DLI Accelerated Data Science Teaching Kit

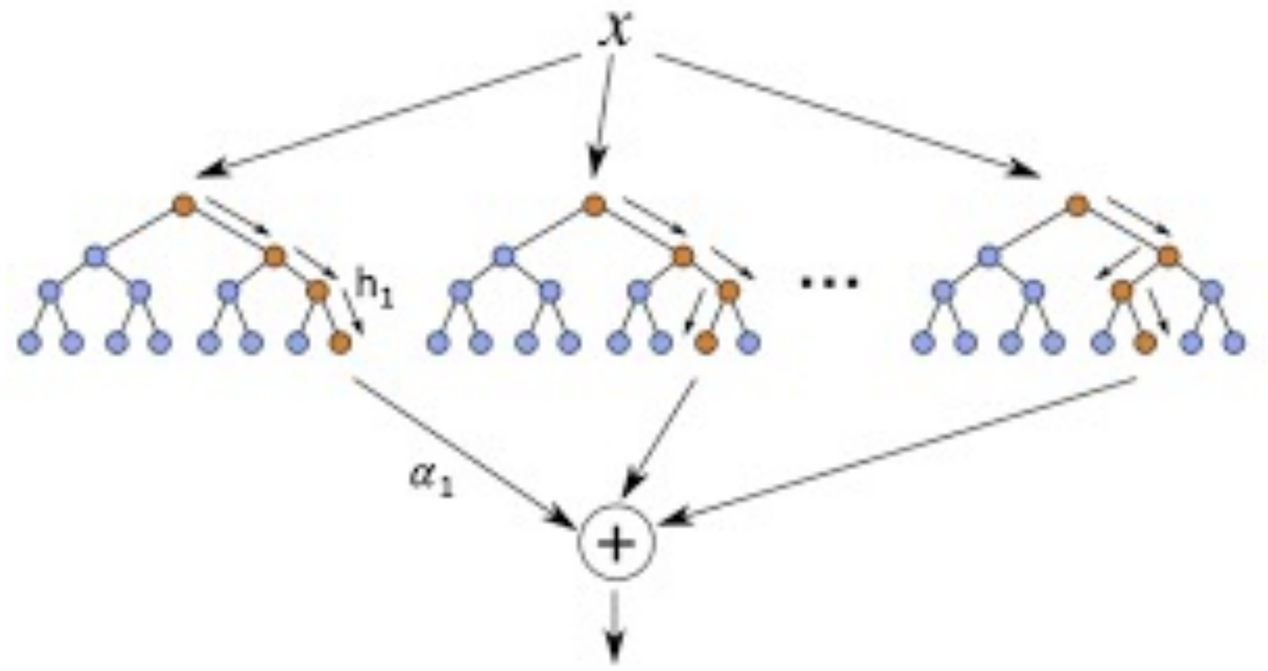
Lecture 14.12 - XGBoost with RAPIDS

What is XGBoosting?

- A more robust and flexible version of gradient boosting
- What does it do?
  - Uses second-order gradients of the loss function in addition to the first-order gradients, based on Taylor expansion of the loss function
- Transforms the loss function into a more sophisticated objective function containing regularization terms

How does XGBoosting improve on Gradient Boosting?

- The extended loss function inhibits overfitting
    - Adds penalty proportional to size of the leaf weights
- This inhibits the growth of the model and prevents it from growing too large
- If the model overfits on the training data, it will not generalize well to new data



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Example of XGBoost

- Let's consider a scenario in which we are trying to predict the income of an individual
- Instead of following the process used for gradient boosting, we will use quantiles:
  - Cut points that divide a feature into equal-sized groups

Reference: Nvidia RAPIDS

Original Dataset

Instance	Age	Has Job	Owns House	Income
0	12	N	N	0
1	32	Y	Y	90
2	25	Y	Y	50
3	48	N	N	25
4	67	N	Y	35
5	18	Y	N	10

Converted Quantile Dataset

- Reprocess each feature using quantiles:
  - Age separated into strata:
    - <18: One individual
    - <32: Two individuals
    - <67: Two individuals
    - 67+: One individual
  - Separates datapoints into roughly even groups

Instance	Age	Has Job	Owns House	Income
0	0	0	0	0
1	2	1	1	90
2	1	1	1	50
3	2	0	0	25
4	3	0	1	35
5	1	1	0	10

