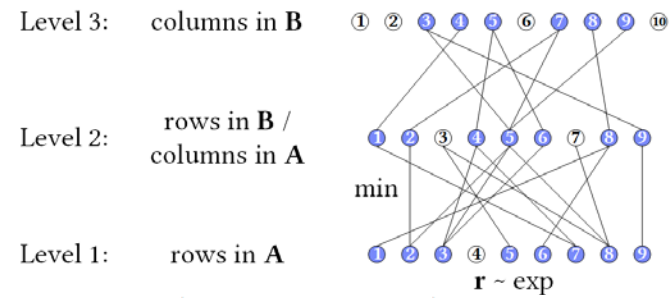


- **#4 Density Map**
  - Store sparsity per b x b block (default b = 256)
  - MM-like estimator (average case estimator for *, probabilistic propagation $s_A + s_B - s_A s_B$ for +)
  - Example: SpMacho [EDBT'15], AT Matrix [ICDE'16]



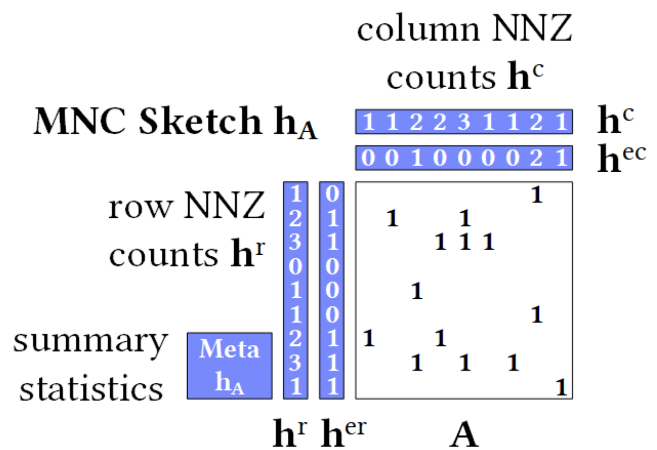
Sparsity Estimation – Estimators, cont.

- **#5 Layered Graph** [J.Comb.Opt.'98]
  - Nodes: rows/columns in mm chain
  - Edges: non-zeros connecting rows/columns
  - Assign r-vectors ~ exp and propagate via min
  - Estimate over roots (output columns)



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

- **#6 MNC Sketch** (Matrix Non-zero Count)
  - Create MNC sketch for inputs A and B
  - Exploitation of structural properties (e.g., 1 non-zero per row, row sparsity)
  - Support for matrix expressions (reorganizations, elementwise ops)
  - Sketch propagation and estimation



$$s_C = \hat{s}_C = h_A^c h_B^r / (ml)$$
if $\max(h_A^r) \leq 1 \lor \max(h_B^c) \leq 1$

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

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**)
- **#1 Costing at Logical vs Physical Level**
  - Costing at physical level takes physical ops and rewrites into account but is much more costly
- **#2 Costing Operators/Graphs vs Plans**
  - Costing plans requires heuristics for **# iterations**, **branches** in general
- **#3 Analytical vs Trained Cost Models**
  - Analytical: **estimate I/O and compute workload**
  - Training: **build regression models** for individual ops

A Personal War Story

Physical, Plans, **Trained** [**PVLDB 2014**]

Physical, Plans, Analytical [**SIGMOD 2015**]

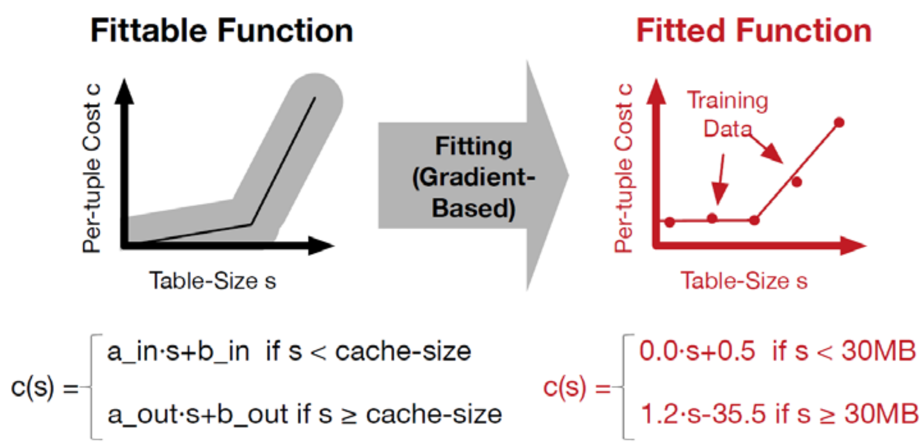
Logical, Graphs, Analytical [**PVDLB 2018**]

Excursus: Differentiable Programming

- **Overview Differentiable Programming**
  - Adoption of auto differentiation concept from ML systems to PLs
  - Yann LeCun (Jan 2018)

"It's really very much like a regular prog[r]am, except it's parameterized, automatically differentiated, and trainable/optimizable."

