Embarrassingly Parallel

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20/02/2019

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https://goo.gl/TJyhmL

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- Several Example Parallel Problems/Techniques
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time permitting:

- The KubeNow Project
- The H2O Platform

Concurrency vs Parallelism

- **Concurrency/Multithreading:** is when two or more tasks can start, run, and complete in overlapping time periods. It doesn't necessarily mean they'll ever be running at the same instant. Eg. multitasking on a single-core machine.
- **Parallelism:** is when tasks literally run at the same time, eg. on a multicore processor.

https://stackoverflow.com/a/1050257

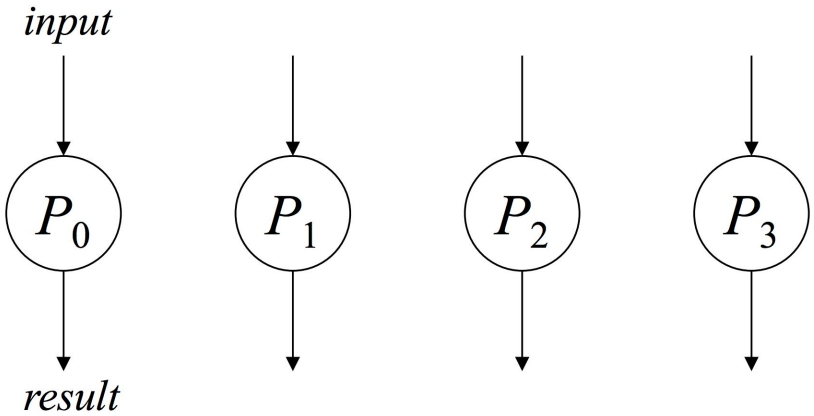
Quoting *Oracle's Multithreaded Programming Guide*:

- **Concurrency:** A condition that exists when at least two threads are making progress. A more generalized form of parallelism that can include time-slicing as a form of virtual parallelism.
- **Parallelism:** A condition that arises when at least two threads are executing simultaneously.

Java Concurrency and Multithreading Tutorial:
http://tutorials.jenkov.com/java-concurrency/index.html

Ideal Parallelism

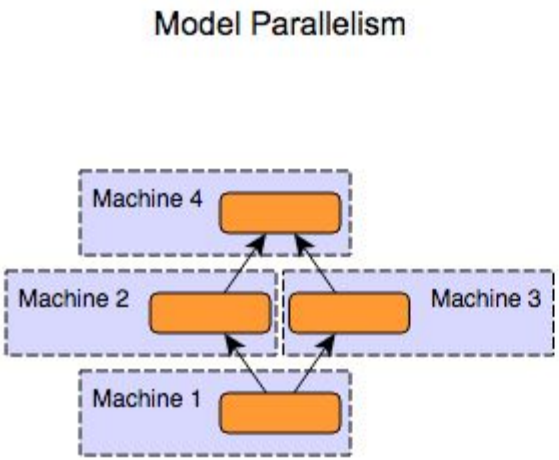
- An ideal parallel computation can be immediately divided into completely independent parts
  - “Embarrassingly parallel”
  - “Naturally parallel”
- No special techniques or algorithms required

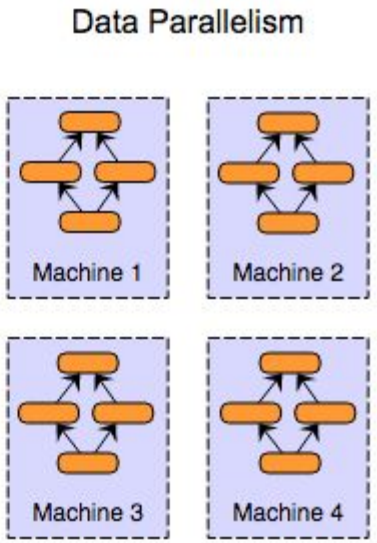


https://www.cs.fsu.edu/~engelen/courses/HPC/Algorithms1.pdf

Parallelisation Approaches

- **Model Parallelism:** different machines in the distributed system are responsible for the computations in different parts of a single network - for example, each layer in the neural network may be assigned to a different machine
- **Data Parallelism:** different machines have a complete copy of the model; each machine simply gets a different portion of the data, and results from each are somehow combined.

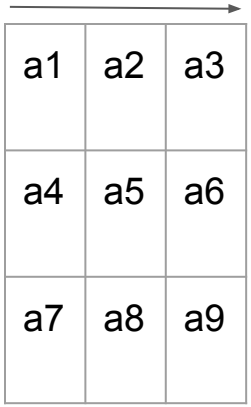


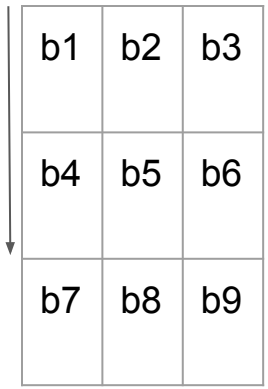


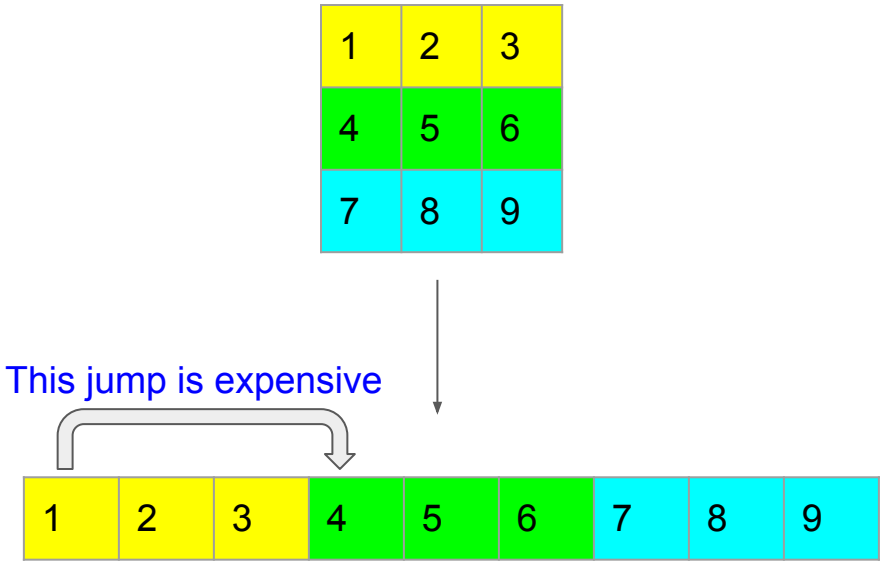
http://engineering.skymind.io/distributed-deep-learning-part-1-an-introduction-to-distributed-training-of-neural-networks

