UC San Diego

DSC 102
Systems for Scalable Analytics

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Topic 3: Parallel and Scalable Data Processing

Part 2: Scalable Data Access

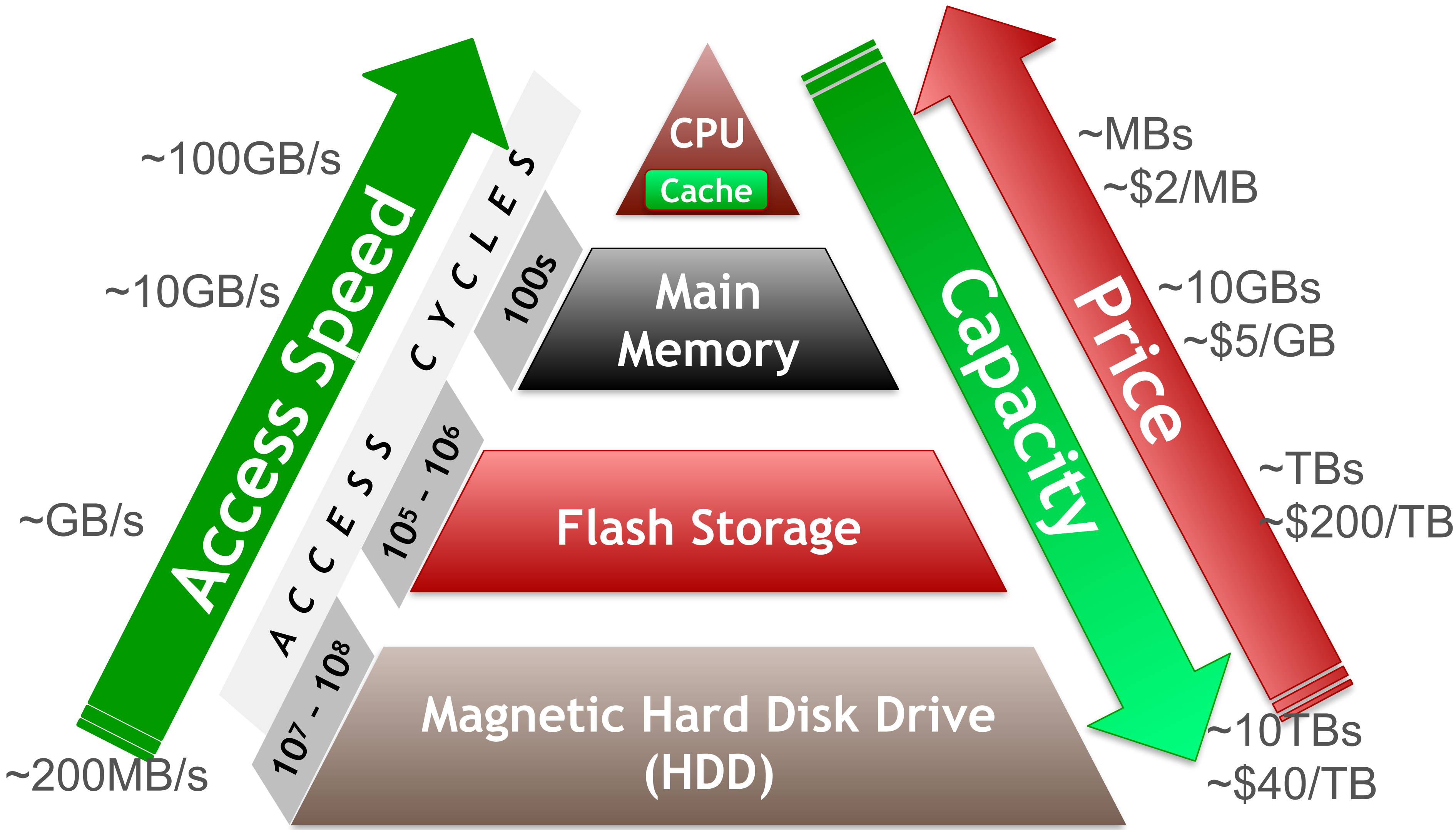
Ch. 9.4, 12.2, 14.1.1, 14.6, 22.1-22.3, 22.4.1, 22.8 of Cow Book

Ch. 5, 6.1, 6.3, 6.4 of MLSys Book

Outline

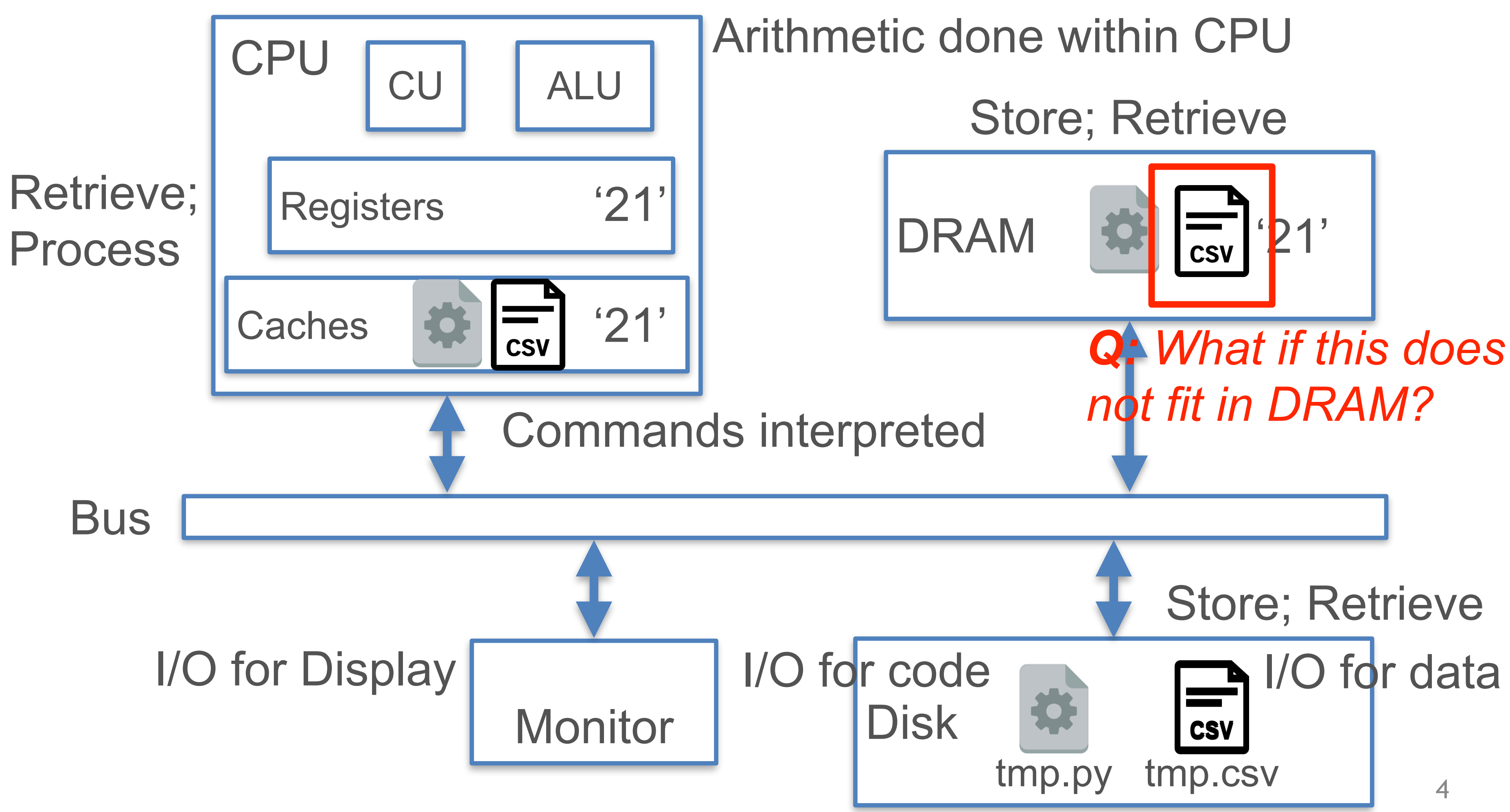
- Basics of Parallelism
  - Task Parallelism; Dask
  - Single-Node Multi-Core; SIMD; Accelerators
- Basics of Scalable Data Access
  - Paged Access; I/O Costs; Layouts/Access Patterns
  - Scaling Data Science Operations
- Data Parallelism: Parallelism + Scalability
  - Data-Parallel Data Science Operations
  - Optimizations and Hybrid Parallelism