- **Example DBMS Fitting**
  - Implement DBMS components as **differentiable functions**
  - E.g.: cost model components
  - Q: **What about guarantees** (memory, size)?



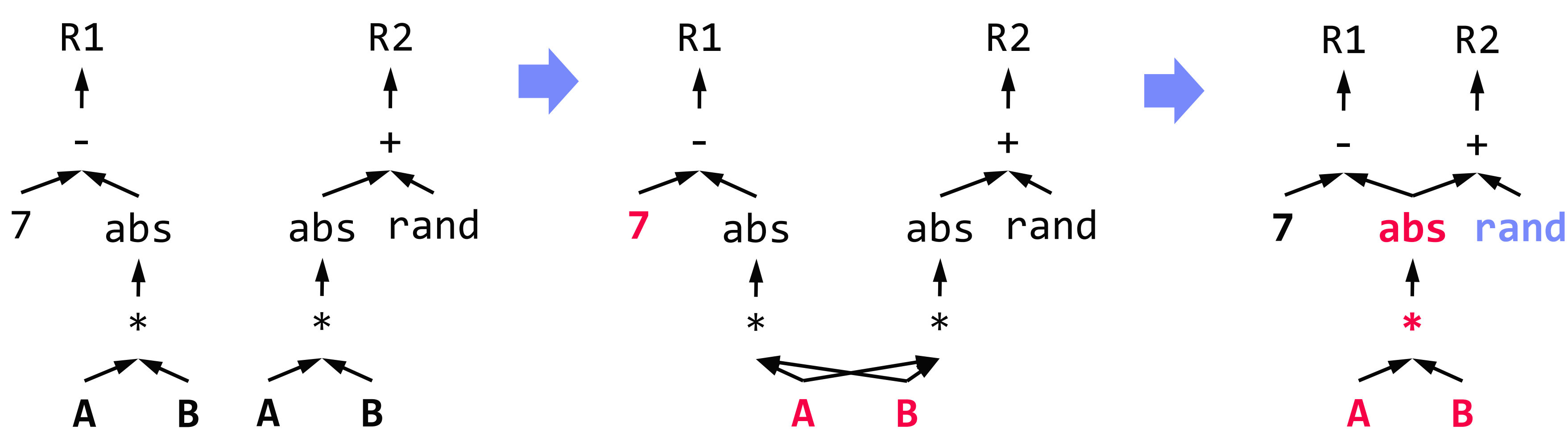
[Benjamin Hilprecht et al: DBMS Fitting: Why should we learn what we already know? **CIDR 2020**]

Rewrites and Operator Selection

Traditional PL Rewrites

- **#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**)
  - **Example:**

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



Traditional PL Rewrites, cont.

- **#2 Constant Folding**
  - After constant propagation, fold sub-DAGs over literals into a single literal
  - **Approach:** recursively compile and execute runtime instructions with special handling of one-side constants

