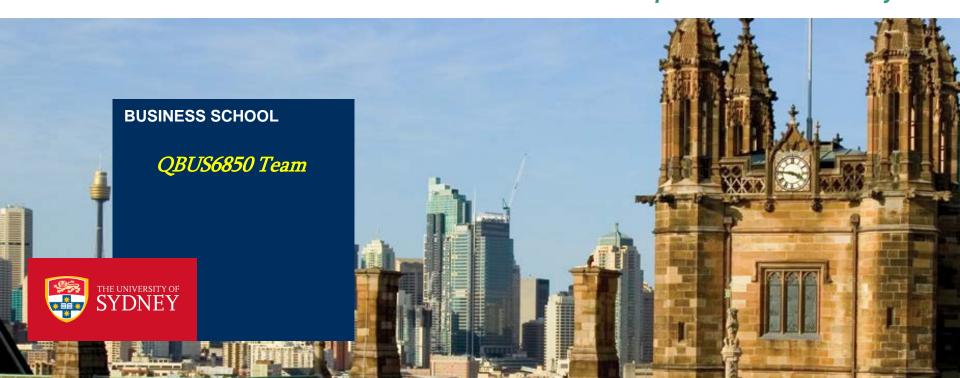
QBUS6850 Lecture 13 Machine Learning with Big Data

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□ Topics covered

- Big Data & High Performance Computing (HPC)
- Batch Gradient Descent (BGD)
- Stochastic Gradient Descent (SGD)
- Mini-batch Gradient Descent
- Map reduce

□ References

- Chu, et al. (2007): Map-Reduce for Machine Learning on Multicore
- Dean and Ghemawat (2008): MapReduce: Simplified Data Processing on Large Cluster



Learning Objectives

- Understand how Stochastic Gradient Descent works
- Understand how Mini-batch Gradient Descent works
- Understand the advantageous and disadvantageous of Batch Gradient Descent, Stochastic Gradient Descent and Mini-batch Gradient Descent
- Understand Map reduce procedure



Big Data & HPC



Big Data

- In 2012, Gartner updated the definition of big data as follows: "Big Data is high-volume, high-velocity and/or high-variety information assets that demand cost-effective, innovative forms of information processing that enable enhanced insight, decision making, and process automation."
- Big Data has three main characteristics: Volume (amount of data),
 Velocity (speed of data in and out), Variety (range of data types and sources).
 - Volume Volume describes the amount of data generated by organizations or individuals. Big data doesn't sample: it just observes and tracks what happens.
 - Velocity Velocity describes the frequency at which data is generated, captured and shared. Big data is often available in realtime
 - Variety Big data means much more than rows and columns. It means unstructured text, video, audio that can have important impacts on company decisions – if it's analyzed properly in time.



Big Data Examples

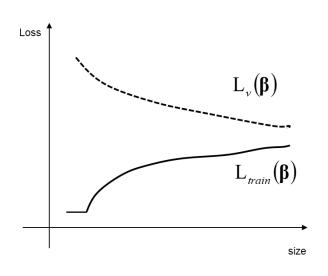
- Twitter CEO Dick Costolo revealed that the company has gone from 90 million tweets per day in September of 2010 to 100 million at the beginning of 2011 to 1/4 billion tweets per day as of Oct 17 2011
- eBay uses two data warehouses at 7.5 petabytes and 40PB as well as a 40PB Hadoop cluster for search, consumer recommendations, and merchandising. (May 10 2013)
- Walmart handles more than 1 million customer transactions every hour, which are imported into databases estimated to contain more than 2.5 petabytes (2560 terabytes) of data – the equivalent of 167 times the information contained in all the books in the US Library of Congress.

Note: the numbers are from online resources and can be out of dated and inaccurate

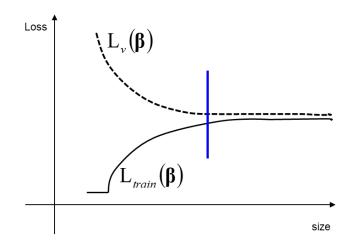


When to get more data?

High Variance Problem.



High bias Problem.



- Do a sanity check based on a small subset (m = 10,000), and check how the learning curves looks like
 - If left (high variance problem), then run the algorithm with more data
 - If right (high bias problem), more data will probably not really help much=> we should take actions on fixing the high bias problem.