Reference: Nvidia RAPIDS

Finding Splits in Decision Trees

- We want to optimize trees that limit the depth of the overall model
- To achieve this, we need to build nodes that split the data well by minimizing error, in this case sum of squared error (SSE)
  - We can reformat the SSE equation into a split loss equation that can be used in our RAPIDS code

$$Split\ Loss\ (R_a,\ R_b,\ n_a,\ n_b)\ =\ -\frac{1}{2}\left(\frac{R_a^2}{n_a}\right) - \frac{1}{2}\left(\frac{R_b^2}{n_b}\right)$$

Reference: Nvidia RAPIDS

Apply Split Loss Function to Dataset

The split (<18) has the greatest reduction in the SSE function

Quantile	*n*	Quantile Sum *r*	Inclusive Scan *n*	Inclusive Scan *r*	*Split Loss*
<18	1	0	1	0	4410
<32	2	60	3	60	4350
<67	2	115	5	175	3675
67+	1	35	6	210	

Performing XGBoost on RAPIDS

- To run XGBoost efficiently using CUDA, RAPIDS uses bit compression and memory compression
  - Implements parallel primitives for processing sparse CSR (Compressed Sparse Row) format input
  - Uses symbol compression to store the quantised input matrix
- Next, we will see an example of XGBoost on the UCI Higgs dataset

Reference: Nvidia RAPIDS

Example: Setting up GPUs

```
import csv
import numpy as np
import os.path
import pandas
import time
import xgboost as xgb
import sys
if sys.version_info[0] >= 3:
    from urllib.request import urlretrieve
else:
    from urllib import urlretrieve

data_url = "https://archive.ics.uci.edu/ml/machine-learning-databases/00280/HIGGS.csv.gz"
dmatrix_train_filename = "higgs_train.dmatrix"
dmatrix_test_filename = "higgs_test.dmatrix"
csv_filename = "HIGGS.csv.gz"
train_rows = 10500000
test_rows = 500000
num_round = 1000

plot = True
```

Download the Higgs Dataset

Example: Load Higgs Dataset

```
# return xgboost dmatrix
def load_higgs():
    if os.path.isfile(dmatrix_train_filename)
      and os.path.isfile(dmatrix_test_filename):
        dtrain = xgb.DMatrix(dmatrix_train_filename)
        dtest = xgb.DMatrix(dmatrix_test_filename)
        if dtrain.num_row() == train_rows and dtest.num_row() == test_rows:
            print("Loading cached dmatrix...")
            return dtrain, dtest

    if not os.path.isfile(csv_filename):
        print("Downloading higgs file...")
        urlretrieve(data_url, csv_filename)

    df_higgs_train = pandas.read_csv(csv_filename, dtype=np.float32,
                                     nrows=train_rows, header=None)
    dtrain = xgb.DMatrix(df_higgs_train.ix[:, 1:29], df_higgs_train[0])
    dtrain.save_binary(dmatrix_train_filename)
    df_higgs_test = pandas.read_csv(csv_filename, dtype=np.float32,
                                    skiprows=train_rows, nrows=test_rows,
                                    header=None)
    dtest = xgb.DMatrix(df_higgs_test.ix[:, 1:29], df_higgs_test[0])
    dtest.save_binary(dmatrix_test_filename)

    return dtrain, dtest
```

Load the Higgs dataset

Split dataset into training and test

Example: Run on CPU and GPU

```
dtrain, dtest = load_higgs()
param = {}
param['objective'] = 'binary:logitraw'
param['eval_metric'] = 'error'
param['tree_method'] = 'gpu_hist'
param['silent'] = 1

print("Training with GPU ...")
tmp = time.time()
gpu_res = {}
xgb.train(param, dtrain, num_round, evals=[(dtest, "test")],
          evals_result=gpu_res)
gpu_time = time.time() - tmp
print("GPU Training Time: %s seconds" % (str(gpu_time)))

print("Training with CPU ...")
param['tree_method'] = 'hist'
tmp = time.time()
cpu_res = {}
xgb.train(param, dtrain, num_round, evals=[(dtest, "test")],
          evals_result=cpu_res)
cpu_time = time.time() - tmp
print("CPU Training Time: %s seconds" % (str(cpu_time)))
```

Run XGBoost on GPU

Run XGBoost on CPU

Example: Plot CPU/GPU Results

```python
if plot:
    import matplotlib.pyplot as plt
    min_error = min(min(gpu_res["test"][param['eval_metric']]),
                    min(cpu_res["test"][param['eval_metric']]))
    gpu_iteration_time =
        [x / (num_round * 1.0) * gpu_time for x in range(0, num_round)]
    cpu_iteration_time =
        [x / (num_round * 1.0) * cpu_time for x in range(0, num_round)]
    plt.plot(gpu_iteration_time, gpu_res['test'][param['eval_metric']],
             label='Tesla P100')
    plt.plot(cpu_iteration_time, cpu_res['test'][param['eval_metric']],
             label='2x Haswell E5-2698 v3 (32 cores)')
    plt.legend()
    plt.xlabel('Time (s)')
    plt.ylabel('Test error')
    plt.axhline(y=min_error, color='r', linestyle='dashed')
    plt.margins(x=0)
    plt.ylim((0.23, 0.35))
    plt.show()
```