Memory Coalescing 1/2

- 2D matrices are represented as vectors in memory
- Take two **square** Matrices **A** and **B**, we want to: **A.B**
- When Multiplying Matrices, we make expensive moves in **B**

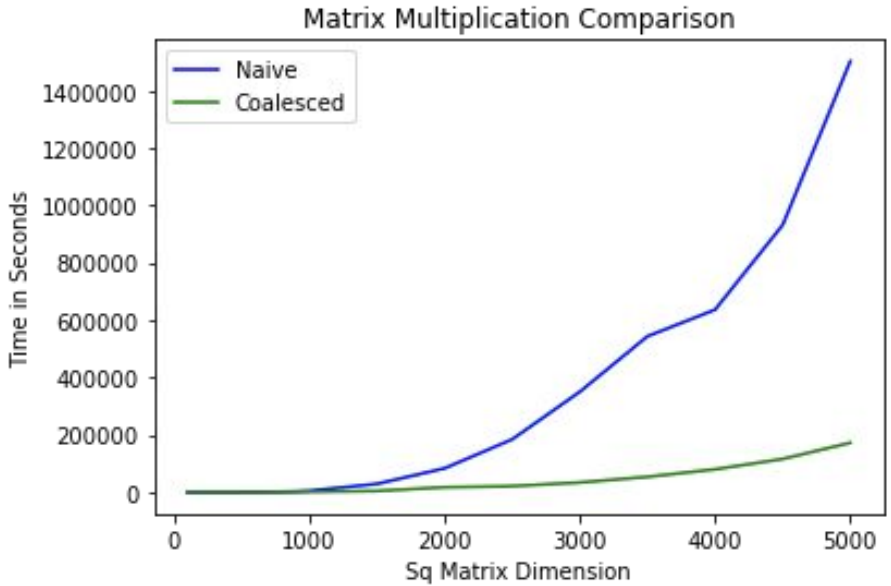






Memory Coalescing 2/2

- Square Matrix Multiplication in Java
- Transpose B
- Move row by row instead of column by column

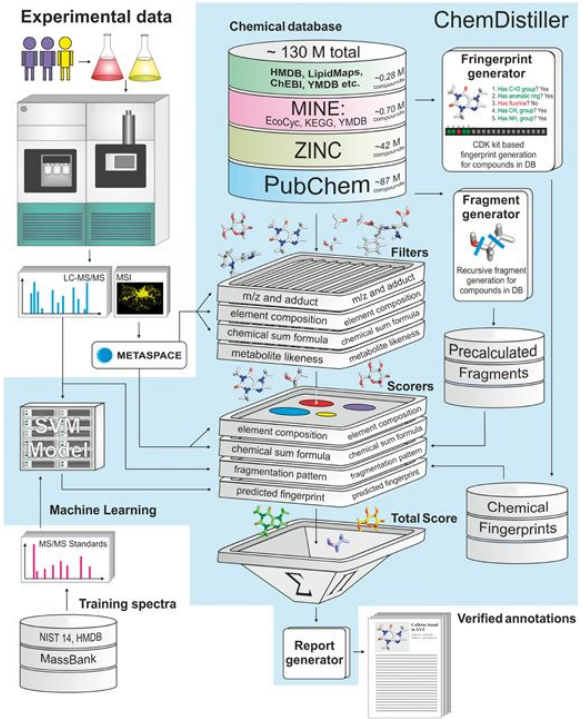


HPC Usage Example 1:

- Task - Permutation test
  - Data: one dataset -> created **10k** datasets by randomising the variables (not the outcome)
  - Run linear regression with 10 fold cross validation on each dataset to obtain a score (e.g. RMSE)
- Performance:
  - When done sequentially, using 1 core, 10k datasets took **> 83 hours**
  - When parallelising the task, using a HPC cluster, 10k datasets took **< 83 minutes**

HPC Usage Example (The ChemDistiller Project):

- Task - Compute Fingerprints for ~130 Million Chemical Compounds
- Data: 13k files, each containing 10k compounds
  - Input compound representation: SMILES
- Performance:
  - Using 1 core, in average, 1 file takes ~ 8 hours, up to 24 hours for files with larger molecules
  - When done sequentially, using 1 core, the 130M compounds would finish in **> 11 YEARS (1-2 years using 8 cores)**
  - **When parallelising the task, using a HPC cluster, 130M compounds took ~ 22 days**