Linear Regression with Big Data

 Below is the gradient descent update rule (one iteration) that we used for the linear regression with one feature.

$$\beta_0 \coloneqq \beta_0 - \alpha \frac{\partial L(\beta_0, \beta_1)}{\partial \beta_0} = \beta_0 - \alpha \frac{1}{N} \sum_{n=1}^N (\beta_0 + \beta_1 x_{n1} - t_n)$$

$$\beta_1 \coloneqq \beta_1 - \alpha \frac{\partial L(\beta_0, \beta_1)}{\partial \beta_1} = \beta_1 - \alpha \frac{1}{N} \sum_{n=1}^N (\beta_0 + \beta_1 x_{n1} - t_n) x_{n1}$$
Update simultaneously

- This seems to be an easy task based on our previous examples
- Now suppose we have some census data of m = 1,000,000,000 examples (this is very possible and realistic)
- Then in order to calculate the above gradient descent update, we need to sum up 1,000,000,000 elements
- This is a very **expense** calculation
- Also called batch gradient descent ("batch" means we use all of the training examples at a time.)



The way the **batch gradient descent** algorithm works with big data:

- We need to stream all of these records through computer, because probably we cannot store all the 1 billion records in computer memory
- We need to read into computer memory all 1 billion records in order to compute the derivative term
- So we need to read through each record, and slowly accumulate the sum in order to compute the derivative
- Complete all the above work, we can take one iteration of batch gradient descent
- Suppose the batch gradient descent needs 10,000 iterations to converge, this whole process can take really really long time



Stochastic Gradient Descent



- Stochastic gradient descent (SGD), also known as incremental gradient descent, is a stochastic approximation of the gradient descent optimization and iterative method for minimizing an objective function that is written as a sum of differentiable functions
- With SGD, the gradient of the loss is estimated each sample at a time and the model is updated along the way with the learning rate
- Stochastic gradient descent can be applied to regression, logistic regression, NN, etc. (Think about their loss functions.)
- We use regression to illustrate the idea of stochastic gradient descent.



Batch Gradient Descent

Batch gradient descent update rule (one iteration) for regression:

$$\beta_j \coloneqq \beta_j - \alpha \frac{\partial L(\boldsymbol{\beta})}{\partial \beta_j} = \beta_j - \alpha \frac{1}{N} \sum_{n=1}^N (f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n) x_{nj}$$

for
$$j = 0,1,2,...,d$$
 where

With large dataset the main pain point is to sum over all the m examples

$$f(\mathbf{x}_n, \boldsymbol{\beta}) = \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \dots + \beta_d x_{nd}$$

- How to solve this pain point?
- Try to do not do this summation $(\sum_{n=1}^{N})$ over all the N examples



Stochastic Gradient Descent

Regression loss function for linear model

$$L(\boldsymbol{\beta}) = \frac{1}{2N} \sum_{n=1}^{N} (f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n)^2$$

Split this $L(\beta)$ into two parts:

Loss(
$$\boldsymbol{\beta}$$
, \mathbf{x}_n , t_n) = $\frac{1}{2}(f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n)^2$

No summation for this loss term

$$L(\boldsymbol{\beta}) = \frac{1}{2} \sum_{n=1}^{N} \text{Loss}(\boldsymbol{\beta}, \mathbf{x}_n, t_n)$$



Stochastic Gradient Descent

Loss(
$$\boldsymbol{\beta}$$
, \mathbf{x}_n , t_n) = $\frac{1}{2}(f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n)^2$

$$\frac{\partial \operatorname{Loss}(\boldsymbol{\beta}, \mathbf{x}_n, t_n)}{\partial \beta_j} = (f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n) x_{nj} \quad \text{(for } j = 0, 1, 2, \dots, n)$$

- Now the partial derivative has no summation term: we can calculate the "small" gradient with respect to each training examples (x_n, t_n)
- Or in other words, we update the parameter based on these "small" gradient/learning, instead of calculating all 1 billion gradients and then sum



SGD- Algorithm

- Choose an initial vector of parameters and learning rate α .
- Repeat the following procedure until an approximate minimum is obtained:
 - Randomize the data set.

• for
$$n=1,2,3,...,N$$
, do Note there is no summation here
$$\beta_j \coloneqq \beta_j - \alpha \frac{\partial \mathrm{Loss}(\boldsymbol{\beta},\mathbf{x}_n,t_n)}{\partial \beta_j} = \beta_j - \alpha (f(\mathbf{x}_n,\boldsymbol{\beta}) - t_n) x_{nj}$$
 (for $j=0,1,2,...,n$)

We used regression as an example for the above SGD algorithm, while other machine learning algorithms like neural network can employ SGD as well.



