Accelerating GPU-based Machine Learning in Python using MPI Library: A Case Study with MVAPICH2-GDR

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Outline

- Background
- MVAPICH2 GDR vs NCCL
- cuML Tech Stack
- cuML Algorithms
- Synthetic Benchmarks
- Results
Background

- Numerous machine learning libraries available
- Features vary between libs
  - Single vs multi node
  - Python interface availability
  - CPU vs GPU support
- Notable libs:
  - Scikit-Learn
  - Apache Spark’s Mllib
  - Apache Mahout
RAPIDS cuML

- RAPIDS
  - Suite of data science libraries built on top of CUDA
  - cuDF: dataframe library
  - cuML: machine learning algorithm library
  - cuGraph: graph algorithm library

- cuML
  - Analogous to Scikit-Learn
  - Multi Node Multi GPU (MNMG)
  - Utilizes NCCL and DASK for communication
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MVAPICH2-GDR vs NCCL

- MPI is the de facto standard for collective communication
- MVAPICH2-GDR has GPU support and years of R&D behind it
- Why not use MVAPICH2-GDR instead of NCCL?
MVAPICH2-GDR vs NCCL

Reduce

Bcast

Allreduce
<table>
<thead>
<tr>
<th>Libraries</th>
<th>GPU Support</th>
<th>MNMG Support</th>
<th>Python Support</th>
<th>High Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scikit-learn</td>
<td>✗</td>
<td>✗</td>
<td>✓</td>
<td>✗</td>
</tr>
<tr>
<td>Spark’s ML lib</td>
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<td>✓</td>
<td>✓</td>
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<td>Mahout</td>
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<td>MPI</td>
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<td>✓</td>
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cuML Tech Stack

- Uses Dask (which uses UCX) for point-to-point communication
- NCCL for collective communication
Collective communication occurs in fit() which is where most communication overhead occurs.
cuML Tech Stack (proposed)

- MPI for collective communication
- Gives users access to MPI operations
cuML Tech Stack (proposed)
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cuML Algorithms

- **K-Means**
  - Separates n points into k clusters using sum of squared error
  - Bcast initial centroid information
  - Cluster cost and centroid selection with Allgather and Allreduce
  - Allreduce for centroid information each iteration

- **Random Forest**
  - Ensemble decision tree classifier
  - No collective communication

- **K-Nearest Neighbor**
  - Data point classification based on k neighboring data points
  - Bcast same subset of data to each worker

- **Linear-Regression**
  - Fit a set of data points into a linear combination of predictors
  - This paper uses SVD over Eigen for benchmarking
  - Bcast at beginning
  - Reduce at each step

- **Truncated SVD**
  - Less computationally intensive SVD
  - Bcast at beginning
  - Reduce and Allgather for matrix computation
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Synthetic Benchmarks

- Attempt to maximize training throughput with given GPU memory
- Utilize make_blobs, make_classification, and make_regression
- Simulate real datasets
  - Cluster: normally distributed clusters
    - Users may set center and standard deviation of each cluster
  - Classification: normally distributed classes with interdependence and random noise and input data containing independent and redundant features
  - Regression: random linear combination of features with noise
    - Users may set sparsity and correlation of features
- Train the Higgs Boson dataset to demonstrate cuML accuracy
  - Use K-Means and Random Forest
  - Use hyperband search to maximize accuracy
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Results

Truncated SVD

K-Means
Results

Linear Regression

Random Forest
Results

Nearest Neighbors
Results

![Graphs showing results for Allreduce, Reduce, and Bcast in K-Means and Nearest Neighbors.](image)
Results

K-Means

Random Forest
Questions?