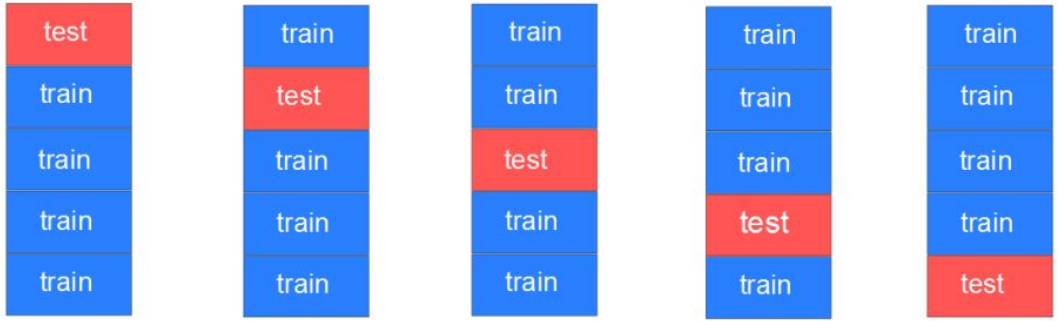


ChemDistiller: an engine for metabolite annotation in mass spectrometry

https://academic.oup.com/bioinformatics/article/34/12/2096/4852828

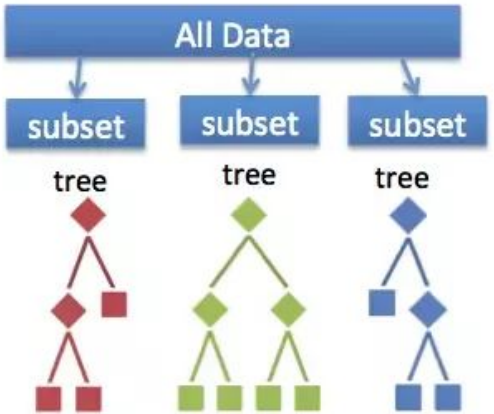
Cross Validation

- A model is trained using **k-1** of the folds as training data
- The resulting model is validated on the remaining part of the data (i.e., it is used as a test set to compute a performance measure such as accuracy).

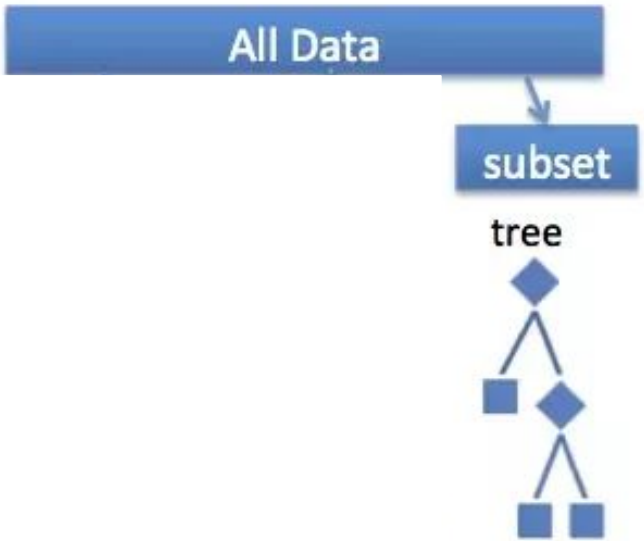


Random Forest

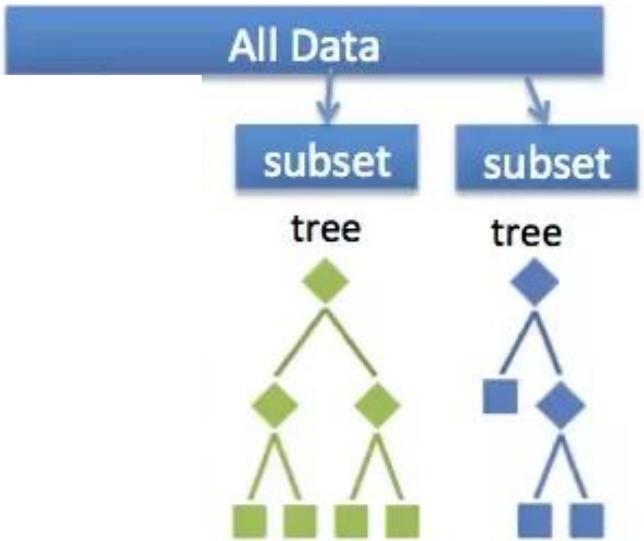
- Random forest algorithm is a supervised classification algorithm. As the name suggests, this algorithm creates the forest with a number of trees
    - In general, the **more trees in the forest** the more robust the forest looks like.
- Bootstrapping algorithm with Decision tree (CART) model.
- Say, we have **n** observations in the complete population with **m** variables.
- Random forest tries to build multiple CART models with different samples and different initial variables.
    - For instance, it will take a random sample of **i** observations and **j** randomly chosen initial variables to build a CART model (**j << m**).
    - It will repeat the process (say) **k** times and then make a final prediction on each observation.
    - Final prediction can simply be the mean (or mode) of each prediction.