SGD Properties

- The **randomization** (shuffling) of the data is done to avoid a bias in the optimization algorithm by providing the data examples in a particular order.
- Stochastic gradient descent is a popular algorithm for training a wide range of models in machine learning, including support vector machines, logistic regression and graphical models. When combined with the backpropagation algorithm, it is the de facto standard algorithm for training neural networks.
- The convergence of stochastic gradient descent has been analysed using the theories of convex minimization and of stochastic approximation.
- Stochastics gradient descent can find good approximated estimates compared to the ones from batch gradient descent.



Example 1

Input data size: N = 10000 examples, d = 1000 features

```
# Estiamte coefficients
t0 = time.time()
lr_obj_big.fit(x_big, y_big)
t1 = time.time()
total = t1-t0
print("BGD Running Time {0}".format(total))
clf = linear_model.SGDRegressor()
t0 = time.time()
clf.fit(x_big, y_big)
t1 = time.time()
total = t1-t0
print("SGD Running Time {0}".format(total))
```

BGD Running Time 1.125 seconds SGD Running Time 0.18799996376 seconds

 Generally, the stochastic gradient descent method will get close to the optimal parameter much faster than the batch gradient descent method.

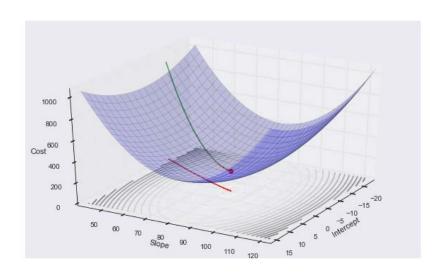


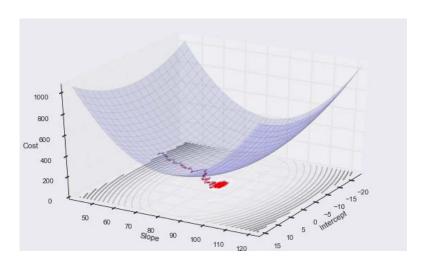
Example 2

Parameter Update Path with SGD & BGD

Batch gradient descent

Stochastic gradient descent



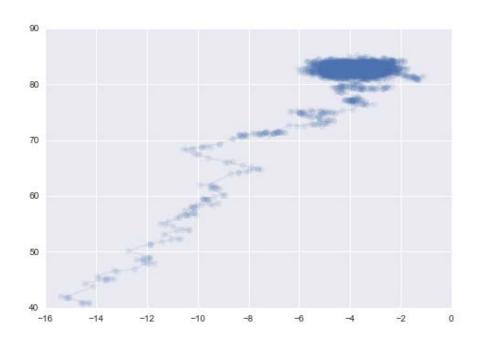


SGD in general has lower accuracy compared to BGD



Example 2

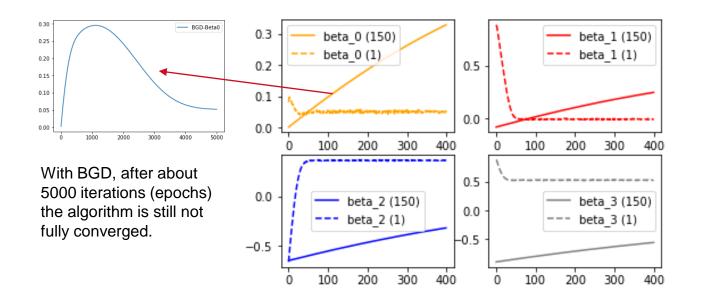
Parameter Update Path with SGD





Example 3 (Tutorial 12)

N = 150 training examples. 2 layer NN for regression. "(150)" represents BGD method, and "(1)" represents SGD method.



Stochastic gradient descent method will get close to the optimal parameter **much faster** than BGD.

In Keras, epoch is an arbitrary cutoff, generally defined as "one pass over the entire dataset", used to separate training into distinct phases, which is useful for logging and periodic evaluation.

https://keras.io/getting-started/faq/#what-does-sample-batch-epoch-mean



Mini-batch Gradient Descent



Mini-batch Gradient Descent

- Mini-batch gradient descent is a trade-off between stochastic gradient descent and batch gradient descent.
- In mini-batch gradient descent, the gradient is summed over a small number of samples. This is between the SGD batch size of 1 sample, and the BGD batch size of all the training samples.
- Mini-batch gradient descent computation can make use of vectorization libraries rather than computing each step separately.
- It may also result in smoother convergence, as the gradient computed at each step uses more training examples than SGD.



Mini-batch Gradient Descent

- To summarize the gradient descent algorithms:
 - Batch gradient descent uses all N examples in each iteration.
 - Stochastic gradient descent uses 1 example in each iteration.
 - Mini-batch gradient descent uses b (b < N) example in each iteration.