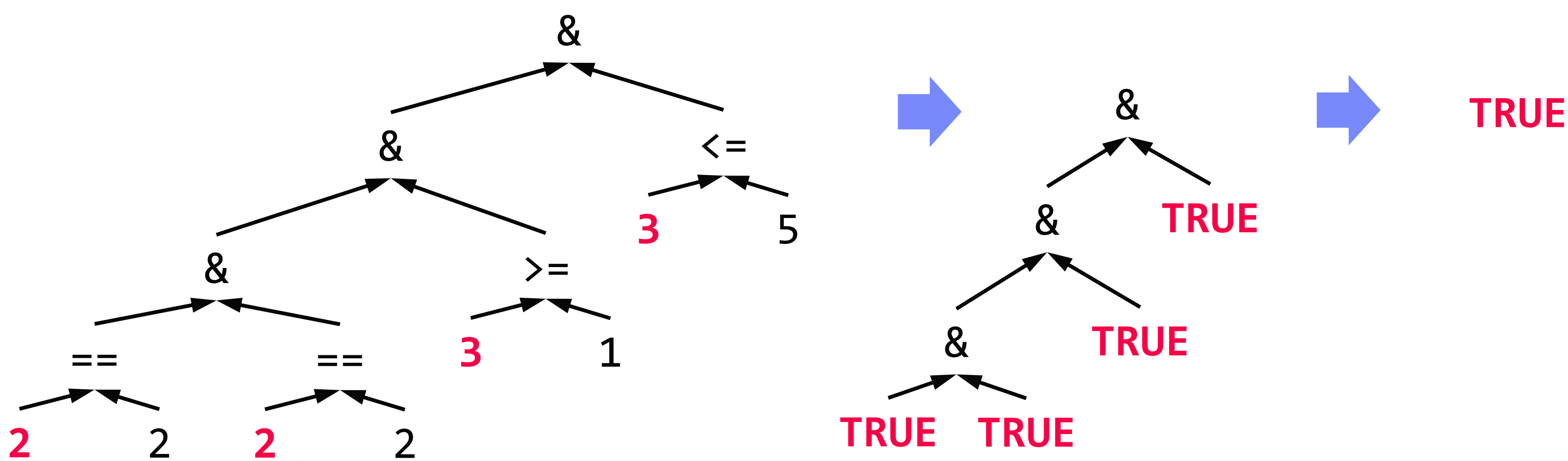
[A. V. Aho, M. S. Lam, R. Sethi, and J. D. Ullman. Compilers – Principles, Techniques, & Tools. Addison-Wesley, 2007]

Turing Award '20

  - **Example** (GLM Binomial probit):

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

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



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

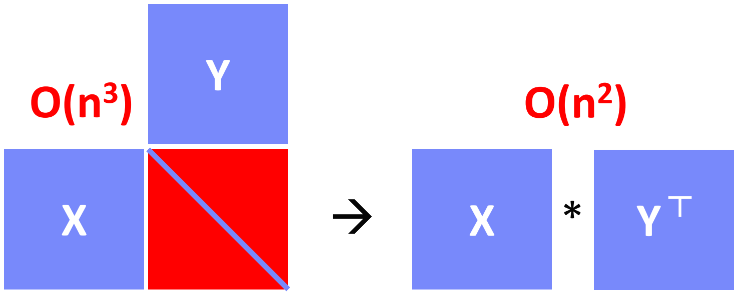
- **#4 Merge of Statement Blocks**
  - **Merge sequences of unconditional blocks** (s1,s2) into a single block
  - Connect matching DAG roots of s1 with DAG inputs of s2

