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Preface

Welcome to the Machine Learning Manual for Bright Cluster Manager 8.0.

0.1 About This Manual

This manual is aimed at helping cluster administrators install, understand, configure, and manage basic machine learning capabilities easily using Bright Cluster Manager. The administrator is expected to be reasonably familiar with the Administrator Manual.

0.2 About The Manuals In General

Regularly updated versions of the Bright Cluster Manager 8.0 manuals are available on updated clusters by default at /cm/shared/docs/cm. The latest updates are always online at http://support.brightcomputing.com/manuals.

- The Installation Manual describes installation procedures for a basic cluster.
- The Administrator Manual describes the general management of the cluster.
- The User Manual describes the user environment and how to submit jobs for the end user.
- The Cloudbursting Manual describes how to deploy the cloud capabilities of the cluster.
- The Developer Manual has useful information for developers who would like to program with Bright Cluster Manager.
- The OpenStack Deployment Manual describes how to deploy OpenStack with Bright Cluster Manager.
- The Big Data Deployment Manual describes how to deploy Big Data with Bright Cluster Manager.
- The UCS Deployment Manual describes how to deploy the Cisco UCS server with Bright Cluster Manager.

If the manuals are downloaded and kept in one local directory, then in most pdf viewers, clicking on a cross-reference in one manual that refers to a section in another manual opens and displays that section in the second manual. Navigating back and forth between documents is usually possible with keystrokes or mouse clicks.

For example: <Alt>-<Backarrow> in Acrobat Reader, or clicking on the bottom leftmost navigation button of xpdf, both navigate back to the previous document.

The manuals constantly evolve to keep up with the development of the Bright Cluster Manager environment and the addition of new hardware and/or applications. The manuals also regularly incorporate customer feedback. Administrator and user input is greatly valued at Bright Computing. So any comments, suggestions or corrections will be very gratefully accepted at manuals@brightcomputing.com.
0.3 Getting Administrator-Level Support

If the reseller from whom Bright Cluster Manager was bought offers direct support, then the reseller should be contacted.

Otherwise the primary means of support is via the website https://support.brightcomputing.com. This allows the administrator to submit a support request via a web form, and opens up a trouble ticket. It is a good idea to try to use a clear subject header, since that is used as part of a reference tag as the ticket progresses. Also helpful is a good description of the issue. The followup communication for this ticket goes via standard e-mail. Section 13.2 of the Administrator Manual has more details on working with support.

0.4 Getting Professional Services

Bright Computing normally differentiates between professional services (customer asks Bright Computing to do something or asks Bright Computing to provide some service) and support (customer has a question or problem that requires an answer or resolution). Professional services can be provided after consulting with the reseller, or the Bright account manager.
1

Introduction And Installing the Machine Learning RPMs

1.1 Introduction
A number of Machine/Deep Learning library and framework RPM packages have been included in Bright Cluster Manager since version 7.3. Bright makes it faster and easier for organizations install the latest state-of-the-art libraries, and to gain insights from rich, complex data.

1.2 Packages Available
Currently the following RPMs are available:

Table 1.1: Machine Learning Packages Included

<table>
<thead>
<tr>
<th>Package name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>caffe</td>
<td>A deep learning framework made with expression, speed, and modularity in mind. Developed by the Berkeley Vision and Learning Center (BVLC) and by community contributors.</td>
</tr>
<tr>
<td>caffe2</td>
<td>The version 2 branch of the lightweight, modular, and scalable Caffe deep learning framework. With MPI support.</td>
</tr>
<tr>
<td>chainer</td>
<td>Chainer is a flexible framework for neural networks. One major goal is flexibility, so it must enable us to write complex architectures simply and intuitively.</td>
</tr>
<tr>
<td>cm-jupyter</td>
<td>Jupyter Notebook is a BSD-licensed web notebook</td>
</tr>
<tr>
<td>cm-jupyterhub</td>
<td>JupyterHub is a multi-user server for notebooks</td>
</tr>
<tr>
<td>cm-ml-distdeps</td>
<td>Meta-package containing library dependencies for Caffe, NVIDIA DIGITS, Theano, Torch, and TensorFlow. This should be installed on the head nodes and the software images</td>
</tr>
</tbody>
</table>