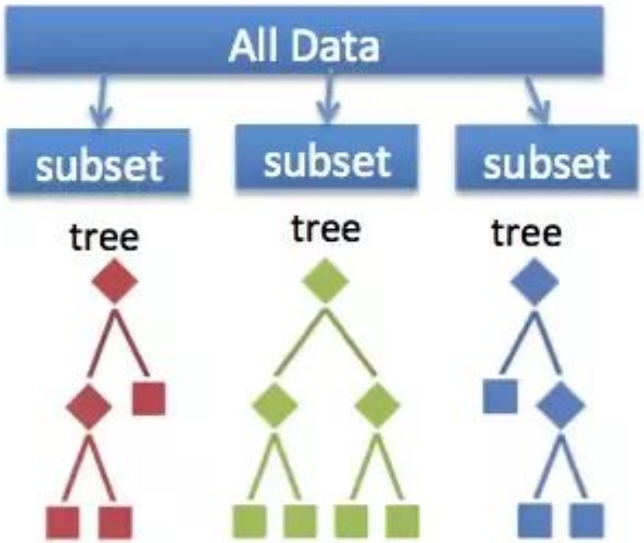
Random Forest



Random Forest



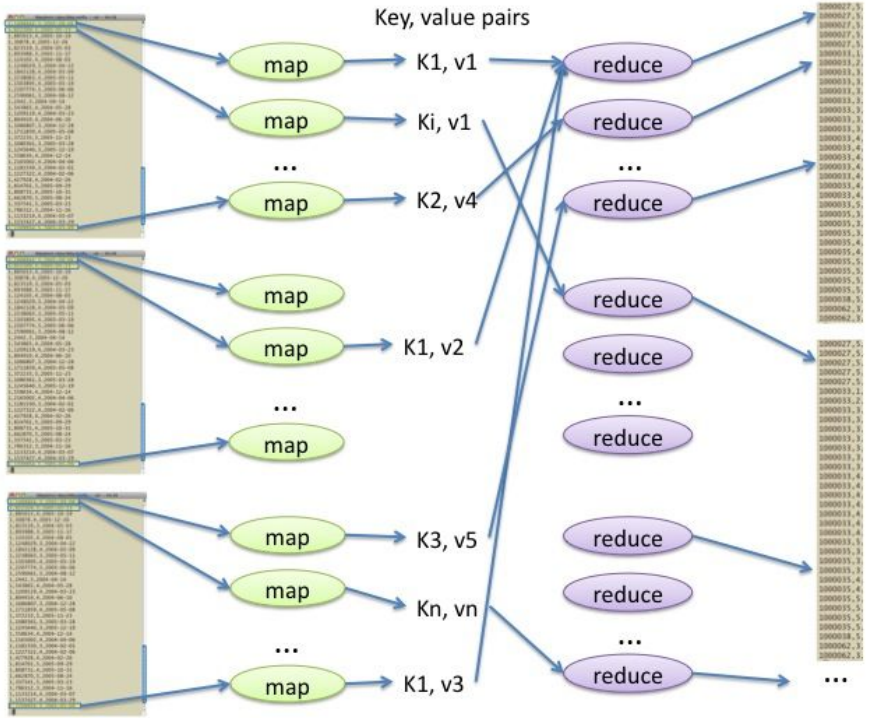
Random Forest



Analysing Very Large Files

- **Map** functions can run in parallel and pass their results to **Reduce** functions
- Results are output in sorted order by the keys created by the reduce function

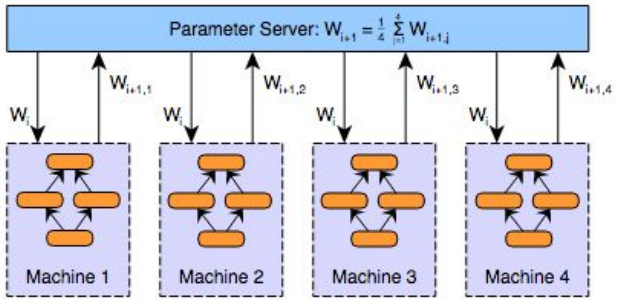
- **Sorting very large files?**



http://selkie.macalester.edu/csinparallel/modules/IntroWMR/build/html/MapReduceIntro/MapReduceIntro.html

Neural Nets Parameter Averaging

1. Initialize the network parameters randomly based on the model configuration
2. Distribute a copy of the current parameters to each worker
3. Train each worker on a subset of the data
4. Set the global parameters to the average the parameters from each worker
5. While there is more data to process, go to step 2



- Steps 2 through 4 are demonstrated in the diagram
- *W* represents the parameters (weights, biases) in the neural network
- Subscripts are used to index the version of the parameters over time, and where necessary for each worker machine

Correlation Matrix

$$r = \frac{1}{n-1} \sum_{i=1}^{n} \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right)$$

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	probeset	ITCC0600	ITCC0601	ITCC0602	ITCC0604	ITCC0607	ITCC0608	ITCC0609	ITCC0611	itcc0001	itcc0002	itcc0003	itcc0008	itcc0009	itcc0010	itcc0013
2	1007_s_at	430.8	226.1	130.6	75	54.9	195.5	124.8	221.5	82.1	57.5	67.1	174	55.8	143.6	110.2
3	1053_at	79.5	95.7	178.8	185.8	144.7	113.1	150.2	157.5	138.4	140.7	198.1	123.7	254.8	130.4	161.5
4	117_at	65.9	14.9	1.8	28.7	4.7	35.2	3	25.5	39.3	17.3	23.7	39.7	4.1	29.8	64.1
5	121_at	203.3	79.4	74.1	60.3	79.7	54.5	60.1	113.3	95.6	85.8	80.1	81.9	72.7	91.9	112.1
6	1255_g_at	5	129.8	177.8	291.1	192.4	20	255.4	5.6	54.9	56.6	63.8	61.2	300	41.1	40.9
7	1294_at	114.6	57.1	40.1	37.1	44.2	50.9	40.4	28.3	56.3	51.6	38.6	127.8	44	79.4	83.8
8	1316_at	113	92.7	115.1	106.5	63.5	103.6	121.6	97.8	26.1	33.2	27	33.5	24	17.3	52.9
9	1320_at	12.1	17.9	1.7	1	2.2	11.2	17.2	16.1	33.2	58.1	27.4	14.3	46.6	37.9	40.4
10	1405_i_at	313.8	135.4	26.1	89.8	164.4	223.2	81	15.7	64.1	29	13	406.7	28.9	149.7	233.3
11	1431_at	18.8	13.7	16.2	8.6	8.2	66	10.3	15.1	33	14.2	79.8	12.5	15.1	7.4	20.9
12	1438_at	2.4	51.9	5.2	9.4	22	6.2	8.3	38.6	69.7	193.6	31.5	107.6	59.1	100.6	120.6
13	1487_at	94	88.9	96	52.1	98.3	67.8	92	91.4	63	99.1	160.7	106.4	54.8	84.4	101.6
14	1494_f_at	30	18.8	33	49	34	33.5	44.9	35.3	26.1	22.9	19.8	18.7	19.8	17	29.1
15	1552256_a_at	33.4	55.5	57.9	53.1	52	60.2	63.7	117	182.2	79.1	185.9	187.1	137.1	143.8	251.8
16	1552257_a_at	109.2	78.6	70	83.8	62.7	97.1	73.4	245.7	126.6	113.4	151.9	117.9	112.2	175.1	159.7
17	1552258_at	31.2	8.3	5.3	20.3	7	20.7	35	22.7	22.6	12.2	11.5	24.9	27.3	18.7	16.5
18	1552261_at	42.2	5.9	5.1	14.1	13.7	6.5	18.9	15.2	19.7	22.5	9.9	29.8	12.8	13.8	24.9

Parallelism at Multiple Levels

- Sometimes the problem at hand is parallelizable at more than one level
- A typical example is when we want to run a parallel algorithm several times
- An example is to run RandomForest on thousands of datasets
- Which level do we choose?