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);
```

Static/Dynamic Simplification Rewrites

- **Examples of Static Rewrites**
  - `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);`



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

- **Examples of Dynamic Rewrites**
  - `t(X) %*% y        → t(t(y) %*% X)` s.t. costs
  - `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`

Static/Dynamic Simplification Rewrites, cont.

[Rasmus Munk Larsen, Tatiana Shpeisman: TensorFlow Graph Optimizations, **Guest Lecture Stanford 2019**]

- **TF Constant Push-Down**
  - `Add(c1,Add(x,c2)) → Add(x,c1+c2)`
  - `ConvND(c1*x,c2) → ConvND(x,c1*c2)`
- **TF Arithmetic Simplifications**
  - Flattening: a+b+c+d → `AddN(a, b, c, d)`
  - Hoisting: `AddN(x * a, b * x, x * c) → x * AddN(a+b+c)`
  - Reduce Nodes Numeric: x+x+x → `3*x`
  - Reduce Nodes Logicial: `!(x > y) → x <= y`
- **TF Broadcast Minimization**
  - `(M1+s1) + (M2+s2) → (M1+M2) + (s1+s2)`
- **TF Better use of Intrinsics**
  - `Matmul(Transpose(X), Y) → Matmul(X, Y, transpose_x=True)`

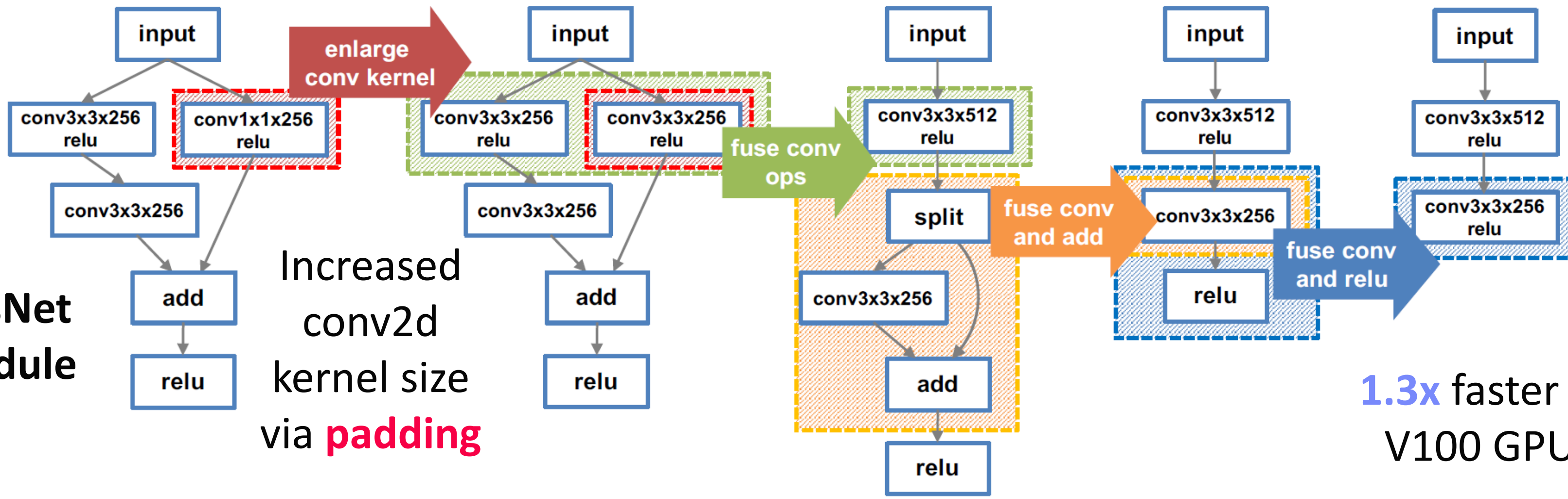
SystemML/SystemDS
`RewriteElementwise-MultChainOptimization`
(orders and collapses matrix, vector, scalar op chains)

Static/Dynamic Simplification Rewrites, cont.

- **Relaxed DNN Graph Substitutions**
  - Allow substitutions that preserve semantics, no matter if faster/slower
  - Backtracking search

[Zhihao Jia, James J. Thomas, Todd Warszawski, Mingyu Gao, Matei Zaharia, Alex Aiken: Optimizing DNN Computation with Relaxed Graph Substitutions. **MLSys 2019**]

ResNet module



Increased conv2d kernel size via **padding**

1.3x faster on V100 GPUs

- **Additional Algorithms**
  - Partial order of substitutions w/ pruning
  - Dynamic programming → substitutions

[Jingzhi Fang, Yanyan Shen, Yue Wang, Lei Chen: Optimizing DNN Computation Graph using Graph Substitutions. **PVLDB 13(11) 2020**]

Static/Dynamic Simplification Rewrites, cont.

- **Rewrites in PyTorch** (Torch Script JIT)
  - Misc: Canonicalization, erase number types and no-ops
  - Fuse linear, fuse relu, fuse graph pipeline
  - Peephole simplifications (e.g., for dtype management)
  - Inlining and loop unrolling
  - Concatenation and fusion rewrites:

PYTORCH

[https://github.com/pytorch/pytorch/blob/master/torch/csrc/jit/passes/subgraph_rewrite.cpp]

```
void SubgraphRewriter::RegisterDefaultPatterns() {
  // TODO: Add actual patterns (like Conv-Relu).
  RegisterRewritePattern(
      R"IR(
graph(%x, %w, %b):
  %c = aten::conv(%x, %w, %b)
  %r = aten::relu(%c)
  return (%r))IR",
      R"IR(
graph(%x, %w, %b):
  %r = aten::convrelu(%x, %w, %b)
  return (%r))IR",
      {{"r", "c"}});
}
```

subgraph_rewrite.cpp (extracted Mar 17, 2022)

Vectorization and Incremental Computation

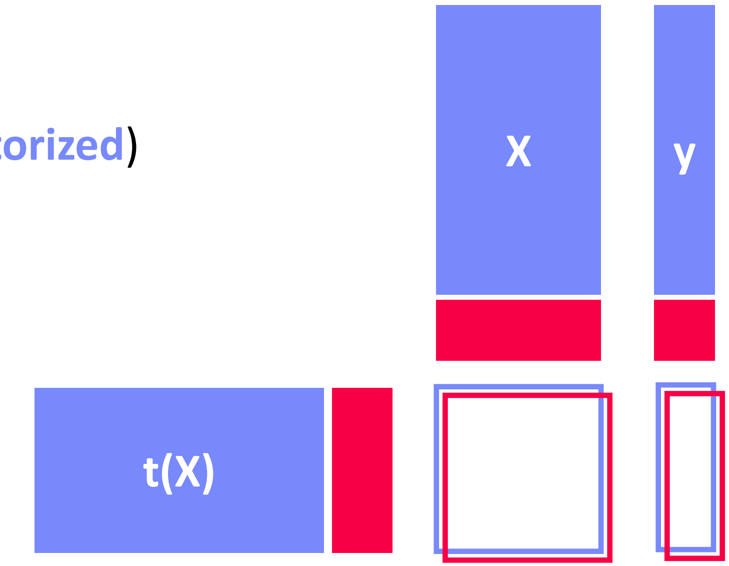
- **Loop Transformations** (e.g., **OptiML**, **SystemML**)
  - **Loop vectorization**
  - Loop hoisting

