## UC San Diego

# DSC 102 Systems for Scalable Analytics

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Topic 3: Parallel and Scalable Data Processing

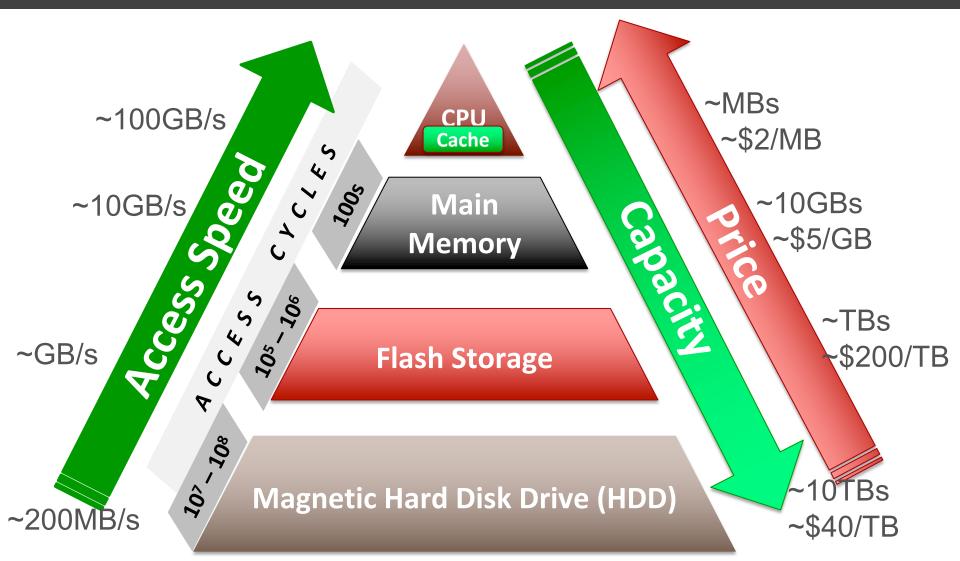
Part 2: Scalable Data Access

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

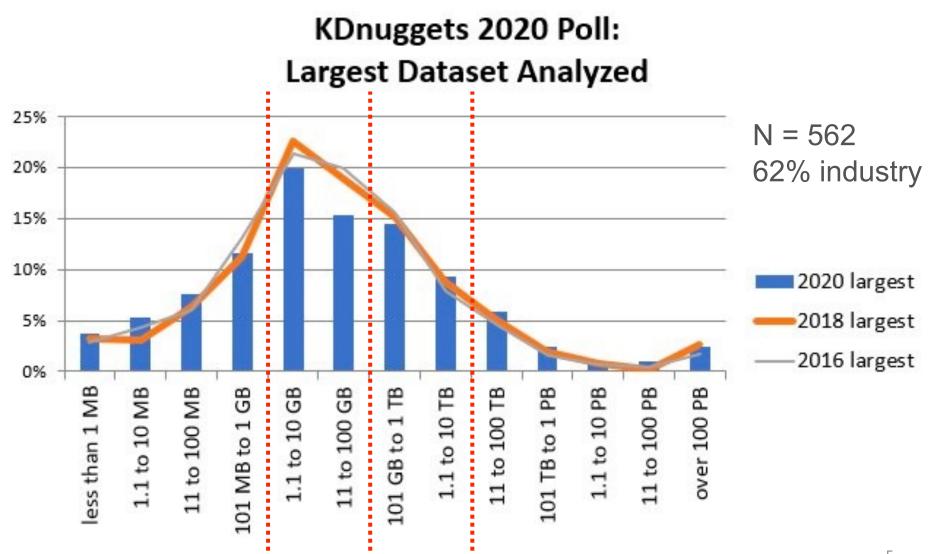
# Recap: Memory Hierarchy



## Memory Hierarchy in Action

Rough sequence of events when program is executed Arithmetic done within CPU **CPU ALU** Store; Retrieve Retrieve: '21' Registers **DRAM Process '21'** Caches What if this does not fit in DRAM? Commands interpreted Bus Store; Retrieve I/O for code I/O for data I/O for Display Disk **Monitor** tmp.py tmp.csv 4