...continues
### Table 1.1: Machine Learning Packages Included...continued

<table>
<thead>
<tr>
<th>Package name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cm-ml-pythondeps</td>
<td>Pre-packaged Python dependencies for Bright’s RPM packages for Caffe, NVIDIA DIGITS, Theano, Torch, and TensorFlow.</td>
</tr>
<tr>
<td>cm-ml-python3deps</td>
<td>This is a monolithic package containing various python libraries needed by caffe, NVIDIA DIGITS, Theano, Torch and TensorFlow. The Python libraries are: Cython, numpy, scipy, python-dateutil, pytz, six, cycler, pyparsing, matplotlib, decorator, networkx, Pillow, toolz, dask, scikit-image, setuptools, pathlib2, pickleshare, simplegeneric, ipython-genutils, traitlets, wcwidth, prompt-toolkit, pygments, pytz, six, cycler, pyparsing, matplotlib, decorator, networkx, Pillow, toolz, dask, scikit-image, setuptools, pathlib2, pickleshare, simplegeneric, ipython-genutils, traitlets, wcwidth, prompt-toolkit, pygments, ptyprocess, pexpect, backports.shutil-get-terminal-size, ipython, h5py, leveldb, nose, pandas, prototub, python-gflags, pyyaml. All of these libraries will be installed in /cm/shared/apps/cm-ml-python3deps so as to avoid conflicts. The Lmod/Tmod environment module will set the environment for these.</td>
</tr>
<tr>
<td>cntk</td>
<td>The Cognitive Toolkit by Microsoft Research, is a unified deep-learning toolkit</td>
</tr>
<tr>
<td>cub</td>
<td>Reusable software components for CUDA</td>
</tr>
<tr>
<td>cudnn</td>
<td>CUDA deep neural network primitives library</td>
</tr>
<tr>
<td>digits</td>
<td>DIGITS is a web frontend to Caffe and Torch, developed by NVIDIA</td>
</tr>
<tr>
<td>dynet</td>
<td>DyNet is a neural network library developed by Carnegie Mellon University and many others. It is written in C++ (with bindings in Python) and is designed to be efficient when run on either CPU or GPU, and to work well with networks that have dynamic structures that change for every training instance. For example, these kinds of networks are particularly important in natural language processing tasks, and DyNet has been used to build state-of-the-art systems for syntactic parsing, machine translation, morphological inflection, and many other application areas.</td>
</tr>
<tr>
<td>horovod</td>
<td>Deep learning library that uses MPI, used for Theano and TensorFlow.</td>
</tr>
<tr>
<td>keras</td>
<td>Meta-framework deep learning library, used to provide a standard interface for Theano, TensorFlow, cntk, pytorch, mxnet.</td>
</tr>
<tr>
<td>keras-python3</td>
<td>Python 3 Keras package</td>
</tr>
<tr>
<td>mlnpython</td>
<td>MLPython is a library for organizing machine learning research.</td>
</tr>
<tr>
<td>mxnet</td>
<td>A flexible, compact, and highly scalable Deep Learning library.</td>
</tr>
<tr>
<td>mxnet-python3</td>
<td>Python 3 MXNet package</td>
</tr>
<tr>
<td>nccl</td>
<td>(pronounced &quot;Nickel&quot;) NVIDIA Collective Communication Library — A standalone CUDA library similar in concept to MPI. It has communication routines that have been optimized to achieve high bandwidth over PCIe and other interconnects</td>
</tr>
</tbody>
</table>

...continues
### 1.3 Requirements

The following packages are planned for the future:

<table>
<thead>
<tr>
<th>Package name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>caffeonspark</td>
<td>CaffeOnSpark brings deep learning to Hadoop and Spark clusters. By combining salient features from deep learning framework Caffe and big-data frameworks Apache Spark and Apache Hadoop, CaffeOnSpark enables distributed deep learning on a cluster of GPU and CPU servers.</td>
</tr>
<tr>
<td>biddmach</td>
<td>BIDMach is a very fast machine learning library.</td>
</tr>
</tbody>
</table>

#### 1.3.1 Software Installation

**Compute Nodes Installation**

The `cm-ml-distdeeps` RPM package must be installed onto all compute nodes that are to run machine learning applications. The `cm-ml-distdeeps` meta-package instructs YUM to install the necessary system libraries as well as the development packages, e.g. `blas-devel`.