Use b = 5 as example in mini-batch gradient descent

$$((\mathbf{x}_i, t_i), (\mathbf{x}_{i+1}, t_{i+1}), (\mathbf{x}_{i+2}, t_{i+2}), (\mathbf{x}_{i+3}, t_{i+3}), (\mathbf{x}_{i+4}, t_{i+4}))$$

$$\beta_j \coloneqq \beta_j - \alpha \frac{\partial L(\boldsymbol{\beta})}{\partial \beta_j} = \beta_j - \alpha \frac{1}{5} \sum_{n=i}^{i+4} (f(\mathbf{x}_n, \boldsymbol{\beta}) - t_n) x_{nj}$$

Each mini-batch we have 5 examples=> make parameter update with summation over every 5 examples



Mini-batch GD- Algorithm

Suppose
$$N = 1000, b = 5$$

- Choose an initial vector of parameters and learning rate α .
- Repeat the following procedure until an approximate minimum is obtained:
 - Randomize the data set.

• for i = 1,6,11,16,21...,996 do

Summation over
$$b = 5$$
 examples

$$\beta_{j} \coloneqq \beta_{j} - \alpha \frac{\partial L(\boldsymbol{\beta})}{\partial \beta_{j}} = \beta_{j} - \alpha \frac{1}{5} \sum_{n=i}^{i+4} (f(\mathbf{x}_{n}, \boldsymbol{\beta}) - t_{n}) x_{nj}$$
(for $j = 0, 1, 2, ..., d$)

We used regression as an example for the above Mini-batch GD algorithm, while other machine learning algorithms like neural network can employ Mini-batch GD as well.



Property

- Mini-batch GD can perform significantly better than SGD, because the code can make use of vectorization libraries rather than computing each step separately, to realize parallel computing
- Mini-batch GD reduces the variance of the parameter updates, which can lead to more stable and smoother convergence compared with SGD, as the gradient computed at each step uses more training examples than SGD
- An potential issue: suppose we have 1050 training samples and we choose b=100 in Mini-batch GD. Algorithm takes first 100 examples (from 1st to 100th) from the training dataset and update. Next it takes second 100 examples (from 101st to 200th) and update again. The problem usually happens with the last set of samples. In our example we've used 1050 which is not divisible by 100 without remainder. **The simplest solution is just to use the rest 50 examples and update.**

http://ruder.io/optimizing-gradient-descent/



Configuration

- Mini-batch sizes b, commonly called "batch size" for brevity, are often tuned to an aspect of the computational architecture on which the implementation is being executed, such as a power of 2 that fits the memory requirements of the GPU or CPU hardware like 32, 64, 128, 256, etc.
- Batch size b is a slider on the learning process.
 - Small values give a learning process that converges quickly at the cost of noise in the training process.
 - Large values give a learning process that converges slowly with accurate estimates of the error gradient.
- A good default for batch size b might be 32.
- It is a good idea to review learning curves of model validation loss against training time with different batch sizes when tuning the batch size.
- Tune batch size and learning rate after tuning all other hyperparameters.

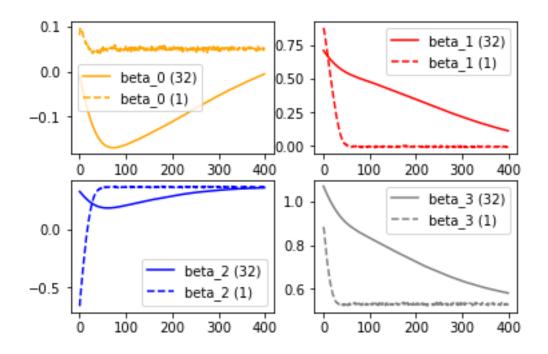
https://machinelearningmastery.com/gentle-introduction-minibatch-gradient-descent-configure-batch-size/



Python Example



N=150 training examples. 2 layer NN for regression. "(32)" represents mini-batch GD method with b=32, and "(1)" represents SGD method.



Mini-batch GD results in smoother convergence, while SGD gets close to the optimal parameter much faster.



BGD SGD Mini-batch GD Comparison



- This stochastic gradient approach allows us to start making progress on the minimization problem right away. It is computationally cheaper, but it results in a larger variance of the parameter update in comparison with batch gradient descent.
- Generally, the stochastic gradient descent method will get close to the optimal parameter much faster than the batch method. Thus the stochastic gradient descent method is useful when we want a quick approximation for the solution to our optimization problem.
- Mini-batch GD has the advantage that the variance of parameter update is reduced compared with SGD, while the computational burden is still reasonable compared with BGD as we do not use all examples for each update.