Measuring Scaling Performance

Strong Scaling:

- Fixed data size (ex: 10000 datasets)
- Change number of parallel processes
- Check performance

Weak Scaling:

- Variable data size (ex: 10, 100, 1000, 10000 datasets)
- Number of parallel processes changes with data size
- Check performance

Metrics:

- Speedup $S(n) = \frac{T_1}{T_n}$

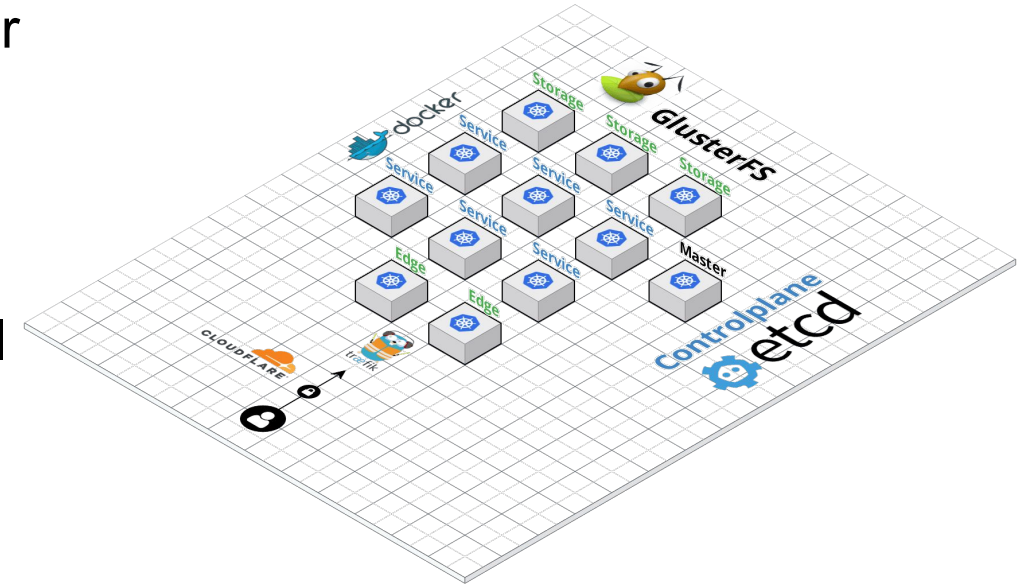
Scaling Efficiency $E(S) = \frac{T_1}{nT_n} = \frac{S(n)}{n}$

Summary

1. Embarrassingly Parallel problems are everywhere
2. It is a mindset .. a way of thinking about problem solving
3. Plenty of platforms
4. Sometimes it is a matter of mapping the problem into a format that a parallel platform can process
5. Many real life examples show it is worth the effort!

KubeNow

- A cloud agnostic platform for microservices, based on Docker and Kubernetes
- Fast Kubernetes operations
- Helps you in lifting your final application configuring DNS records and distributed storage



