Announcements and Feedback

- If you have not registered your team yet, please do so ASAP
  - For those that have registered, you should have gotten an introduction email from your assigned TA
- Example problem statements will be posted to Piazza
- Many questions on data set
- Phase 2 and 3 are coming this week!
Do I Need More Data?

- 2000 lines is just a minimum
- Part of the Phase 1 process is where you have to determine if your data is going to work towards your goals
  - Think back to the demo in class with Real Estate data
  - If my goal was to look specifically at single family homes across different neighborhoods, I would probably need more data
- Don't be afraid to get data from multiple sources!
What to Turn In and How

- One submission **per team** (will fix in the handout)
- Your submission will consist of your code as well as a write up
  - The write up will describe **why** you did the operations you did and explain **what you learned**
- Submission will probably be through UBLearns, but that is still TBD
What to Expect from Phase 2 and 3

- Phase 2 will focus on applying modeling and algorithms to your data to address your problem statement, and visualizing the results
  - You will be required to try a certain number of statistical models/ML algorithms. Some from class, some from external sources.
  - You must explain the motivation for using a particular technique and what you learned from applying it.
- Phase 3 will focus on building a data product based on your findings
  - You will also record a short demo of your product
Recap from Last Class

- Live demo of MapReduce execution on local instance of Hadoop
  - Viewed/manipulated our local Hadoop instance via browser and command-line
  - Defined a Mapper, Reducer, and main for a simple word count problem
  - Executed our job and updated our code based on observations

- Very simple code — scales up without change
- The execution/parallelization details are handled by Hadoop
Where is MR Actually Used?

- Google uses it (we think) for wordcount, adwords, pagerank, indexing
- Simple algorithms such as grep, text-indexing, reverse indexing
- Bayesian classification: data mining
- Facebook uses it for various things, ie demographic information
- Financial services use it for analytics
- Astronomy: Gaussian analysis for location extra-terrestrial objects
- Expected to play a critical role in semantic web and web3.0
Where is MR Actually Used?

- Google uses it (we think) for wordcount, adwords, pagerank, indexing
- Simple algorithms such as grep, text-indexing, reverse indexing
- Bayesian classification: data mining
- Facebook uses it for various things, i.e., demographic information
- Financial services use it for analytics
- Astronomy: Gaussian analysis for location extra-terrestrial objects
- Expected to play a critical role in semantic web and web3.0
- **Bioinformatics and Next-Generation Sequencing (NGS)**
Case Study: Optimizing MapReduce

- Many applications in BioInformatics revolve around next-generation sequencing
  - "NGS has become the leading application area in the domain of bioinformatics" [1]
- Process of analyzing sequences such as DNA to understand different characteristics of an organism
- Very large DNA strings (sequences of A,C,G,T bases)
  - Hundreds of GB of sequence data can be generated from single experiments
- A number of different problems arise: k-mer counting, sequence quality assessment, read alignment, fast similarity search, etc
- Two sources of knowledge required: domain specific, and big data

Case Study: Optimizing MapReduce

- Many applications in BioInformatics revolve around next-generation sequencing
  - "NGS has become the leading application area in the domain of bioinformatics" [1]
- Process of analyzing sequences such as DNA to understand different characteristics of an organism
- Very large DNA strings (sequences of A,C,G,T bases)
  - Hundreds of GB of sequence data can be generated from single experiments
- A number of different problems arise: k-mer counting, sequence quality assessment, read alignment, fast similarity search, etc
- Two sources of knowledge required: domain specific, and big data

Many established MapReduce libraries exist for Bioinformatics and NGS

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CloudBLAST [9]</td>
<td>Combining MapReduce and virtualization on distributed resources for Bioinformatics applications</td>
</tr>
<tr>
<td>CloudBurst [10]</td>
<td>Highly sensitive read mapping with MapReduce</td>
</tr>
<tr>
<td>Crossbow [12]</td>
<td>Searching for SNPs with cloud computing</td>
</tr>
<tr>
<td>GATK [13]</td>
<td>A MapReduce framework for analyzing next-generation DNA sequencing data</td>
</tr>
<tr>
<td>Myrna [14]</td>
<td>Cloud-scale RNA-sequencing differential expression analysis</td>
</tr>
<tr>
<td>Galaxy [15]</td>
<td>A comprehensive approach for supporting accessible, reproducible, and transparent computational research in the life sciences</td>
</tr>
<tr>
<td>SEAL [16]</td>
<td>A distributed short read mapping and duplicate removal tool</td>
</tr>
<tr>
<td>CloudAligner [17]</td>
<td>A fast and full-featured MapReduce based tool for sequence mapping</td>
</tr>
<tr>
<td>Contrail [18]</td>
<td>A de Bruijn Genome assembler that uses Hadoop</td>
</tr>
<tr>
<td>FX [19]</td>
<td>an RNA-Seq analysis tool on the cloud</td>
</tr>
<tr>
<td>BioPig [20]</td>
<td>A Hadoop-based analytic toolkit for large-scale sequence data</td>
</tr>
<tr>
<td>SeqPig [21]</td>
<td>Simple and scalable scripting for large sequencing data sets in Hadoop</td>
</tr>
<tr>
<td>Halvade [22]</td>
<td>Scalable sequence analysis with MapReduce</td>
</tr>
</tbody>
</table>
k-mer Counting