Recap: Memory Hierarchy

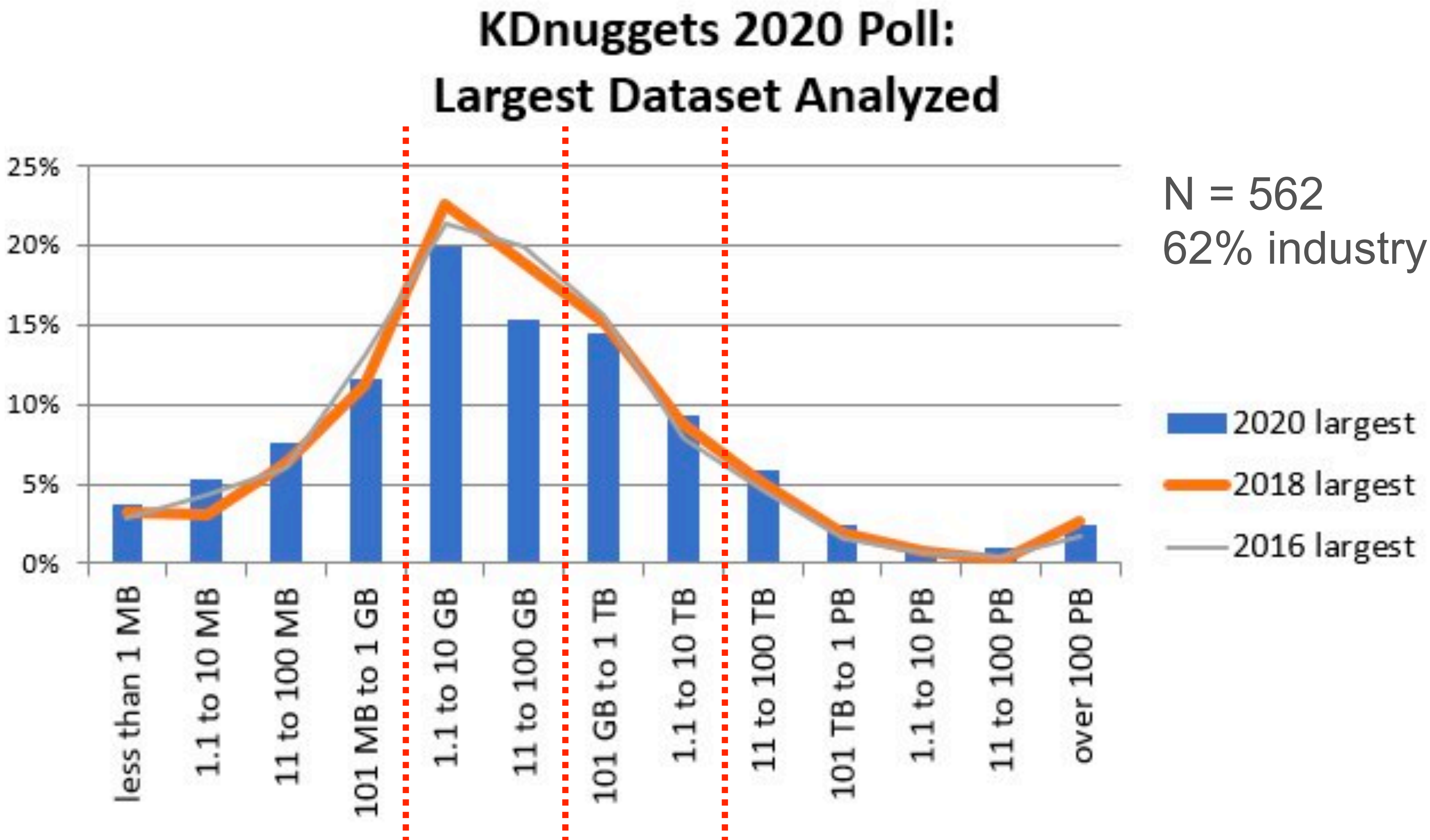


Memory Hierarchy in Action

Rough sequence of events when program is executed



Scale of Datasets in Practice



N = 562
62% industry

https://www.kdnuggets.com/2020/07/poll-largest-dataset-analyzed-results.html

Scalable Data Access

Central Issue: Large data file does not fit entirely in DRAM

Basic Idea: Divide-and-conquer again!
"Split" data file (virtually or physically) and *stage reads* of its pages from disk to DRAM; vice versa for writes

4 key regimes of scalability / staging reads:

- **Single-node disk**: Paged access from file on local disk
- **Remote read**: Paged access from disk(s) over a network
- **Distributed memory**: Data fits on a cluster's total DRAM
- **Distributed disk**: Use entire memory hierarchy of cluster

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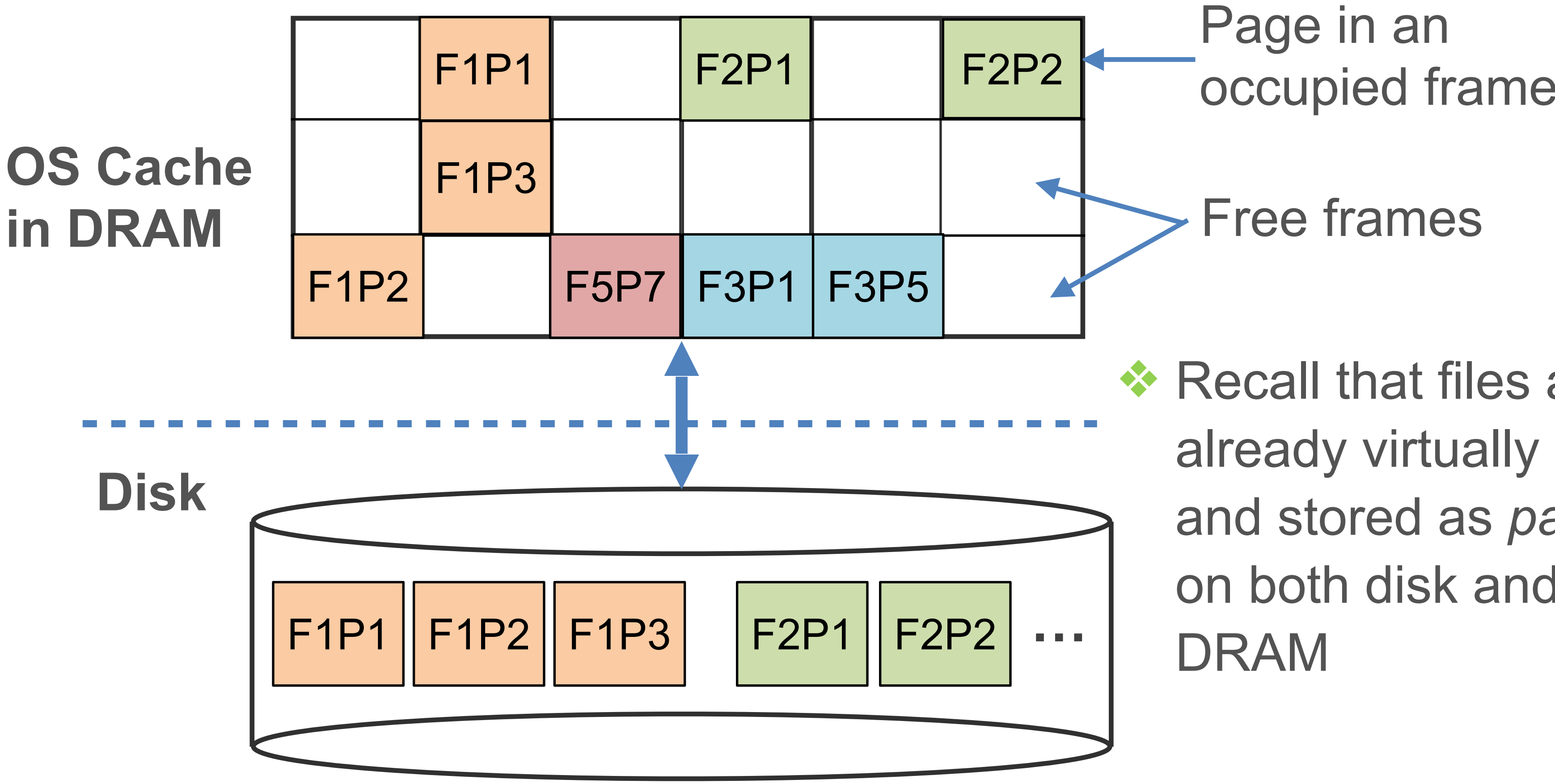
Paged Data Access to DRAM