```
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
```



- **"Decremental"/Unlearning** (GDPR)

[Sebastian Schelter: "Amnesia" – Machine Learning Models That Can Forget User Data Very Fast. **CIDR 2020**]

[Sebastian Schelter, Stefan Grafberger, Ted Dunning: HedgeCut: Maintaining Randomised Trees for Low-Latency Machine Unlearning. **SIGMOD 2021**]

Update-in-place

- **Example: Cumulative Aggregate via Strawman Scripts**
  - **But:** R, Julia, Matlab, SystemDS, 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)

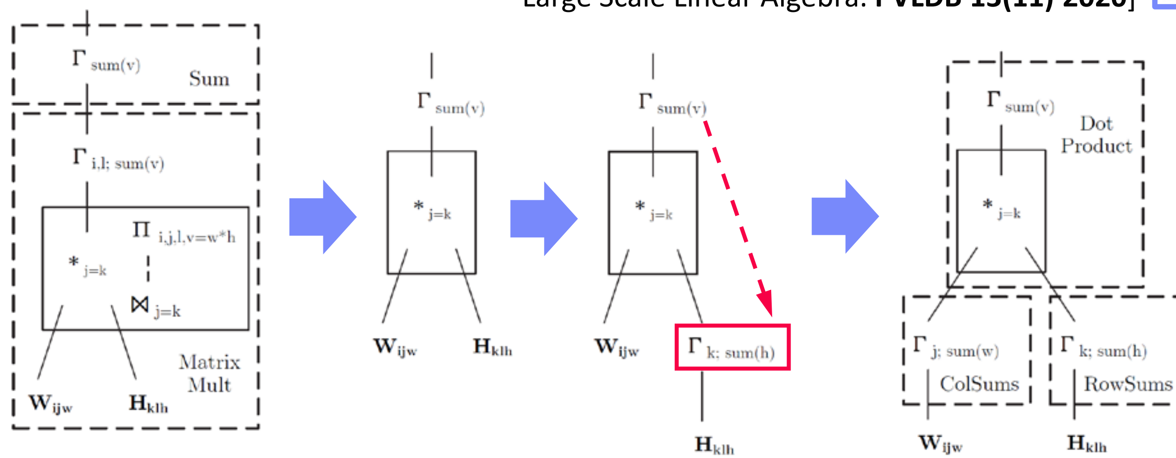
- **Update in place** (w/ O(n))
  - **SystemDS:** via rewrites (**why do the above scripts apply?**)
  - **R:** via reference counting
  - **Julia:** by default, otherwise explicit **B = copy(A)** necessary

Excursus: Automatic Rewrite Generation

- **SPOOF/SPORES (Sum-Product Optim.)**
  - **Break up** LA ops into basic ops (RA)
  - **Elementary sum-product/RA rewrites**
  - **Example:**
    `sum(W%*%H)`