- k-mer counting is a critical first step for many NGS applications
- A k-mer refers to all the possible subsequences of length k in a DNA/RNA sequence
- k-mer counting returns a count of every k-mer present in a sequence

"When the k-mer size is large and billions of reads need to be processed, k-mer counting becomes the most difficult problem in Bioinformatics" [1]
k-mer Counting Mapper

$k = 3$

ACGGCTAGAACGCTAACCAGATCAGTCAGCTAGAC...

<"ACG",1>
k-mer Counting Mapper

k = 3

ACGGCTAGAACGCTAACCGATCAGTCAGCTAGAC...

<"ACG",1>

<"CGC",1>
k-mer Counting Mapper

k = 3

ACGGCTAGAACGCTAAACCGATCAGTCAGCTAGAC...

<"ACG",1>  <"GGC",1>

<"CGC",1>
k-mer Counting Mapper

$k = 3$

ACGGCTAGAACGCTAAACCGATCAGTCAGCTAGAC...

- <"ACG",1>
- <"CGC",1>
- <"GGC",1>
- <"GCT",1>
- <"CGC",1>
k-mer Counting Mapper

k = 3

ACGGCTAGAACGCTAAACCGATCAGTCAGCTAGAC...

"ACG",1
"GCT",1
"CGC",1
"GCT",1
"CTA",1
"TAG",1
"AGA",1
"GAA",1
"AAC",1
"AAG",1
etc...
k-mer Counting Mapper

map(input):
    for i in [0,input.length - k):
        emit(input[i:i+k], 1)
Optimizing k-mer Counting

● Primary goal of the paper is to study optimization techniques for k-mer counting (in BPiG library)
● Studied many different configuration parameters, segmented into four groups:
  ○ CPU, Memory, I/O, and Network
CPU and Memory are obviously important, however many data-intensive MapReduce applications are I/O and network bound. Primary parameters in CPU/Memory relate to the number of available cores, and the memory allocated to each container. These are heavily dependent on the particular cluster being used. The one parameter they did look at in a bit more detail is control over Java garbage collection (GC).
Disk Relevant Parameters

- Intermediate data (largely from mappers) is also stored in HDFS.
- Hadoop applications are often I/O bound; managing intermediate data size and I/O costs can provide large benefits.
- Relevant parameters are block size and data compression.
Network Parameters

- Mapping phase does not require network usage (computation is performed local to the data!)
- Reduce phase requires significant network usage
  - Shuffle – can run during map phase, but finishes after map completes
  - Sort – runs after shuffle completes
  - Reduce – runs after sort completes
- MapReduce allows overlap of shuffle and map phases
Network Parameters

Fig. 2. Decomposition of reducer phases. [1]
Network Parameters

Fig. 2. Decomposition of reducer phases. [1]
Intermediate Data

- Intermediate data is the data that is produced during MapReduce execution (primarily from mappers)
- This data is also stored in HDFS
- Intermediate data is HUGE in k-mer counting
  - Think about how many key-value pairs are produced for a single character in the input string...
Intermediate Data

Table 5
Characteristics of intermediate data for common Hadoop applications.

<table>
<thead>
<tr>
<th>Job Name</th>
<th>Input data Size (TB)</th>
<th>Int. data Size (TB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogProc</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>NdayModel</td>
<td>3.54</td>
<td>3.54</td>
<td>100%</td>
</tr>
<tr>
<td>BehaviorModel</td>
<td>3.60</td>
<td>9.47</td>
<td>263%</td>
</tr>
<tr>
<td>ClickAttribution</td>
<td>6.80</td>
<td>8.20</td>
<td>121%</td>
</tr>
<tr>
<td>SegmentExploder</td>
<td>14.10</td>
<td>25.20</td>
<td>179%</td>
</tr>
<tr>
<td>LogRead</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>LogCount</td>
<td>1.10</td>
<td>0.04</td>
<td>4%</td>
</tr>
</tbody>
</table>

Table 6
Characteristics of intermediate data for k-mer (k=20) counting.