Basic Idea: "Split" data file (virtually or physically) and *stage reads* of its pages from disk to DRAM (vice versa for writes)



- Recall that files are already virtually split and stored as *pages* on both disk and DRAM

Page Management in DRAM Cache

- **Caching**: Retaining pages read from disk in DRAM
- **Eviction**: Removing a page frame's content in DRAM
- **Spilling**: Writing out pages from DRAM to disk
  - If a page in DRAM is "**dirty**" (i.e., some bytes were written), eviction requires a spill; o/w, ignore that page
- The set of DRAM-resident pages typically changes over the lifetime of a process
- **Cache Replacement Policy**: The algorithm that chooses which page frame(s) to evict when a new page has to be cached but the OS cache in DRAM is full
  - Popular policies include Least Recently Used, Most Recently Used, etc. (more shortly)

Quantifying I/O: Disk and Network

- Page reads/writes to/from DRAM from/to disk incur latency
- **Disk I/O Cost**: Abstract counting of number of page I/Os; can map to bytes given page size
- Sometimes, programs read/write data over network
- **Communication/Network I/O Cost**: Abstract counting of number of pages/bytes sent/received over network
- I/O cost is *abstract*; mapping to latency is *hardware-specific*

Example: Suppose a data file is 40GB; page size is 4KB

I/O cost to read file = 10 million page I/Os

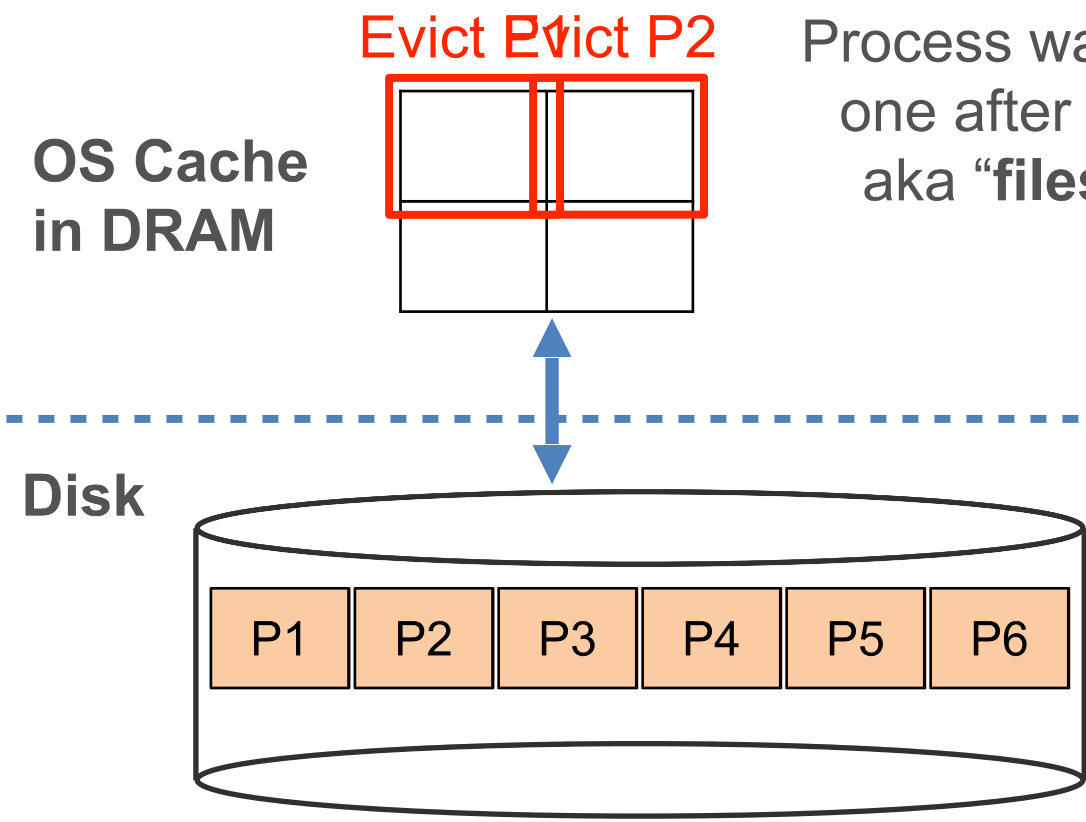
Disk with I/O throughput: 800 MB/s → 40GB/800MBps = 50s

Network with speed: 200 MB/s → 40GB/200MBps = 200s

Scaling to (Local) Disk

Basic Idea: Split data file (virtually or physically) and *stage reads* of its pages from disk to DRAM (vice versa for writes)

Suppose OS Cache has only 4 frames; initially empty



Process wants to read file's pages one after another, then discard: aka "**filescan**" access pattern

Read P1
Read P2
Read P3
Read P4
Read P5
Read P6

Cache is full!
Cache Repl. needed

Total I/O cost: **6**

Scaling to (Local) Disk

- In general, *scalable programs stage access* to pages of file on disk and efficiently use available DRAM
  - Recall that typically DRAM size << Disk size
- Modern DRAM sizes can be 10s of GBs; so we read a "chunk"/ "block" of file at a time (say, 1000s of pages)
  - On magnetic hard disks, such chunking leads to *more sequential I/Os*, raising throughput and lowering latency!
  - Similarly, write a chunk of dirtied pages at a time

Generic Cache Replacement Policies

***Q:** What to do if number of page frames is too few for file?*

- **Cache Replacement Policy**: Algorithm to decide which page frame(s) to evict to make space
  - Typical frame ranking criteria: recency of use, frequency of use, number of processes reading it
  - Typical optimization goal: Reduce total page I/O costs
- A few well-known policies:
  - **Least Recently Used (LRU)**: Evict page that was used the longest time ago
  - **Most Recently Used (MRU)**: Opposite of LRU
  - ML-based caching policies are “hot” nowadays! :)

Ad: Take CSE 132C for more on cache replacement policies

Data Layouts and Access Patterns

- Recall that *data layouts* and *data access patterns* affect what data subset gets cached in higher level of memory hierarchy
  - Recall matrix multiplication example and CPU caches
- **Key Principle:** Optimizing layout of data file on disk based on data access pattern can help reduce I/O costs
  - Applies to both magnetic hard disk and flash SSDs
  - But especially critical for former due to vast differences in latency of random vs sequential access!