For example, if the name of the software image is `gpu-image`, then the administrator can install the RPM as follows:
Introduction And Installing the Machine Learning RPMs

Example

[root@bright80 ~]# yum install --installroot=/cm/images/gpu-image cm-ml-distdeps

The preceding command must be applied to all software images that are used to run machine learning applications.

Head Node Installation

The head node must also have the `cm-ml-distdeps` RPM package installed on it. If it is not already installed, then it should be installed:

Example

[root@bright80 ~]# yum install cm-ml-distdeps

The Bright Cluster Manager machine learning packages have proper RPM dependencies defined. This means that the cluster administrator does not need to spend time figuring out what needs to be installed.

For example, if the administrator wants to install NVIDIA’s DIGITS, then all that needs to be done is to run the following command on the head node:

[root@bright80 ~]# yum install digits

In general, a `yum install <name of desired package>` should do installation for supported machine learning packages. That is, YUM then automatically installs `cm-ml-pythondeps`, `cm-ml-distdeps`, `cudnn`, `caffe`, `torch` and `cuda80-toolkit` as dependencies if needed.

At the time of writing (October 2017) there is a minor bug open for CentOS 7.3, which may prevent `cm-ml-pythondeps` installing. A workaround for it is to first install `http-parser` as explained in section 4.1.1.

The RPMs get installed in the `/cm/shared` directory, which is exported over NFS. The RPMS are therefore available to all the compute nodes. The installation of the machine learning libraries is therefore done within minutes, rather than the days that it typically takes to build and install all the necessary dependencies.

Software Libraries Useful For Developers

Developers that work on extending the machine learning libraries typically do not want to use the pre-packaged RPMs. For this use case, Bright can help minimize the time spent to get started.

By installing the `cm-ml-distdeps` on the head node and compute nodes, and the `cm-ml-pythondeps` and `cudnn` RPM packages on the head node, a developer can get ready for machine learning development within minutes and spend time on the interesting application at hand, rather than wasting time in dependency hell.

1.3.2 Module Installation

Bright provides environment module definitions for all the machine learning packages. The environment module files are also compatible with the Lmod software introduced in Bright Cluster Manager 7.3.

The machine learning environment modules automatically load additional environment modules as dependencies.

For example, loading the DIGITS module with:

```bash
module load shared digits
```

automatically loads additional modules such `cudnn`, `openblas`, `hdf5_18`, and so on. Those modules are the dependencies needed to use DIGITS.

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1.3 Requirements

Example

[root@bright80 ~]# module list
Currently Loaded Modulefiles:
  1) shared 2) cmsh 3) cmd 4) cluster-tools/8.0

[root@bright80 ~]# module load digits
[root@bright80 ~]# module list
Currently Loaded Modulefiles:
  1) shared 8) cuda80/toolkit/8.0.61 15) caffe/0.16.2
  2) cmsh 9) hdf5_18/1.8.18 16) cudnn/5.1
  3) cmd 10) openmpi/gcc/64/1.10.3 17) torch7/7.0
  4) cluster-tools/8.0 11) nccl/1.3.4 18) tensorflow/1.3.0
  5) cm-ml-pythondeps/1.11.0 12) protobuf/3.1.0 19) digits/6.0.0
  6) cudnn/6.0 13) opencv3/3.1.0
  7) openblas/dynamic/0.2.18 14) gcc5/5.4.0

[root@bright80 ~]#

The module dependencies are achieved via the module definition files:

[root@bright80 ~]# module show digits
-----
/cm/shared/modulefiles/digits/6.0.0:

module-whatis adds nVidia Deep Neural Network Library to your environment variables
module load caffe
module load torc7
module load cm-ml-pythondeps
module load openblas
module load cuda80/toolkit
module load hdf5_18
module load tensorflow
prepend-path PATH /cm/shared/apps/digits/6.0.0/
prepend-path PYTHONPATH /cm/shared/apps/digits/6.0.0
-----

1.3.3 Further Reading

Additional information about the usage of each individual framework may be found in the user manual.
Running Caffe

This chapter goes through an example workflow in order to train a Caffe model to recognize handwritten digits. It closely follows the sample run by NVIDIA's Luke Yeager at https://github.com/NVIDIA/DIGITS/blob/master/docs/GettingStarted.md.