<table>
<thead>
<tr>
<th>Input size (GB)</th>
<th>Int. data size (GB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.5</td>
<td>1350%</td>
</tr>
<tr>
<td>5</td>
<td>67.7</td>
<td>1354%</td>
</tr>
<tr>
<td>10</td>
<td>135.4</td>
<td>1354%</td>
</tr>
<tr>
<td>20</td>
<td>270.9</td>
<td>1355%</td>
</tr>
<tr>
<td>40</td>
<td>541.5</td>
<td>1354%</td>
</tr>
<tr>
<td>60</td>
<td>830.0</td>
<td>1383%</td>
</tr>
<tr>
<td>100</td>
<td>1381.0</td>
<td>1381%</td>
</tr>
</tbody>
</table>
## Intermediate Data

### Table 5
Characteristics of intermediate data for common Hadoop applications.

<table>
<thead>
<tr>
<th>Job Name</th>
<th>Input data Size (TB)</th>
<th>Int. data Size (TB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogProc</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>NdayModel</td>
<td>3.54</td>
<td>3.54</td>
<td>100%</td>
</tr>
<tr>
<td>BehaviorModel</td>
<td>3.60</td>
<td>9.47</td>
<td>263%</td>
</tr>
<tr>
<td>ClickAttribution</td>
<td>6.80</td>
<td>8.20</td>
<td>121%</td>
</tr>
<tr>
<td>SegmentExploder</td>
<td>14.10</td>
<td>25.20</td>
<td>179%</td>
</tr>
<tr>
<td>LogRead</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>LogCount</td>
<td>1.10</td>
<td>0.04</td>
<td>4%</td>
</tr>
</tbody>
</table>

### Table 6
Characteristics of intermediate data for k-mer (k=20) counting.

<table>
<thead>
<tr>
<th>Input size (GB)</th>
<th>Int. data size (GB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.5</td>
<td>1350%</td>
</tr>
<tr>
<td>5</td>
<td>67.7</td>
<td>1354%</td>
</tr>
<tr>
<td>10</td>
<td>135.4</td>
<td>1354%</td>
</tr>
<tr>
<td>20</td>
<td>270.9</td>
<td>1355%</td>
</tr>
<tr>
<td>40</td>
<td>541.5</td>
<td>1354%</td>
</tr>
<tr>
<td>60</td>
<td>830.0</td>
<td>1383%</td>
</tr>
<tr>
<td>100</td>
<td>1381.0</td>
<td>1381%</td>
</tr>
</tbody>
</table>
# Intermediate Data

More than 10 fold increase to data size

## Table 5
Characteristics of intermediate data for common Hadoop applications.

<table>
<thead>
<tr>
<th>Job Name</th>
<th>Input data Size (TB)</th>
<th>Int. data Size (TB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogProc</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>NdayModel</td>
<td>3.54</td>
<td>3.54</td>
<td>100%</td>
</tr>
<tr>
<td>BehaviorModel</td>
<td>3.60</td>
<td>9.47</td>
<td>263%</td>
</tr>
<tr>
<td>ClickAttribution</td>
<td>6.80</td>
<td>8.20</td>
<td>121%</td>
</tr>
<tr>
<td>SegmentExploder</td>
<td>14.10</td>
<td>25.20</td>
<td>179%</td>
</tr>
<tr>
<td>LogRead</td>
<td>1.10</td>
<td>1.10</td>
<td>100%</td>
</tr>
<tr>
<td>LogCount</td>
<td>1.10</td>
<td>0.04</td>
<td>4%</td>
</tr>
</tbody>
</table>

## Table 6
Characteristics of intermediate data for k-mer (k=20) counting.

<table>
<thead>
<tr>
<th>Input size (GB)</th>
<th>Int. data size (GB)</th>
<th>Int./Input</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>13.5</td>
<td>1350%</td>
</tr>
<tr>
<td>5</td>
<td>67.7</td>
<td>1354%</td>
</tr>
<tr>
<td>10</td>
<td>135.4</td>
<td>1354%</td>
</tr>
<tr>
<td>20</td>
<td>270.9</td>
<td>1355%</td>
</tr>
<tr>
<td>40</td>
<td>541.5</td>
<td>1354%</td>
</tr>
<tr>
<td>60</td>
<td>830.0</td>
<td>1383%</td>
</tr>
<tr>
<td>100</td>
<td>1381.0</td>
<td>1381%</td>
</tr>
</tbody>
</table>

*More than 10 fold increase to data size*
Data Compression

- Compressing data can help balance work between I/O and CPU.
- I/O bound applications often find it worth it to spend extra CPU cycles to compress data so that I/O burden is lesser.
  - Also helps with communication burden on the network.
- For BPigs k-mer counting, enabling compression resulted in more than 50% drop in disk I/O and ~10% decrease in runtime.
## Data Compression Results

### Table 7

IO Improvement from data compression.