Row-store vs Column-store Layouts

- A common dichotomy when serializing 2-D structured data (relations, matrices, DataFrames) to file on disk

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

Say, a page can fit only 4 cell values

Row-store:	1a,1b,1c,1d	2a,2b,2c,2d	3a,3b,3c,3d	…
Col-store:	1a,2a,3a,4a	5a,6a	1b,2b,3b,4b	…

- Based on data access pattern of program, I/O costs with row- vs col-store can be orders of magnitude apart!

Row-store vs Column-store Layouts

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

Say, a page can fit only 4 cell values

Row-store: 1a,1b,1c,1d | 2a,2b,2c,2d | 3a,3b,3c,3d | …

Col-store: 1a,2a,3a,4a | 5a,6a | 1b,2b,3b,4b | …

***Q:** What is the I/O cost with each to compute, say, a sum over B?*

- With row-store: need to fetch *all* pages; I/O cost: 6 pages
- With col-store: need to fetch only B's pages; I/O cost: 2 pages
- This difference generalizes to higher dim. for tensors

Hybrid/Tiled/"Blocked" Layouts

- Sometimes, it is beneficial to do a hybrid, especially for analytical RDBMSs and matrix/tensor processing systems

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

Say, a page can fit only 4 cell values

Hybrid stores with 2x2 tiled layout:

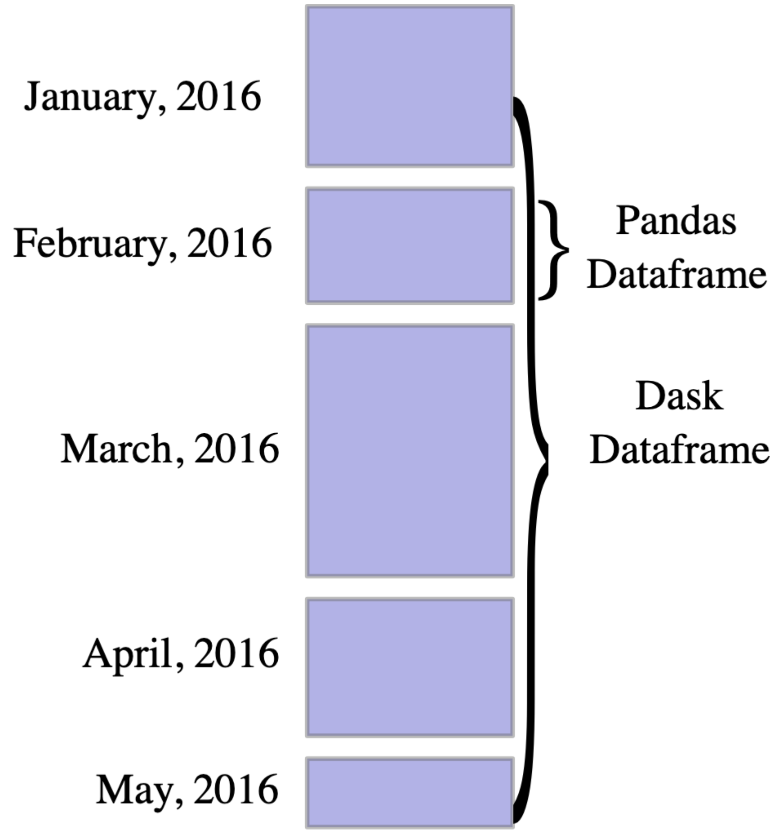
1a,1b,2a,2b	1c,1d,2c,2d	3a,3b,4a,4b	…
1a, 2a, 1b, 2b	1c, 2c, 1d, 2d	3a, 4a, 2b, 3b	…

Key Principle: What data layout will yield lower I/O costs (row vs col vs tiled) depends on data access pattern of the program!

Example: Dask's DataFrame

Basic Idea: Split data file (virtually or physically) and *stage reads* of its pages from disk to DRAM (vice versa for writes)

- Dask DF scales to disk-resident data via a row-store
- "Virtual" split: each split is a Pandas DF under the hood
- Dask API is a "wrapper" around Pandas API to scale ops to splits and put all results together
- If file is too large for DRAM, need manual *repartition()* to get physically smaller splits (< ~1GB)

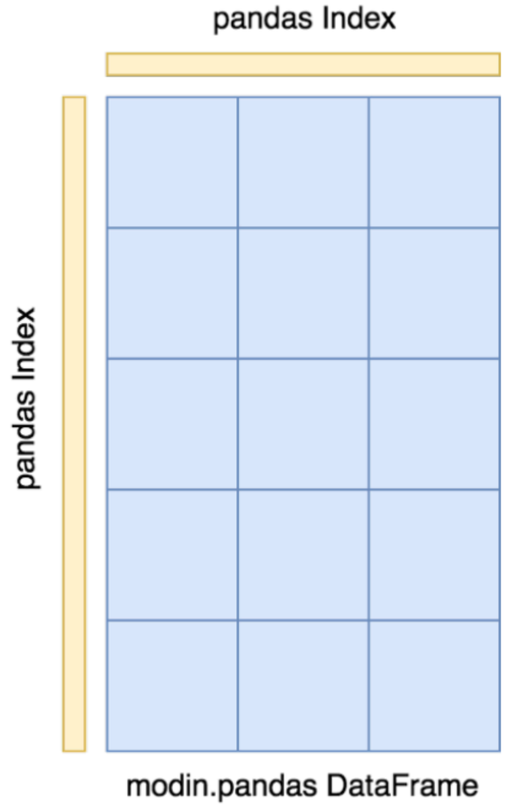


https://docs.dask.org/en/latest/dataframe-best-practices.html#repartition-to-reduce-overhead

Example: Modin's DataFrame

Basic Idea: Split data file (virtually or physically) and *stage reads* of its pages from disk to DRAM (vice versa for writes)

- Modin's DF aims to scale to disk-resident data via a tiled store
- Enables seamless scaling along *both* dimensions
- Easier use of multi-core parallelism
- Many in-memory RDBMSs had this, e.g., SAP HANA, Oracle TimesTen
- ScaLAPACK had this for matrices



https://www2.eecs.berkeley.edu/Pubs/TechRpts/2018/EECS-2018-191.pdf
https://arxiv.org/pdf/2001.00888.pdf

Scaling with Remote Reads

Basic Idea: Split data file (virtually or physically) and *stage reads* of its pages from disk to DRAM (vice versa for writes)

- Similar to scaling to local disk but not "local":
  - Stage page reads from remote disk/disks over the network (e.g., from S3)
- *More restrictive* than scaling with local disk, since spilling is not possible or requires costly network I/Os
  - OK for a *one-shot* filescan access pattern
  - Use DRAM to cache; repl. policies
  - Can also use smaller local disk as cache; you did this in PA1

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Scaling Data Science Operations

- Scalable data access for key representative examples of programs/operations that are ubiquitous in data science:
  - DB systems:
    - Non-deduplicating project
    - Simple SQL aggregates
    - SQL GROUP BY aggregates
  - ML systems:
    - Matrix sum/norms
    - (Stochastic) Gradient Descent