https://github.com/kubenow/KubeNow

Deploy PhenoMeNal with KubeNow

PhenoMeNal
Large-Scale Computing for Medical Metabolomics

KubeNow

https://goo.gl/jZx5sn

kn

kn-destroy

kn-apply

kn-az,gce

kn-ansible

kn-ssh

kn-helm

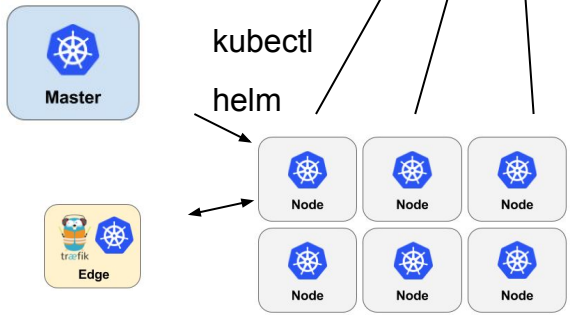
HashiCorp Terraform

ANSIBLE

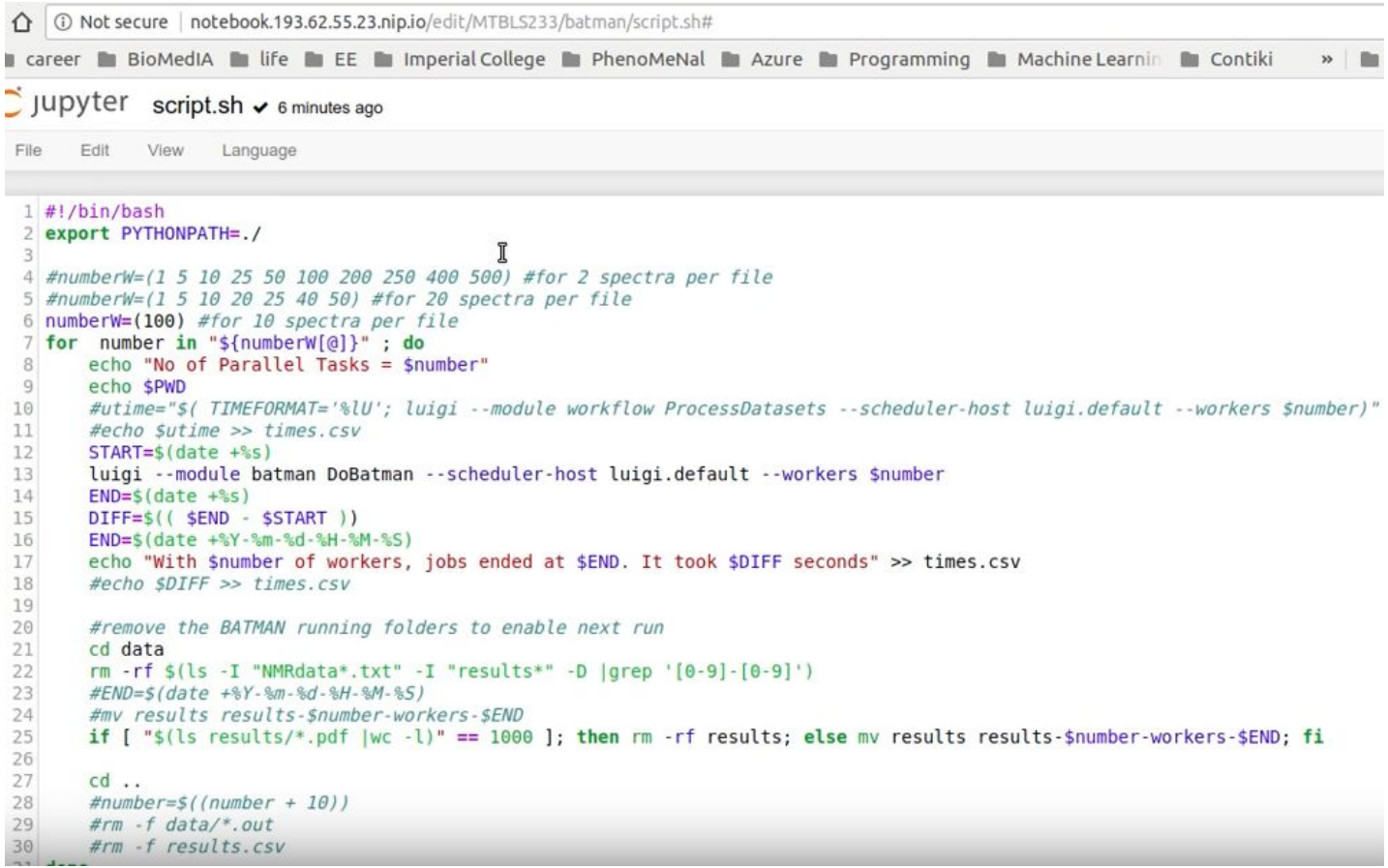
DockerHub

kubectl

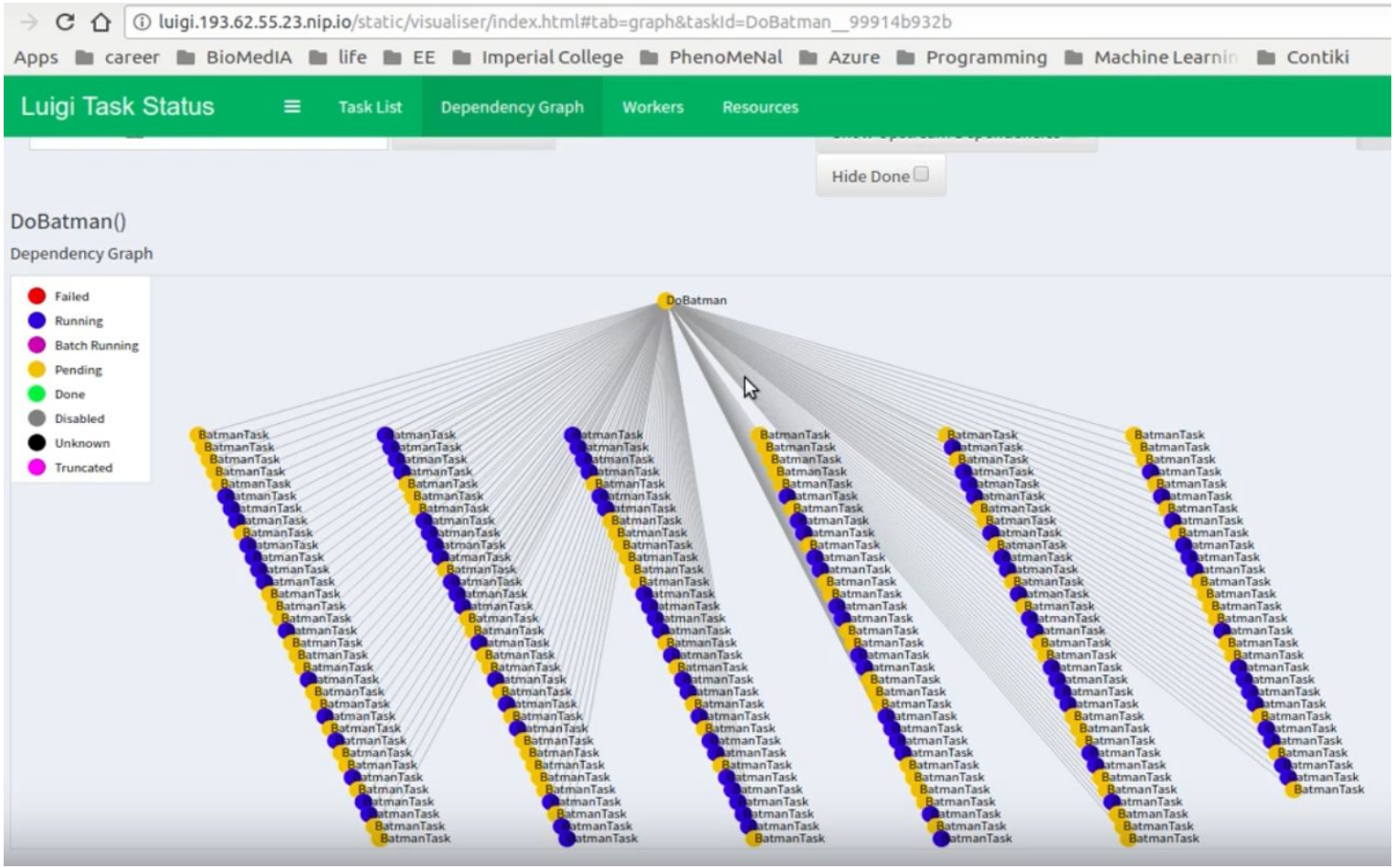
helm



Jupyter


Not secure | notebook.193.62.55.23.nip.io/edit/MTBLS233/batman/script.sh#
career BioMedIA life EE Imperial College PhenoMeNal Azure Programming Machine Learnin Contiki
jupyter script.sh 6 minutes ago
File Edit View Language
#!/bin/bash
export PYTHONPATH=./
#numberW=(1 5 10 25 50 100 200 250 400 500) #for 2 spectra per file
#numberW=(1 5 10 20 25 40 50) #for 20 spectra per file
numberW=(100) #for 10 spectra per file
for number in "${numberW[@]}" ; do
echo "No of Parallel Tasks = $number"
echo $PWD
#utime="$(TIMEFORMAT='%lU'; luigi --module workflow ProcessDatasets --scheduler-host luigi.default --workers $number)"
#echo $utime >> times.csv
START=$(date +%s)
luigi --module batman DoBatman --scheduler-host luigi.default --workers $number
END=$(date +%s)
DIFF=$(($END - $START))
END=$(date +%Y-%m-%d-%H-%M-%S)
echo "With $number of workers, jobs ended at $END. It took $DIFF seconds" >> times.csv
#echo $DIFF >> times.csv
#remove the BATMAN running folders to enable next run
cd data
rm -rf $(ls -I "NMRdata*.txt" -I "results*" -D |grep '[0-9]-[0-9]')
#END=$(date +%Y-%m-%d-%H-%M-%S)
#mv results results-$number-workers-$END
if ["$(ls results/*.pdf |wc -l)" == 1000]; then rm -rf results; else mv results results-$number-workers-$END; fi
cd ..
#number=$((number + 10))
#rm -f data/*.out
#rm -f results.csv