#### Scale of Datasets in Practice



#### 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 <u>stage reads</u> of its pages from disk to DRAM; vice versa for writes

4 key regimes of scalability / staging reads:

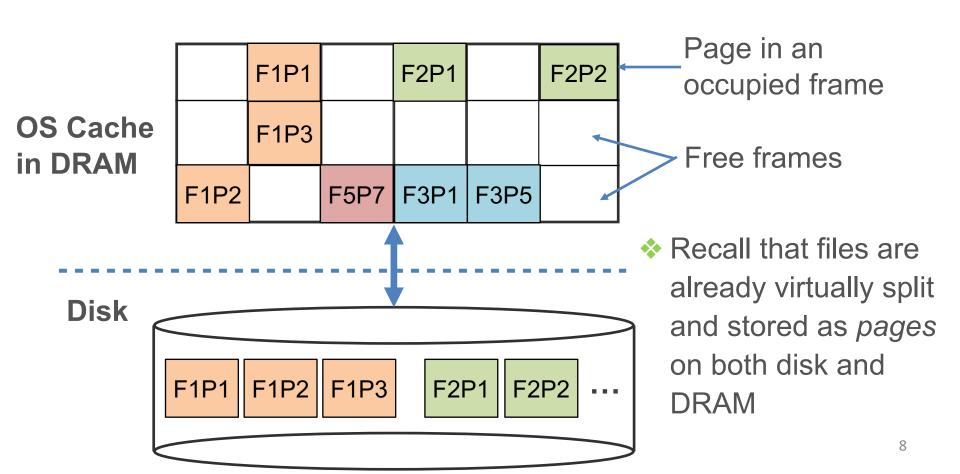
- Single-node disk: Paged access from file on local disk
- Remote read: Paged access from disk(s) over a network
- Distributed memory: Data fits on a cluster's total DRAM
- Distributed disk: Use entire memory hierarchy of cluster

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## Paged Data Access to DRAM

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



## 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

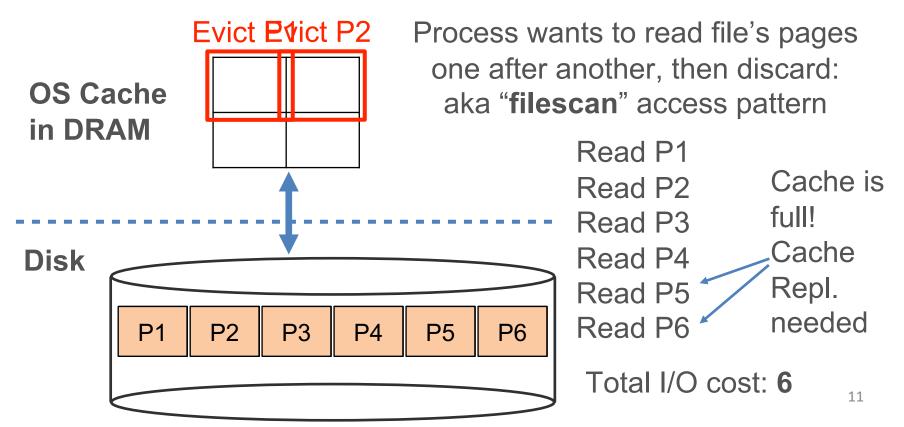
Disk with I/O throughput: 800 MB/s ——— 40GB/800MBps = 50s

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

## Scaling to (Local) Disk

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

Suppose OS Cache has only 4 frames; initially empty



# Scaling to (Local) Disk

- In general, <u>scalable programs stage access</u> to pages of file on disk and efficiently use available DRAM
  - Recall that typically DRAM size << Disk size</p>
- Modern machines have 10s of GBs DRAM; so, read a "chunk"/"block" of file at a time (say, 1000s of pages)
  - On HDDs, such chunking leads to more sequential I/Os, raising throughput and lowering latency
  - Similarly, write a chunk of dirtied pages at a time

## Data Layouts and Access Patterns

- Data Layout: Order in which data is laid out on storage; property of physical level of database
- Data Access Pattern: Order in which a program needs to access data for its computations; property of the program
- Together, the above two affect what data subset gets cached in higher level of memory hierarchy
- Key Principle: Optimizing data layout on disk based on data access pattern can help reduce I/O costs and latency
  - Applies to both HDDs and SSDs but especially critical for HDDs due to its random vs. sequential access latency gap