[Tarek Elgamal et al: SPOOF: Sum-Product Optimization and Operator Fusion for Large-Scale Machine Learning. **CIDR 2017**]

[Yisu Remy Wang et al: SPORES: Sum-Product Optimization via Relational Equality Saturation for Large Scale Linear Algebra. **PVLDB 13(11) 2020**]

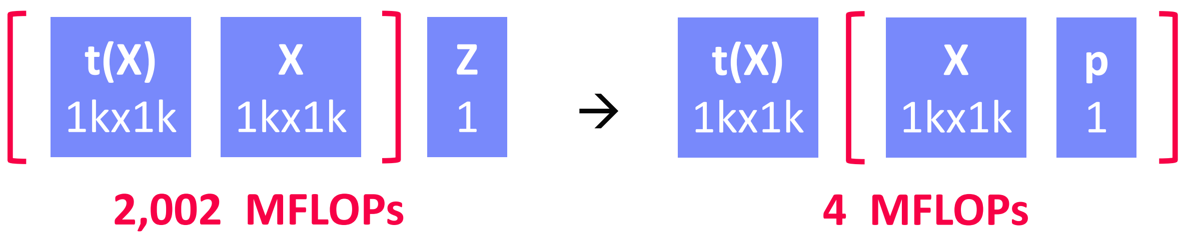


- **TASO (Super Optimization)**
  - List of operator specifications and properties
  - Automatic **generation/verification of graph substitutions** and **data layouts** via cost-based backtracking search

[Zhihao Jia et al: TASO: optimizing deep learning computation with automatic generation of graph substitutions. **SOSP 2019**]

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: O(n log n)

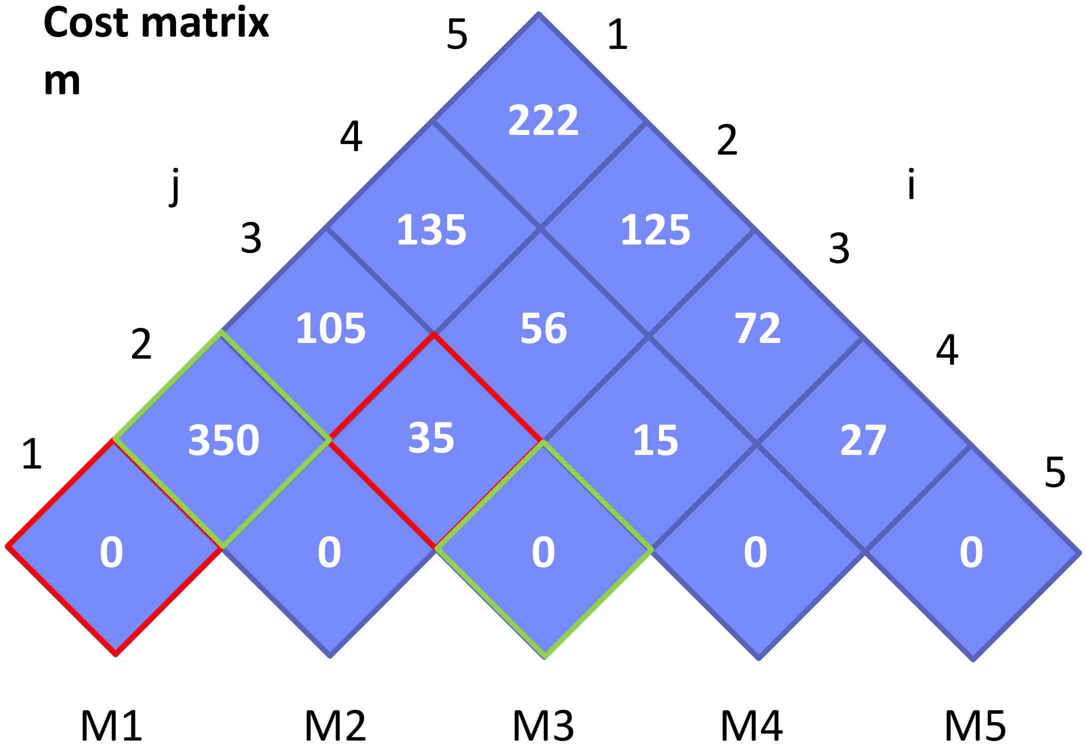
n	C_{n-1}
5	14
10	4,862
15	2,674,440
20	1,767,263,190
25	1,289,904,147,324

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

Matrix Multiplication Chain Optimization, cont.

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)

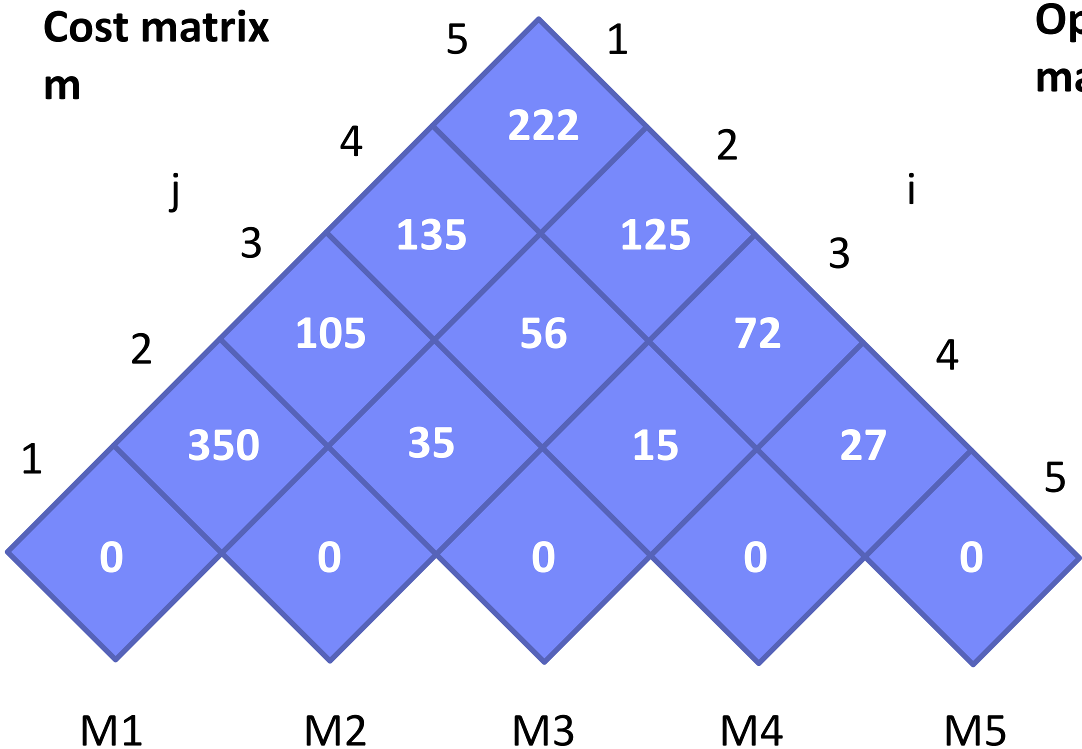
= min(
105,
400)

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