Plot the Results for GPU and CPU

Difference in Performance

- 4.15x speed improvement for the GPU algorithm with the same accuracy as the CPU algorithm

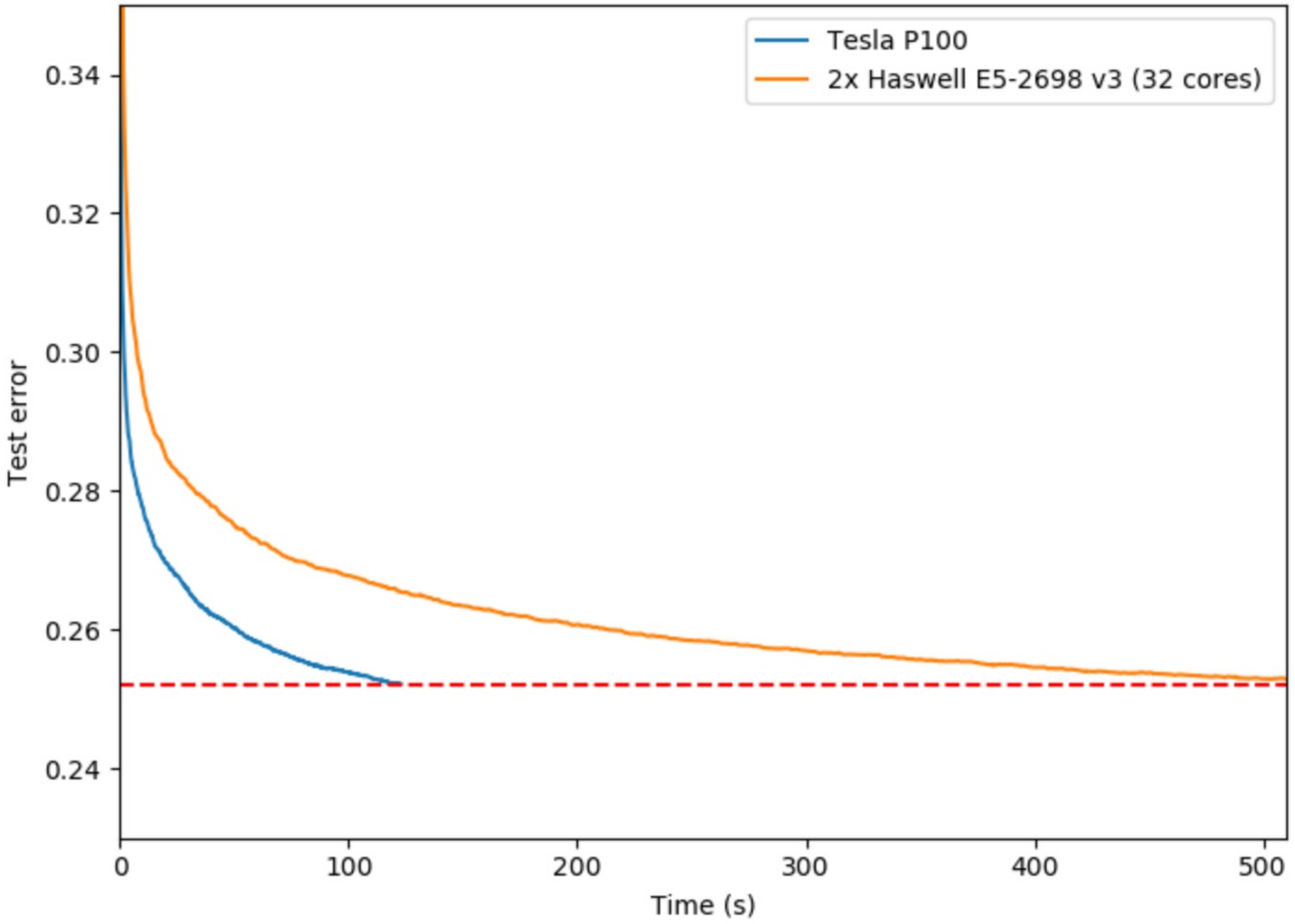

Figure 3. Test error over time for the Higgs dataset, 1000 boosting iterations.

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Thank You