## Row-store vs Column-store Layouts

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

A	В	С	D	Say, a page	can fit on	ly 4 cell v	values	
<b>1</b> a	1b	1c	1d					
2a	2b	2c	2d	Row-store:	1a,1b,1	2a,2b,2	3a,3b,3 c,3d	
3a	3b	3c	3d	Row-store.	c,1d	c,2d	c,3d	•••
4a	4b	4c	4d		10 20 2		1h 2h 2	
5a	5b	5c	5d	Col-store:	1a,2a,3 a,4a	5a,6a	1b,2b,3 b,4b	
6a	6b	6c	6d					

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

Α	В	С	D	Say, a page	can fit on	ly 4 cell v	values	
<b>1</b> a	1b	1c	1d					
2a	2b	2c	2d	Row-store:	1a,1b,1	2a,2b,2	3a,3b,3	
3a	3b	3c	3d	Row-store:	c,1d	c,2d	3a,3b,3 c,3d	• • • •
4a	4b	4c	4d		10 20 2		1h 2h 2	
5a	5b	5c	5d	Col-store:	1a,2a,3 a,4a	5a,6a	1b,2b,3 b,4b	
6a	6b	6c	6d					

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

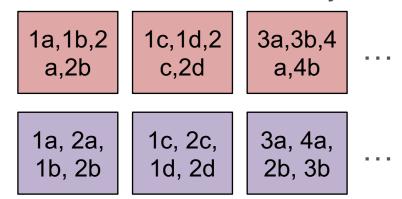
## Hybrid/Tiled/"Blocked" Layouts

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

Α	В	С	D
<b>1</b> a	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:

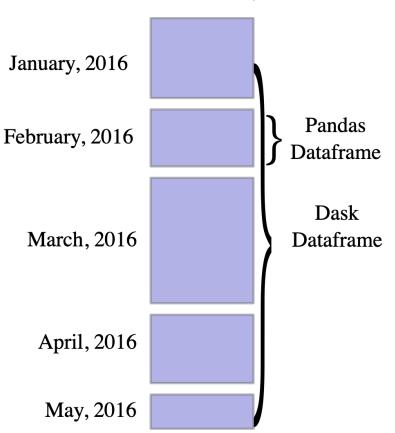


**Key Principle:** Which data layout will yield lower I/O costs (row vs. col vs tiled) depends on data access pattern of the program!

## Example: Dask's DataFrame

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

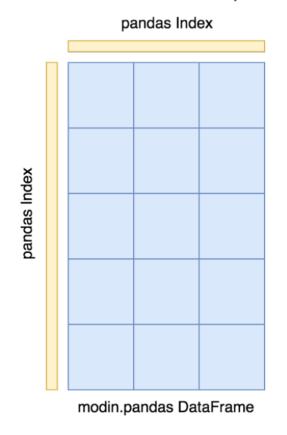
- Dask DF scales to disk-resident data via a row-store
- "Virtual" split: each split is a Pandas DF under the hood
- Dask API is a "wrapper" around Pandas API to scale ops to splits and put all results together
- If file is too large for DRAM, need manual repartition() to get physically smaller splits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



## Example: Modin's DataFrame

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

- Modin's DF aims to scale to diskresident 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



## Scaling with Remote Reads

**Basic Idea**: Split data file (virtually or physically) and <u>stage reads</u> 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

## Peer Instruction Activity

(Switch slides)

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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:
  - Select
  - Non-deduplicating project
  - Simple SQL aggregates
  - GROUP BY aggregates
  - ML systems:
    - Matrix sum/norms
    - (Stochastic) Gradient Descent

## Scaling to Disk: Relational Select

A	В	С	D	R $\sigma_B$	="3 <i>b</i> "	(R)	
<b>1</b> a	1b	1c	1d				
2a	2b	2c	2d	Row-store:	1a,1b,1	2a,2b,2	3a,3b,3
3a	3b	3c	3d	Now-Store.	1a,1b,1 c,1d	c,2d	3a,3b,3 c,3d
4a	4b	4c	4d				
5a	5b	5c	5d		4a,4b,4 c,4d	5a,5b,5 c,5d	6a,6b,6 c,6d
6a	6b	6c	6d		<b>0,</b> -T <b>u</b>	0,00	0,00