Luigi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Apps
career
BioMedIA
life
EE
Imperial College
PhenoMeNal
Azure
Programming
Machine Learnin
Contiki
Luigi Task Status
Task List
Dependency Graph
Workers
Resources
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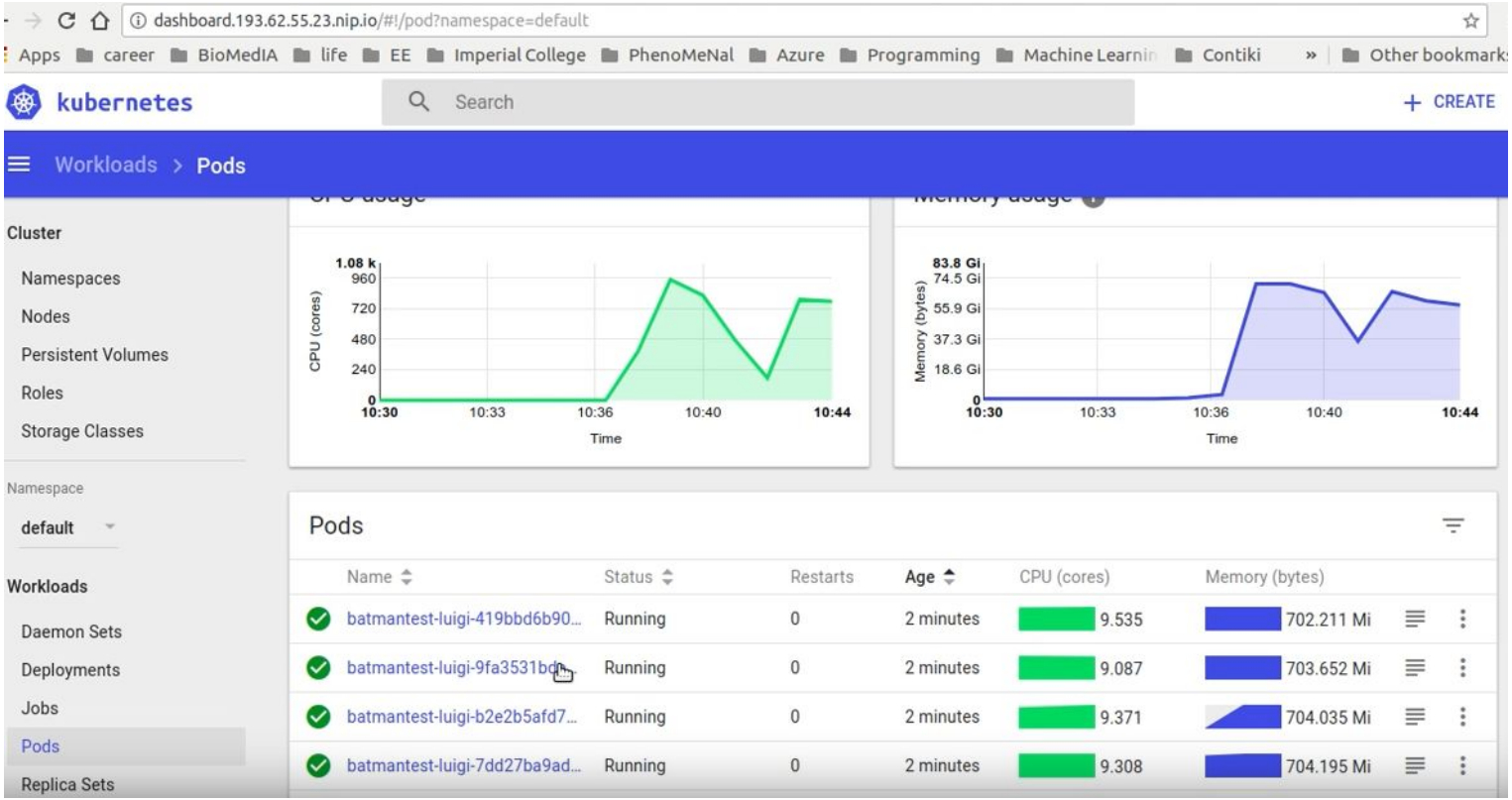
DoBatman
BatmanTask