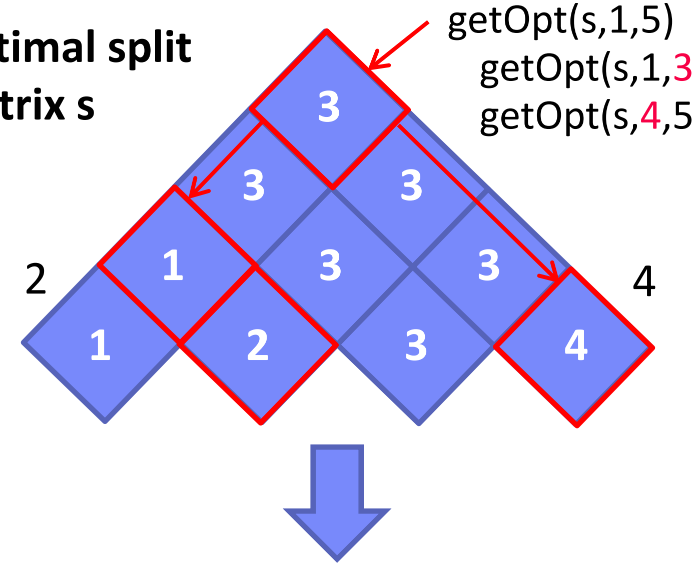
Matrix Multiplication Chain Optimization, cont.

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))

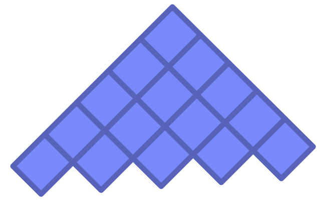
➔ ((M1 (M2 M3)) (M4 M5))

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

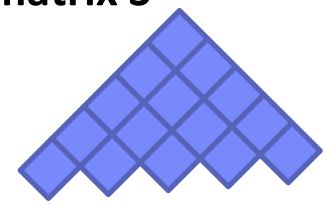
Matrix Multiplication Chain Optimization, cont.

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

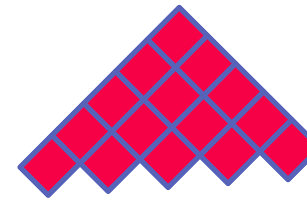
Cost matrix M



Optimal split matrix S



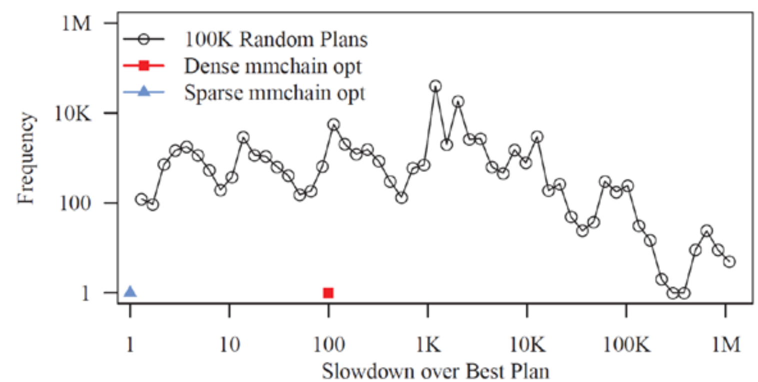
Sketch matrix E



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

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

Example: n=20 matrices



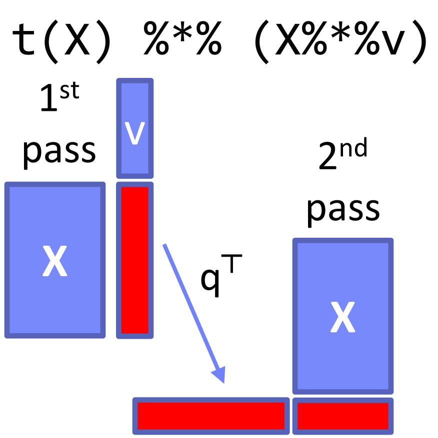
[Johanna Sommer, Matthias Boehm, Alexandre V. Evfimievski, Berthold Reinwald, Peter J. Haas: **MNC:** Structure-Exploiting Sparsity Estimation for Matrix Expressions. **SIGMOD 2019**]

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

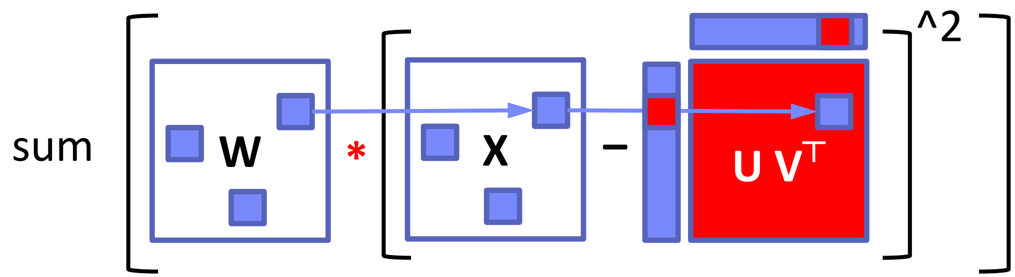