Scaling to Disk: Non-dedup. Project

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

R

SELECT C FROM R

Row-store:

1a,1b,1c,1d	2a,2b,2c,2d	3a,3b,3c,3d
4a,4b,4c,4d	5a,5b,5c,5d	6a,6b,6c,6d

- Straightforward **filescan** data access pattern
  - Read one page at a time into DRAM; may need cache repl.
  - Drop unneeded columns from tuples on the fly
- I/O cost: 6 (read) + output # pages (write)

Scaling to Disk: Non-dedup. Project

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

R

SELECT C FROM R

Col-store:

1a,2a,3a,4a	5a,6a	1b,2b,3b,4b	5b,6b
1c,2c,3c,4c	5c,6c	1b,2b,3b,4b	5b,6b

- Since we only need col C, no need to read other pages!
- I/O cost: 2 (read) + output # pages (write)
- Big advantage for col-stores over row-stores for SQL analytics queries (projects, aggregates, etc.), aka “OLAP”
  - Rationale for col-store RDBMS (e.g., Vertica) and Parquet

Scaling to Disk: Simple Aggregates

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

R

SELECT MAX(A) FROM R

Row-store:

1a,1b,1c,1d	2a,2b,2c,2d	3a,3b,3c,3d
4a,4b,4c,4d	5a,5b,5c,5d	6a,6b,6c,6d

- Again, straightforward **filescan** data access pattern
  - Similar I/O behavior as non-deduplicating project
- I/O cost: 6 (read) + output # pages (write)

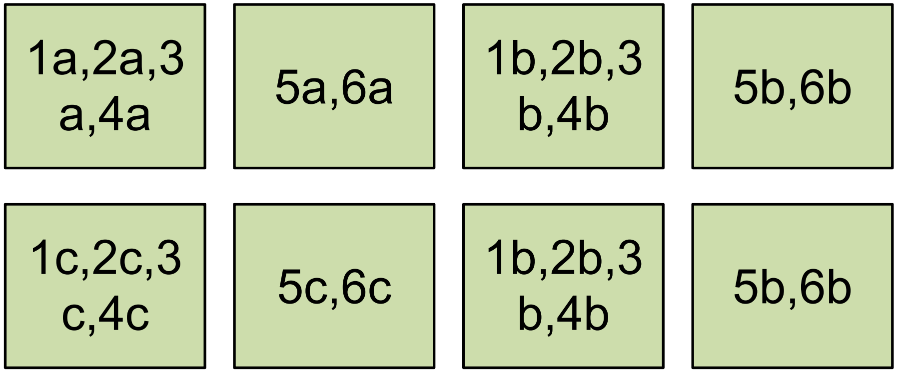
Scaling to Disk: Simple Aggregates

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

R

SELECT MAX(A) FROM R

Col-store:



- Similar to the non-dedup. project, we only need col A; no need to read other pages!
- I/O cost: 2 (read) + output # pages (write)

Scaling to Disk: Group By Aggregate

A	B	C	D
a1	1b	1c	4
a2	2b	2c	3
a1	3b	3c	5
a3	4b	4c	1
a2	5b	5c	10
a1	6b	6c	8

R

SELECT A, SUM(D)
FROM R GROUP BY A

- Now it is not straightforward due to the GROUP BY!
- Need to "collect" all tuples in a group and apply agg. func. to each
- Typically done with a **hash table** maintained in DRAM
  - Has 1 record per group and maintains "running information" for that group's agg. func.
  - Built on the fly during filescan of R; holds the output in the end

Hash table (output)

A	Running Info.
a1	17
a2	13
a3	1

Scaling to Disk: Group By Aggregate

A	B	C	D
a1	1b	1c	4
a2	2b	2c	3
a1	3b	3c	5
a3	4b	4c	1
a2	5b	5c	10
a1	6b	6c	8

R

SELECT A, SUM(D)
FROM R GROUP BY A

Row-store:

a1,1b,1c,4	a2,2b,2c,3	a1,3b,3c,5
a3,4b,4c,1	a2,5b,5c,10	a1,6b,6c,8

Hash table in DRAM

A	Running Info.
a1	4 -> 9 -> 17
a2	3 -> 13
a3	1

- Note that the sum for each group is constructed *incrementally*
- I/O cost: 6 (read) + output # pages (write); just one filescan again!

***Q:** But what if hash table > DRAM size?!*

Scaling to Disk: Group By Aggregate

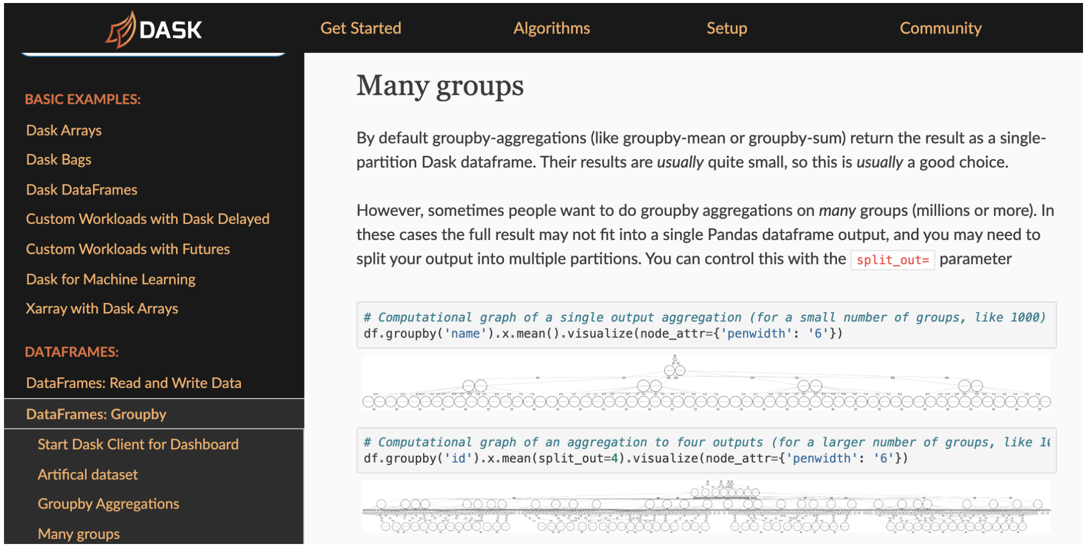
SELECT A, SUM(D) FROM R GROUP BY A

***Q:** But what if hash table > DRAM size?*

- Program will likely just crash! OS may keep swapping pages of hash table to/from disk; aka “thrashing”

***Q:** How to scale to large number of groups?*

- Divide and conquer! Split up R based on values of A
- HT for each split may fit in DRAM alone
- Reduce running info. size if possible



Ad: Take CSE 132C for more on how GROUP BY is scaled

Scaling to Disk: Matrix Sum/Norms

2	1	0	0
2	1	0	0
0	1	0	2
0	0	1	2
3	0	1	0
3	0	1	0

M_{6x4}

$$||M||_2^2$$

Row-store:

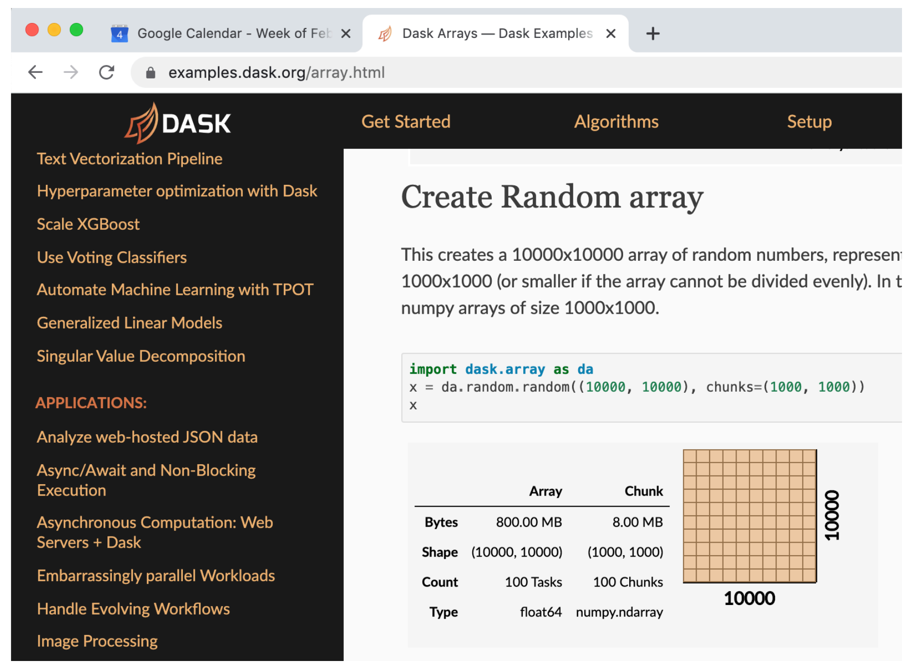
2,1, 0,0	2,1 0,0	0,1, 0,2
0,0, 1,2	3,0, 1,0	3,0, 1,0

- Again, straightforward **filescan** data access pattern
  - Very similar to relational simple aggregate
  - Running info. in DRAM for sum of squares of cells
    - 0 -> 5 -> 10 -> 15 -> 20 -> 30 -> 40
- I/O cost: 6 (read) + output # pages (write)
- Col-store and tiled-store also have I/O cost 6; why?

Scalable Matrix/Tensor Algebra

- In general, tiled partitioning is more common for matrix/tensor ops
  - More DRAM/cache-efficient implementations

- DRAM-to-disk scaling:
  - pBDR, SystemDS, and Dask Arrays for matrices
  - SciDB, Xarray for n-d arrays
- CUDA for DRAM-GPU caches scaling of matrix/tensor ops



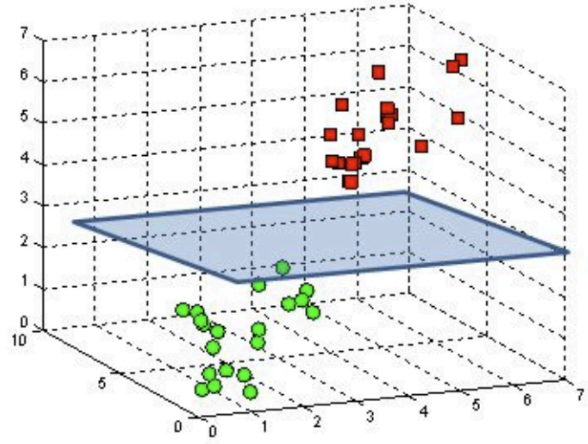
Numerical Optimization in ML

- Many regression and classification models in ML are formulated as a (constrained) *minimization* problem
  - E.g., logistic and linear regression, linear SVM, etc.
  - Aka "Empirical Risk Minimization" (ERM) approach
  - Computes "loss" of predictions over labeled examples

$$\mathbf{w}^* = argmin_{\mathbf{w}} \sum_{i=1}^{n} l(y_i, f(\mathbf{w}, x_i))$$

- Hyperplane-based models aka Generalized Linear Models (GLMs) use f() that is a scalar function of distances: $\mathbf{w}^T x_i$

A hyperplane in $\mathbb{R}^3$ is a plane

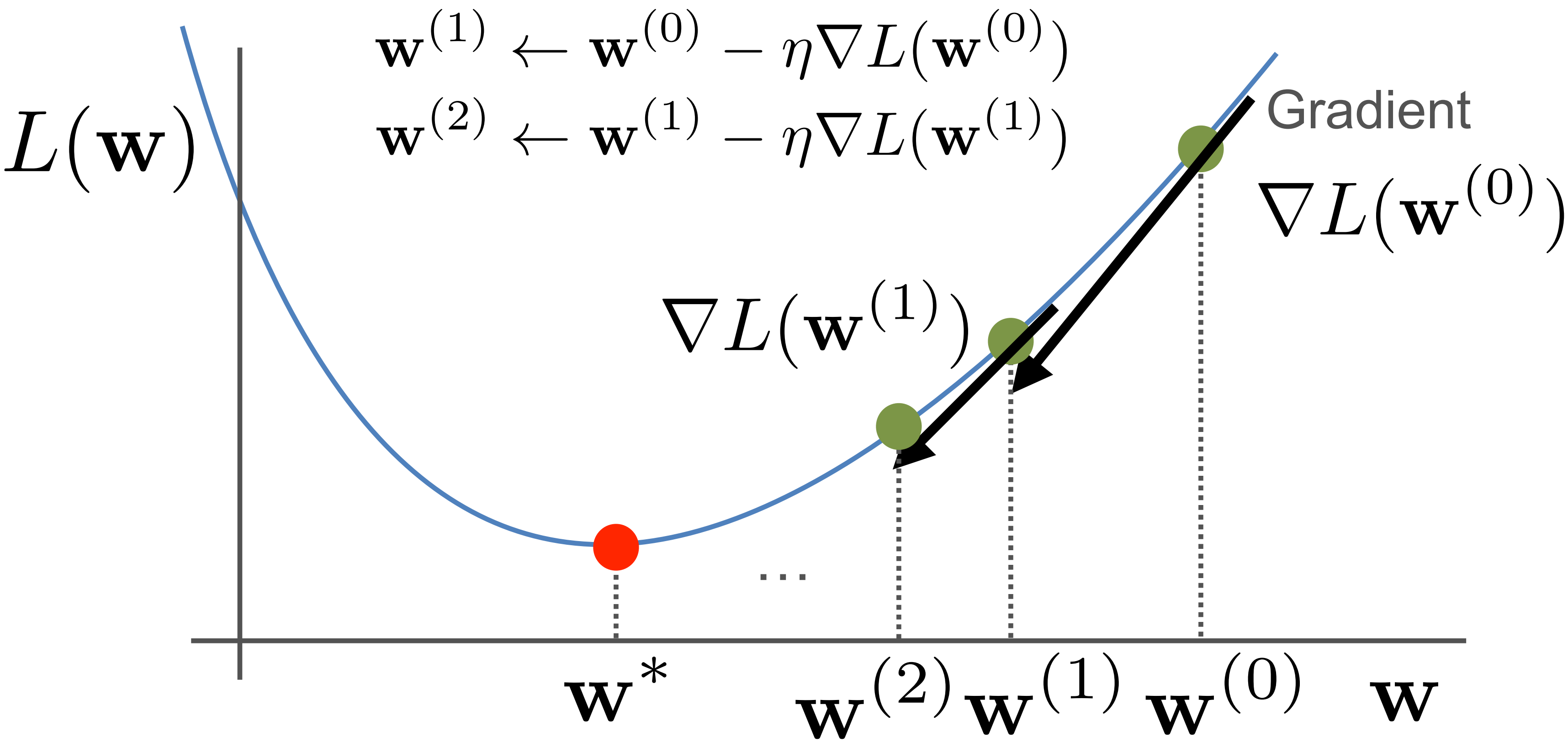


Batch Gradient Descent for ML

$$L(\mathbf{w}) = \sum_{i=1}^{n} l(y_i, f(\mathbf{w}, x_i))$$

- In many cases, **loss function** l() is **convex**; so is L()
- Closed-form minimization typically infeasible
- **Batch Gradient Descent:**
  - Iterative numerical procedure to find an optimal **w**
  - Initialize **w** to some value $\mathbf{w}^{(0)}$
  - Compute **gradient**: $$\nabla L(\mathbf{w}^{(k)}) = \sum_{i=1}^{n} \nabla l(y_i, f(\mathbf{w}^{(k)}, x_i))$$
  - Descend along gradient:
    (Aka **Update Rule**) $$\mathbf{w}^{(k+1)} \leftarrow \mathbf{w}^{(k)} - \eta \nabla L(\mathbf{w}^{(k)})$$
  - Repeat until we get close to **w***, aka **convergence**