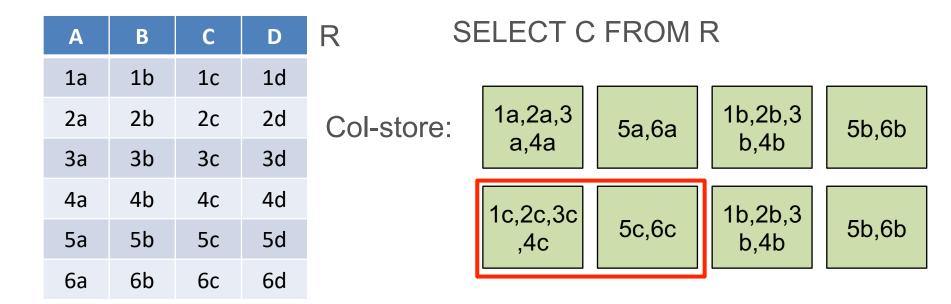
- Straightforward filescan data access pattern
  - Read pages/chunks from disk to DRAM one by one
  - CPU applies predicate to tuples in pages in DRAM
  - Copy satisfying tuples to temporary output pages
  - Use LRU for cache replacement, if needed
- I/O cost: 6 (read) + output # pages (write)

# Scaling to Disk: Non-dedup. Project

A	В	С	D	R SELECT C FROM R			
<b>1</b> a	1b	1c	1d				
2a	2b	2c	2d	Row-store:	1a,1b,1	2a,2b,2	3a,3b,3
3a	3b	3c	3d	Now-Store.	1a,1b,1 c,1d	2a,2b,2 c,2d	3a,3b,3 c,3d
4a	4b	4c	4d				
5a	5b	5c	5d		4a,4b,4 c,4d	5a,5b,5 c,5d	6a,6b,6 c,6d
6a	6b	6c	6d		<b>0,</b> -T <b>0</b>	0,00	0,00

- 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



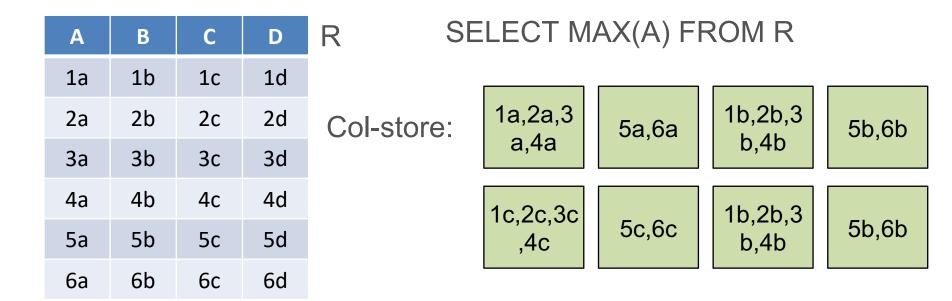
- Since we only need col C, no need to read other pages
- I/O cost: 2 (read) + output # pages (write)
- Big advantage for col-stores over row-stores for SQL analytics queries (projects, aggregates, etc.), aka "OLAP"
  - Rationale for col-store RDBMS (e.g., Vertica) and Parquet

# Scaling to Disk: Simple Aggregates

Α	В	С	D	R SELECT MAX(A) FROM R			
<b>1</b> a	1b	1c	1d				
2a	2b	2c	2d	Row-store:	1a,1b,1	2a,2b,2	3a,3b,3
3a	3b	3c	3d	Row-Store.	1a,1b,1 c,1d	c,2d	3a,3b,3 c,3d
4a	4b	4c	4d				
5a	5b	5c	5d		4a,4b,4 c,4d	5a,5b,5 c,5d	6a,6b,6 c,6d
6a	6b	6c	6d		0,40	0,00	0,00

- 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



- 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

Α	В	С	D	F
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 (output)