- **#2 Broadcast-Based Operators** (aka broadcast join)
  - SystemML **mapmm**, **mapmmchain**
- **#3 Co-Partitioning-Based Operators** (aka improved repartition join)
  - SystemML **zipmm**; Emma, Samsara OpAtB
- **#4 Shuffle-Based Operators** (aka repartition join)
  - SystemML **cpmm**, **rmm**; Samsara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

Sparsity-Exploiting Operators

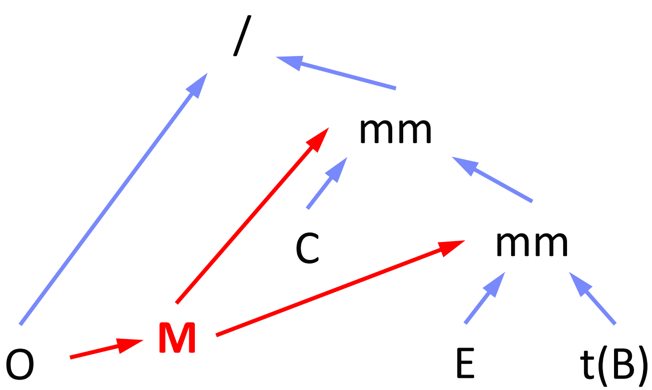
- **Goal:** Avoid dense intermediates and unnecessary computation
- **#1 Fused Physical Operators**
  - E.g., SystemML [PVLDB'16] wsloss, wcemm, wdivmm
  - Selective computation over non-zeros of "sparse driver"

`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**
  - **Rewrites and operator selection**

➔ **Impact of Size Inference and Costs**
  - Advanced optimization of LA 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 (next week: bye)**
  - **04 Operator Fusion and Runtime Adaptation** [Apr 01] (advanced compilation, operator scheduling, JIT compilation, operator fusion / codegen, MLIR)