<table>
<thead>
<tr>
<th>Data size</th>
<th>Counter group(GB)</th>
<th>Uncompressed</th>
<th>COMPRESSED</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Map</td>
<td>Reduce</td>
<td>Total</td>
</tr>
<tr>
<td>40GB</td>
<td>Number of bytes read</td>
<td>604</td>
<td>598</td>
<td>1202</td>
</tr>
<tr>
<td></td>
<td>Number of bytes written</td>
<td>1200</td>
<td>598</td>
<td>1798</td>
</tr>
<tr>
<td>60GB</td>
<td>Number of bytes read</td>
<td>929</td>
<td>917</td>
<td>1846</td>
</tr>
<tr>
<td></td>
<td>Number of bytes written</td>
<td>1839</td>
<td>917</td>
<td>2756</td>
</tr>
</tbody>
</table>
# Data Compression Results

## Table 7

<table>
<thead>
<tr>
<th>Data size</th>
<th>Counter group(GB)</th>
<th>Uncompressed</th>
<th></th>
<th>Compressed</th>
<th></th>
<th>Difference</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Map</td>
<td>Reduce</td>
<td>Total</td>
<td>Map</td>
<td>Reduce</td>
<td>Total</td>
</tr>
<tr>
<td>40GB</td>
<td>Number of bytes read</td>
<td>604</td>
<td>598</td>
<td>1202</td>
<td>283</td>
<td>131</td>
<td>414</td>
</tr>
<tr>
<td></td>
<td>Number of bytes written</td>
<td>1200</td>
<td>598</td>
<td>1798</td>
<td>550</td>
<td>131</td>
<td>681</td>
</tr>
<tr>
<td>60GB</td>
<td>Number of bytes read</td>
<td>929</td>
<td>917</td>
<td>1846</td>
<td>442</td>
<td>167</td>
<td>609</td>
</tr>
<tr>
<td></td>
<td>Number of bytes written</td>
<td>1839</td>
<td>917</td>
<td>2756</td>
<td>853</td>
<td>167</td>
<td>1020</td>
</tr>
</tbody>
</table>
Spilling

- I/O is a big bottleneck, we want to reduce this cost as much as we can.
- What happens when we run out of memory while working with intermediated data:
  - The data must be written to disk. This is called a spill.
  - Spills during mapping are particularly problematic.
- For k-mer counting, the large intermediate data can cause significant spilling overheads:
  - Spill behavior can be controlled by block size and memory per container.
Spilling

Fig. 1. The flow of data processing across MapReduce tasks.
Spilling

When this runs out of space, a spill occurs!

**Fig. 1.** The flow of data processing across MapReduce tasks.
The Cost of Spilling

- One "spill" per map task is the ideal case (intermediate data just written out to disk once when task completes)
- If there is more than one spill for a map task, it results in 3x the I/O cost because the previous spill data must be read in, and sorted and merged with the current overflow data
- Keeping the number of spills to 1 per map task can be one of the most effective ways to improve MapReduce performance
Spilling and Block Size

- Big block size is good to lower startup overhead for mappers
  - But it can lead to more spilling — especially with the large intermediate data size of k-mer
- Experimentation with BPig actually found lower block size to be better overall due to decrease in spill count
- Lower block size still left some mappers with multiple spills, so more memory was allocated to the maps ring buffer
Spilling and Block Size
Spilling and Block Size

Job Execution Time (mins)

Up to ~25% performance improvement
Networking

- Overlapping map and shuffle can lead to benefits but can also interfere with mapping, and leave long running reduce tasks dangling.
- Experimental results from this work showed best performance with no overlap whatsoever.
Networking

**Fig. 5.** Impact of reducer start time.
Networking

Long running shuffle tasks

![Diagram showing average stage execution time with categories Map, Shuffle, Merge, and Reduce.]

**Fig. 5.** Impact of reducer start time.
Overall Results

Fig. 6. Impact factors.

Fig. 7. Performance comparison.
Overall Results

Spill reduction had a huge impact!

Fig. 6. Impact factors.

Fig. 7. Performance comparison.
Summary

- Bioinformatics has a number of relevant use cases for MapReduce
  - k-mer counting is a critical component for many other types of analysis
- I/O bottlenecks can cause significant issues for data-intensive MapReduce applications
- Tuning to eliminate extra spills and to keep I/O costs low can yield significant improvement
- Application stayed simple (and the same). Flexibility and simplicity of MapReduce is still a win!