Batch Gradient Descent for ML



- Learning rate is a **hyper-parameter** selected by user or "AutoML" tuning procedures
- Number of iterations/epochs of BGD also hyper-parameter

Data Access Pattern of BGD at Scale

- The data-intensive computation in BGD is the gradient
  - In scalable ML, dataset D may not fit in DRAM
  - Model **w** is typically small and DRAM-resident

$$\nabla L(\mathbf{w}^{(k)}) = \sum_{i=1}^{n} \nabla l(y_i, f(\mathbf{w}^{(k)}, x_i))$$

***Q:** What SQL op is this reminiscent of?*

- Gradient is like SQL SUM over vectors (one per example)
- At each epoch, 1 **filescan** over D to get gradient
- Update of **w** happens normally in DRAM
- Monitoring across epochs for convergence needed
- Loss function L() is also just a SUM in a similar manner

I/O Cost of Scalable BGD

$$\nabla L(\mathbf{w}^{(k)}) = \sum_{i=1}^{n} \nabla l(y_i, f(\mathbf{w}^{(k)}, x_i))$$

D

Y	X1	X2	X3
0	1b	1c	1d
1	2b	2c	2d
1	3b	3c	3d
0	4b	4c	4d
1	5b	5c	5d
0	6b	6c	6d

Row-store:

0,1b, 1c,1d	1,2b, 2c,2d	1,3b, 3c,3d
0,4b, 4c,4d	1,5b, 5c,5d	0,6b, 6c,6d

- Straightforward **filescan** data access pattern for SUM
  - Similar I/O behavior as non-dedup. project and simple SQL aggregates
- I/O cost: 6 (read) + output # pages (write for final **w**)

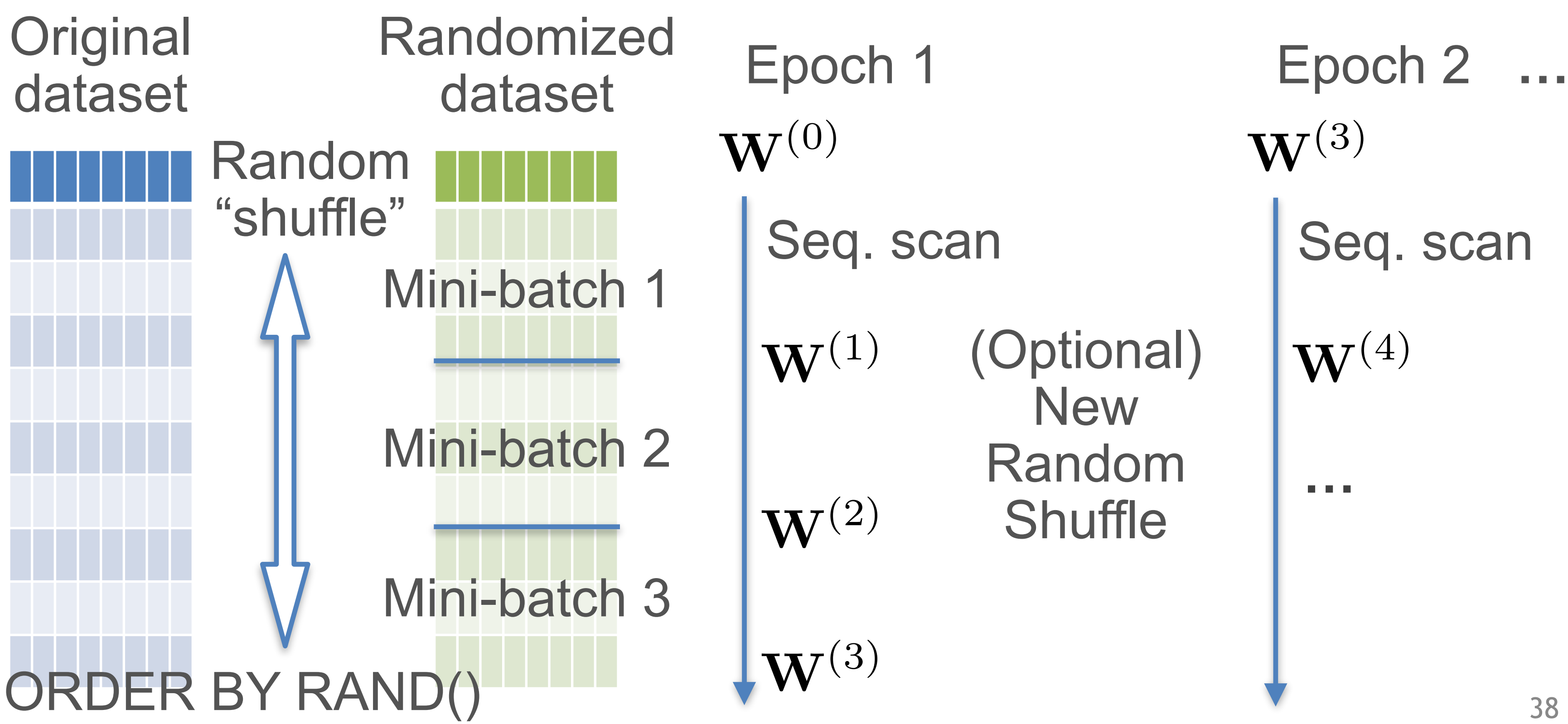
Stochastic Gradient Descent for ML

- Two key cons of BGD:
  - Often, too many epochs to reach optimal
  - Each update of **w** needs full scan: costly I/Os
- Stochastic GD (SGD) mitigates both cons
- **Basic Idea:** Use a *sample* (**mini-batch**) of D to approximate gradient instead of "full batch" gradient
  - Done *without replacement*
  - Randomly reorder/shuffle D before every epoch
  - Sequential pass: sequence of mini-batches
- Another big pro of SGD: works well for *non-convex* loss too, especially DL; BGD does not
- SGD often called the "workhorse" of modern ML/DL

Access Pattern of Scalable SGD

$$\mathbf{W}^{(t+1)} \leftarrow \mathbf{W}^{(t)} - \eta \nabla \tilde{L}(\mathbf{W}^{(t)}) \qquad \nabla \tilde{L}(\mathbf{W}) = \sum_{i \in B} \nabla l(y_i, f(\mathbf{W}, x_i))$$

Sample mini-batch from dataset without replacement



I/O Cost of Scalable SGD

- I/O cost of random shuffle is non-trivial; need so-called "external merge sort" (skipped in this course)
  - Typically amounts to 1 or 2 passes over file
- Mini-batch gradient computations: 1 **filescan** per epoch:
  - As filescan proceeds, count # examples seen, accumulate per-example gradient for mini-batch
  - Typical mini-batch sizes: 10s to 1000s
  - Orders of magnitude more model updates than BGD!
- Total I/O cost per epoch: 1 shuffle cost + 1 filescan cost
  - Often, shuffling only once upfront suffices
- Loss function L() computation is same as before (for BGD)