MapReduce



Intuition

- MapReduce is a programming model and an associated implementation for processing and generating big data sets with a parallel, distributed algorithm on a cluster.
- A MapReduce program is composed of:
 - a Map procedure (method) that performs filtering and sorting (such as sorting students by first name into queues, one queue for each name)
 - a Reduce method that performs a summary operation (such as counting the number of students in each queue, yielding name frequencies).
- The "MapReduce System" (also called "infrastructure" or "framework")
 orchestrates the processing by marshalling the distributed servers,
 running the various tasks in parallel, managing all communications and
 data transfers between the various parts of the system, and providing for
 redundancy and fault tolerance.



An example

- Power of parallel computing
- Map: filtering and sorting of data
- Reduce: summary operations

For the 400 examples to be calculated in min-batch gradient descent of regression

$$b = 400, N = 1,000,000,000$$

$$((\mathbf{x}_i, t_i), (\mathbf{x}_{i+1}, t_{i+1}), \dots, (\mathbf{x}_{i+399}, t_{i+399}))$$

Summation over b = 400 examples to produce one parameter update

$$\beta_j \coloneqq \beta_j - \alpha \frac{\partial L(\boldsymbol{\beta})}{\partial \beta_j} = \beta_j - \alpha \frac{1}{400} \sum_{k=i}^{i+399} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

Suppose we have a computer cluster.

Can we speed up this process?



Step 1

Compute 1

Compute 2

Compute 3

Compute 4

$$((\mathbf{x}_{i}, t_{i}), (\mathbf{x}_{i+1}, t_{i+1}), \dots, (\mathbf{x}_{i+99}, t_{i+99}))$$

$$\sum_{k=i}^{i+99} (f(\mathbf{x}_{k}, \boldsymbol{\beta}) - t_{k}) x_{kj}$$

$$((\mathbf{x}_{i+100}, t_{i+100}), (\mathbf{x}_{i+101}, t_{i+101}), \dots, (\mathbf{x}_{i+199}, t_{i+199}))$$

$$\sum_{k=i+100}^{i+199} (f(\mathbf{x}_{k}, \boldsymbol{\beta}) - t_{k}) x_{kj}$$

$$((\mathbf{x}_{i+200}, t_{i+200}), (\mathbf{x}_{i+201}, t_{i+201}), \dots, (\mathbf{x}_{i+299}, t_{i+299}))$$

$$\sum_{k=i+200}^{i+299} (f(\mathbf{x}_{k}, \boldsymbol{\beta}) - t_{k}) x_{kj}$$

$$((\mathbf{x}_{i+300}, t_{i+300}), (\mathbf{x}_{i+301}, t_{i+301}), \dots, (\mathbf{x}_{i+399}, t_{i+399}))$$

$$\sum_{k=i+399}^{i+399} (f(\mathbf{x}_{k}, \boldsymbol{\beta}) - t_{k}) x_{kj}$$



Step 2

Compute 1

$$\sum_{k=i}^{i+99} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

Compute 2

$$\sum_{k=i+100}^{i+199} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

Compute 3

$$\sum_{k=i+200}^{i+299} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

Compute 4

$$\sum_{k=i+300}^{i+399} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

Then we usually use a single computer to combine results from the 4 map reduce computers

$$\frac{1}{400} \sum_{k=i}^{i+399} (f(\mathbf{x}_k, \boldsymbol{\beta}) - t_k) x_{kj}$$

- Theoretically, this process is 4-fold faster than the non-parallel approach
- However, this speed uplift can be affected by network latency and other overhead associated with MapReduce



When can we use MapReduce?

- We have multiple computers (computer cluster)
- We have one computer
 - multiple cores of the CPU
 - multiple cores of the GPU

CPU core 1
CPU core 2
CPU core 3
CPU core 4

GPU core 1
GPU core 2
GPU core 3
GPU core 4



MapReduce Application

- Many machine learning algorithms can be expressed as a summation form over the training set:
 - Regression
 - Logistic regression
 - K-means
 - SVM
 - NN
 - Naive Bayes (NB)
 - Gaussian Discriminative Analysis (GDA)
 - Principal Components Analysis (PCA)
 - Expectation Maximization (EM)
 - We did not talk about the models highlighted in red in our unit
- These parameter estimation process can be paralleled by MapReduce

Chu, et al. (2007)



Further Readings

- Hadoop
 - http://hadoop.apache.org/
- Online learning
 - https://en.wikipedia.org/wiki/Online_machine_learning
- Cloud computing
 - https://en.wikipedia.org/wiki/Cloud_computing