Α	Running Info.
a1	17
a2	13
a3	1

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

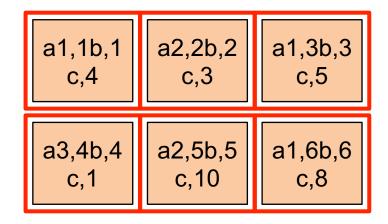
- Now it is not straightforward due to the **GROUP BY!**
- Need to "collect" all tuples in a group and apply agg. func. to each
- Typically done with a hash table maintained in DRAM
  - Has 1 record per group and maintains "running information" for that group's agg. func.
  - Built on the fly during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

# Scaling to Disk: Group By Aggregate

Α	В	С	D	R
a1	1b	1c	4	
a2	2b	2c	3	
a1	3b	3c	5	
a3	4b	4c	1	
a2	5b	5c	10	
a1	6b	6c	8	

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

Row-store:



Hash table in DRAM

Α	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

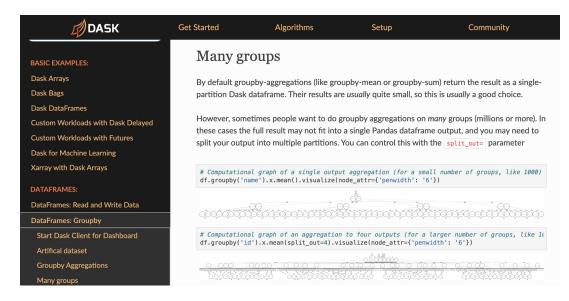
#### SELECT A, SUM(D) FROM R GROUP BY A

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 Data Science Operations

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

## Scaling to Disk: Matrix Sum/Norms

2	1	0	0	M6x4	I	$\ M\ _{2}^{2}$	
2	1	0	0				
0	1	0	2	Row-store:	2,1,	2,1	0,1,
0	0	1	2		0,0	0,0	0,2
3	0	1	0		0,0,	3,0,	3,0,
3	0	1	0		1,2	1,0	1,0

- Again, straightforward filescan data access pattern
  - Very similar to relational simple aggregate
  - Running info. in DRAM for sum of squares of cells

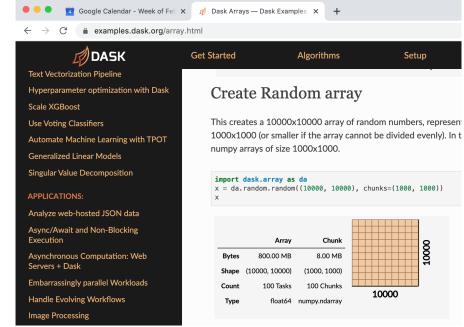
- I/O cost: 6 (read) + output # pages (write)
- Col-store and tiled-store also have I/O cost 6; why?

# 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





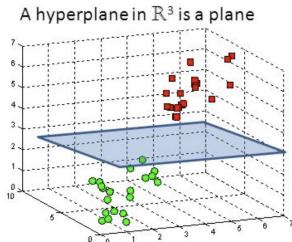


## Numerical Optimization in ML

- 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:  $\mathbf{w}^T x_a$ 

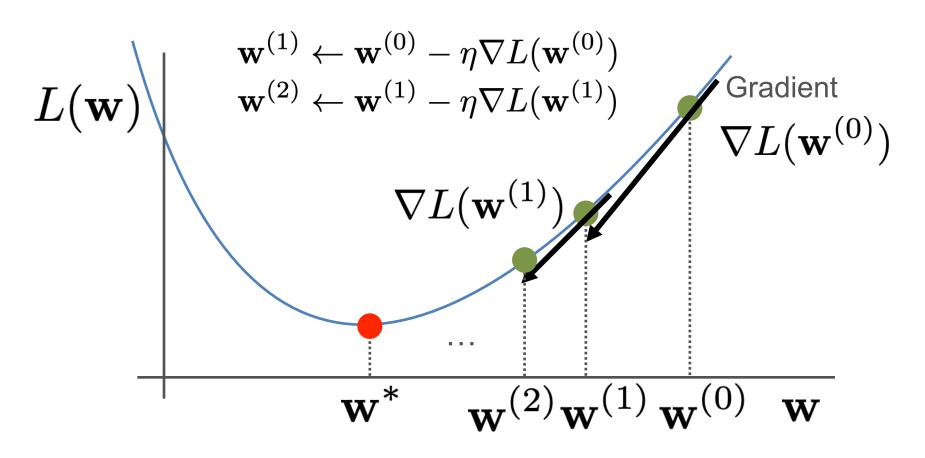


## **Batch Gradient Descent for ML**

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

- In many cases, loss function I() 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 w<sup>(0)</sup>
  - riangle Compute **gradient**:  $\nabla L(\mathbf{w}^{(k)}) = \sum_{i=1}^n \nabla l(y_i, f(\mathbf{w}^{(k)}, x_i))$
  - ullet 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