Kubernetes Dashboard

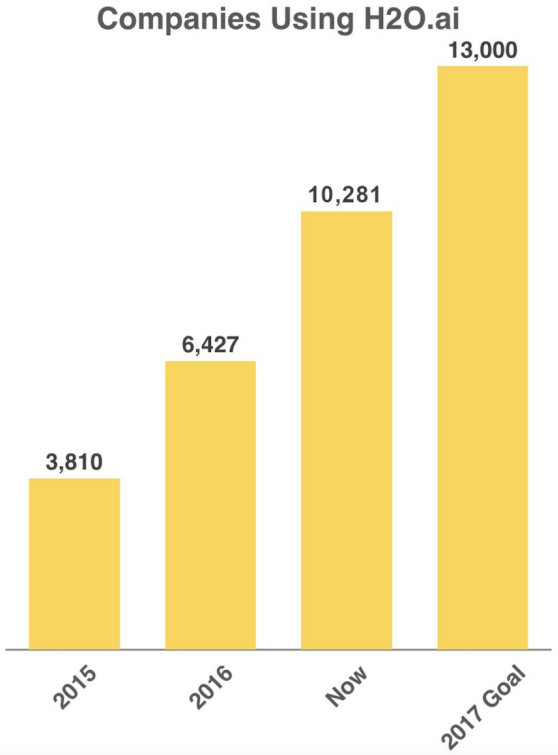


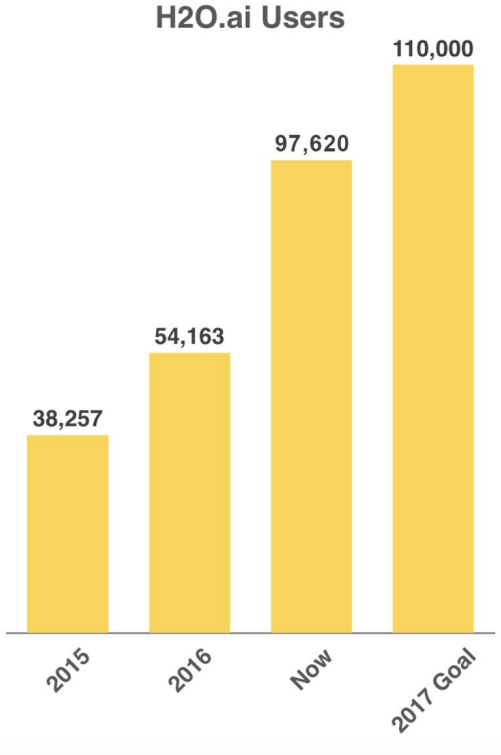
H2O.ai

- Founded in 2012, Mountain View, CA Stanford Math & Systems Engineers
- It is produced by the company *H2O.ai* (formerly *0xdata*)
- Open Source Software
- Ease of Use via Web Interface or API
- Cutting Edge Machine Learning Algorithms
- R, Python, Scala, Spark & Hadoop Interfaces Distributed Algorithms Scale to Big Data
- Simple deployment without intermediary transformations
- In-Memory Parallel Processing

- https://github.com/h2oai
- http://docs.h2o.ai
- https://www.stat.berkeley.edu/~ledell/docs/h2o_hpccon_oct2015.pdf

H2O Community





H2O: Current Algorithm Overview

Statistical Analysis

- Linear Models (GLM)
- Cox Proportional Hazards
- Naïve Bayes

Ensembles

- Random Forest
- Distributed Trees
- Gradient Boosting Machine
- R Package - Super Learner Ensembles

Deep Neural Networks

- Multi-layer Feed-Forward Neural Network
- Auto-encoder
- Anomaly Detection
- Deep Features

Clustering

- K-Means

Dimension Reduction

- Principal Component Analysis
- Generalized Low Rank Models

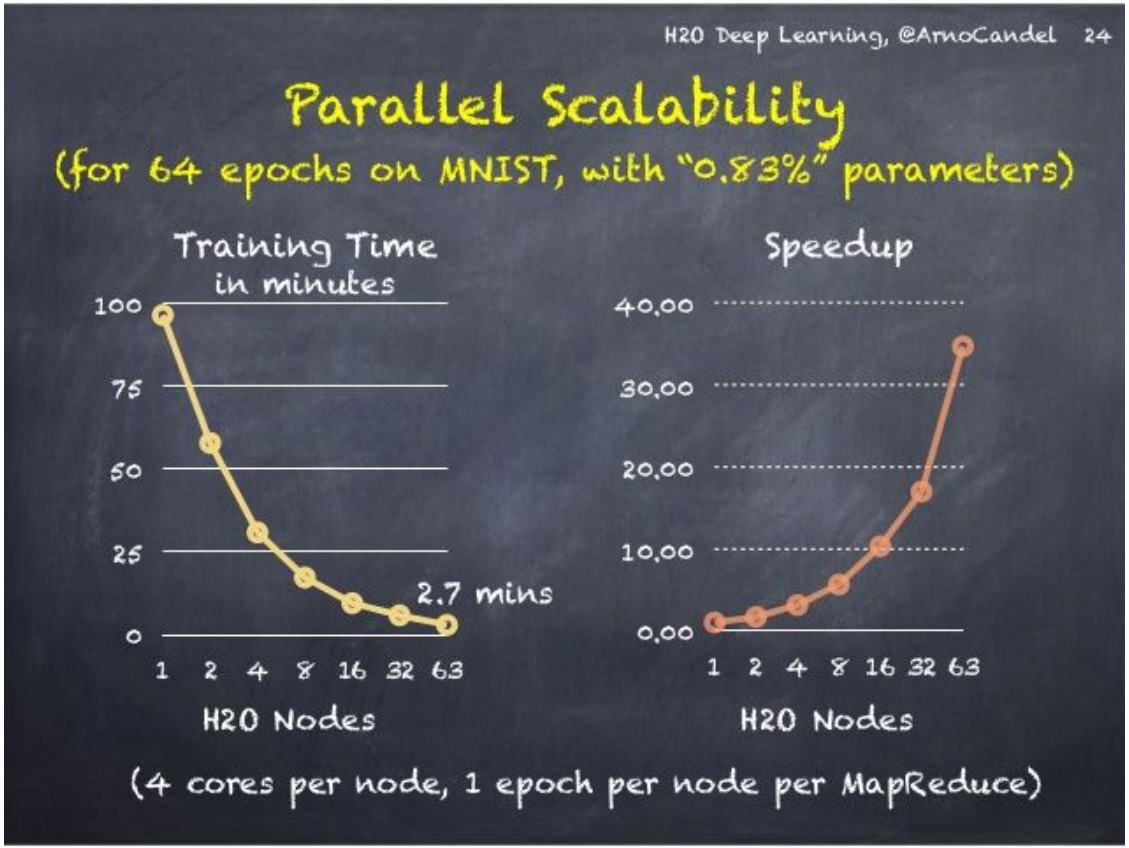
Solvers & Optimization

- Generalized ADMM Solver
- L-BFGS (Quasi Newton Method)
- Ordinary Least-Square Solver
- Stochastic Gradient Descent

Data Munging

- Integrated R-Environment
- Slice, Log Transform

H2O Scalability



Thank you