Scaling Data Science Operations

- Scalable data access for key representative examples of programs/operations that are ubiquitous in data science:
  - DB systems:
    - Relational select
    - Non-deduplicating project
    - Simple SQL aggregates
    - SQL GROUP BY aggregates
  - ML systems:
    - Matrix sum/norms
    - (Stochastic) Gradient Descent

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Review Questions

1. What are the 4 main regimes of scalable data access?
2. Briefly explain 1 pro and 1 con of scaling with local disk vs scaling with remote reads.
3. You are given a DataFrame serialized as a 100 GB Parquet columnar file. All 20 columns are of same fixed-length data type. You compute a sum over 4 columns. What is the I/O cost (in GB)?
4. Which is the most flexible layout format for 2-D structured data?
5. You layout a 1 TB matrix in tile format with a shape 2000x500. What is the I/O cost (in GB) of computing its full matrix sum?
6. Briefly explain 1 pro and 1 con of SGD vs BGD.
7. Suppose you use scalable SGD to train a DL model. The dataset has 100 mil examples. You use a mini-batch size of 50. How many iterations (number of model update steps) will SGD finish in 20 epochs?
8. What is the precise runtime tradeoff involved in shuffle-once-upfront vs shuffle-every-epoch for SGD?

Optional: More Examples of Scaling Data Science Operations

Not included in syllabus

Scaling to Disk: Relational Select

A	B	C	D
1a	1b	1c	1d
2a	2b	2c	2d
3a	3b	3c	3d
4a	4b	4c	4d
5a	5b	5c	5d
6a	6b	6c	6d

R

$$\sigma_{B=\text{“}3b\text{”}}(R)$$

Row-store:

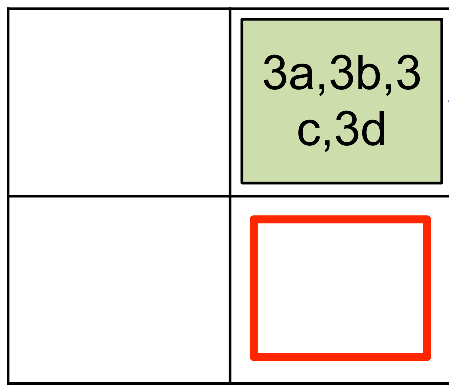
1a,1b,1c,1d	2a,2b,2c,2d	3a,3b,3c,3d
4a,4b,4c,4d	5a,5b,5c,5d	6a,6b,6c,6d

- Straightforward **filescan** data access pattern
  - Read pages/chunks from disk to DRAM one by one
  - CPU applies predicate to tuples in pages in DRAM
  - Copy satisfying tuples to temporary output pages
  - Use LRU for cache replacement, if needed
- I/O cost: 6 (read) + output # pages (write)

Scaling to Disk: Relational Select

$$\sigma_{B=\text{``}3b\text{''}}(R)$$

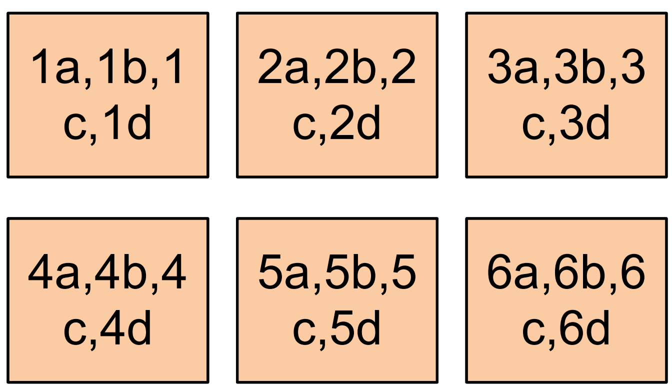
OS Cache in DRAM



Reserved for writing output data of program (may be spilled to a temp. file)

CPU finds a matching tuple!
Copies that to output page

Disk



Need to evict some page
LRU says kick out page 1
Then page 2 and so on
…

Scaling to Disk: Gramian Matrix

2	1	0	0
2	1	0	0
0	1	0	2
0	0	1	2
3	0	1	0
3	0	1	0

M_{6x4}

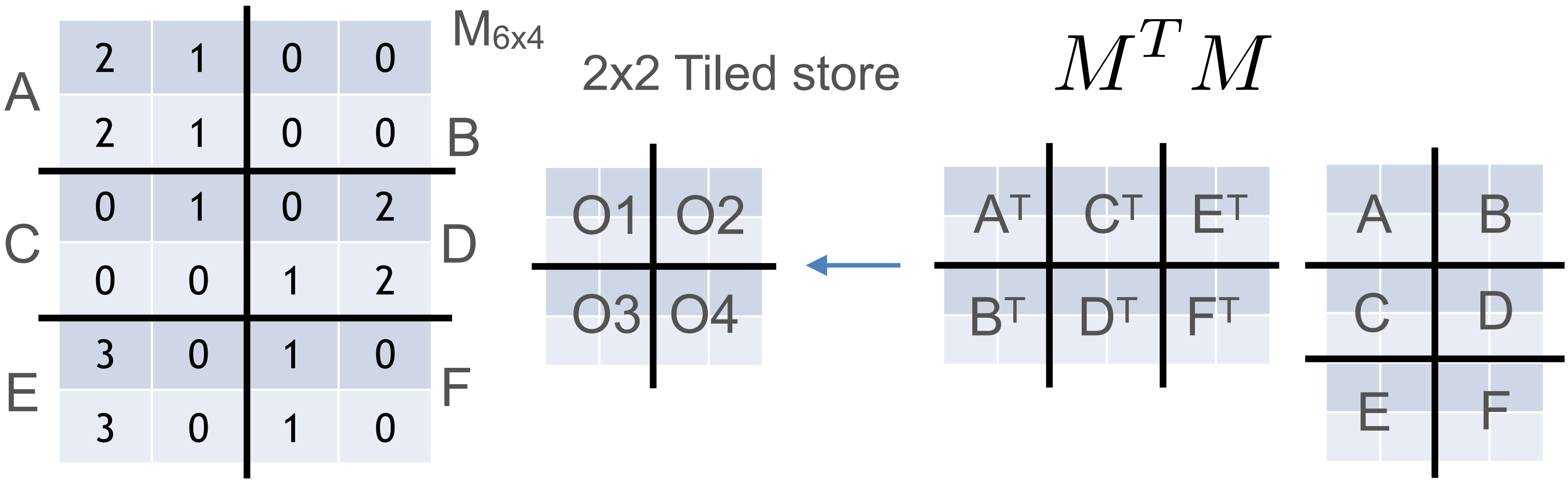
$$M^T M$$

Row-store:

2,1, 0,0	2,1 0,0	0,1, 0,2
0,0, 1,2	3,0, 1,0	3,0, 1,0

- A bit tricky, since output may not fit entirely in DRAM
  - Similar to GROUP BY difficult case
- Output here is 4x4, i.e., 4 pages; only 3 can be in DRAM!
  - Each row will need to update entire output matrix
  - Row-store can be a poor fit for such matrix algebra
- What about col-store or tiled-store?

Scaling to Disk: Gramian Matrix



- Read A, C, E one by one to get O1 = $A^TA + C^TC + E^TE$; O1 is incrementally computed; write O1 out; I/O: 3 (r) + 1 (w)
- Likewise with B, D, F for O4; I/O: 3 (r) + 1 (w)
- Read A, B and put A^TB in O2; read C, D to add C^TD to O2; read E, F to add E^TF to O2; write O2 out; I/O: 6 + 1
- Likewise with B,A; D,C; F,E for O3; I/O: 6 + 1
- Max I/O cost: 18 (r) + 4(w); *scalable on both dimensions!*