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

Y	X1	X2	Х3
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,	0,6b,	

- 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)

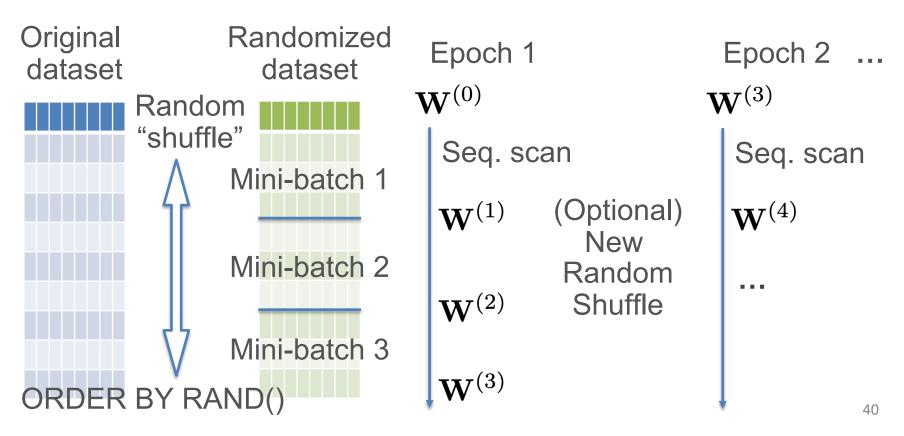
### Stochastic Gradient Descent for ML

- 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:
    - Select
    - Non-deduplicating project
    - Simple SQL aggregates
    - GROUP BY aggregates
  - ML systems:
    - Matrix sum/norms
    - (Stochastic) Gradient Descent

# Peer Instruction Activity

(Switch slides)

### 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. It has 20 columns, all of the 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 data layout format for 2-D structured data?
- 5. You lay out 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 million examples. Mini-batch size is set to 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?

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  - Single-Node Multi-Core; SIMD; Accelerators
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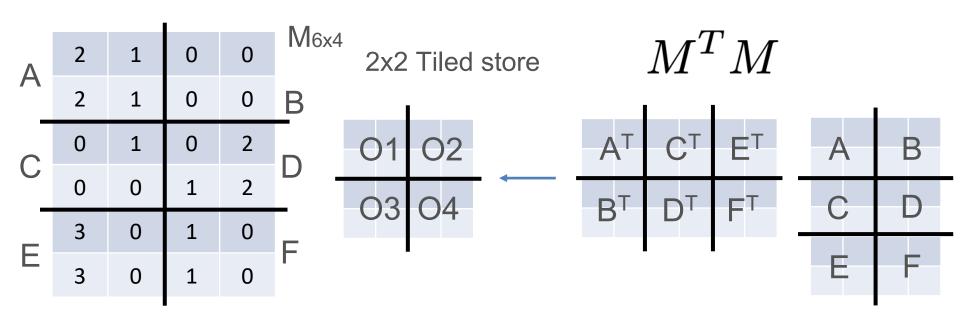
Optional: Another Example of Scaling Data Science Operations
Not included in syllabus

# Scaling to Disk: Gramian Matrix

2	1	0	0	M6x4	$M^{'}$	$^TM$	
2	1	0	0				
0	1	0	2	Row-store:	2,1,	2,1	0,1,
0	0	1	2		0,0	0,0	0,2
3	0	1	0		0,0,	3,0,	3,0,
3	0	1	0		1,2	1,0	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<sup>T</sup>A + C<sup>T</sup>C + E<sup>T</sup>E; 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<sup>T</sup>B in O2; read C, D to add C<sup>T</sup>D to O2; read E, F to add E<sup>T</sup>F 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!