The example uses the MNIST handwritten digit database (http://yann.lecun.com/exdb/mnist) as the input to provide a training and validation dataset, and LeNet-5 (http://yann.lecun.com/exdb/lenet/) for the neural network model that is to be trained to classify the dataset. Both are generously made available by Yann LeCun from his website at http://yann.lecun.com/.

2.1 Downloading The MNIST Data

The MNIST dataset can be downloaded using the DIGITS downloader. For example, a user tim, could unpack the datasets into a directory /mnt as follows):

```
[tim@bright80 ~]$ python /cm/shared/apps/digits/current/digits/download_data/__main__.py \
mnist /home/tim/
Downloading url=http://yann.lecun.com/exdb/mnist/train-images-idx3-ubyte.gz ...
Downloading url=http://yann.lecun.com/exdb/mnist/train-labels-idx1-ubyte.gz ...
Downloading url=http://yann.lecun.com/exdb/mnist/t10k-images-idx3-ubyte.gz ...
Downloading url=http://yann.lecun.com/exdb/mnist/t10k-labels-idx1-ubyte.gz ...
Uncompressing file=train-images-idx3-ubyte.gz ...
Uncompressing file=train-labels-idx1-ubyte.gz ...
Uncompressing file=t10k-images-idx3-ubyte.gz ...
Uncompressing file=t10k-labels-idx1-ubyte.gz ...
Reading labels from /home/tim/train-labels.bin ...
Reading images from /home/tim/train-images.bin ...
Reading labels from /home/tim/test-labels.bin ...
Reading images from /home/tim/test-images.bin ...
Dataset directory is created successfully at '/home/tim/
Done after 64.6851580143 seconds.
[tim@bright80 ~]$
```

2.2 Setting The Default Matplotlib Backend

The administrator can set the default matplotlib GUI backend supported by editing the file:

```
/cm/shared/apps/cm-ml-pythondeps/lib64/python2.7/site-packages/matplotlib/mpl-data/\nmatplotlibrc
```

and, for example, changing the line:

```
backend: agg
```
Running Caffe

to:

backend: gtk3agg

The preceding change allows GTK3 GUI support, if, for example, just basic X11 GUI support is not wanted, and GTK3 is installed.

2.3 Creating A Working Directory

A working directory can be created with, for example:

[tim@bright80 ~]$ mkdir -p /tmp/digits/jobs

The actual path, which is set by the parameter jobs_dir, can be changed by the administrator in DIGITS version 6.0.0 in:

/cm/shared/apps/digits/6.0.0/digits/digits.cfg

2.4 Using The Web App

The DIGITS server can be started with:

[root@bright80 ~]# module load shared digits
[root@bright80 ~]# cd /cm/shared/apps/digits/6.0.0
[root@bright80 6.0.0]# ./digits-devserver

2017-08-11 08:33:45 [INFO ] Loaded 4 jobs.

The server can run with or without a GPU. Running without a GPU is generally not recommended. If run without a GPU the error #35 response is shown in the output. If there is a GPU on the node, and the error #35 response is still displayed, then a possible cause is that the NVIDIA driver has not been loaded, or has loaded incorrectly.

Once the DIGITS server is up and running, a web browser can be used to navigate to the home screen of DIGITS. If all is well, then the server location should be indicated by the last line. The locations are typically at:

- http://localhost/

  or at

- http://localhost:5000/ if using digits-devserver

  or at

- http://localhost:34448/ if using digits-server

  Instead of using localhost in the preceding URLs, the external IP address of the system can be used, if the Shorewall firewall is opened for the appropriate port. Typically the administrator adds lines to the rules file, similar to the output of the following grep:

```bash
[root@bright80 ~]# grep 5000 /etc/shorewall/rules
# -- Allow port 5000 (digits) traffic from elsewhere to master
ACCEPT:info net fw tcp 5000 #DIGITS
```

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After adding the lines, Shorewall should be restarted, with, for example, `service shorewall restart`.

The DIGITS home screen should then show up in the browser (figure 2.1).

![Figure 2.1: DIGITS Home Screen](image)

2.5 Logging In

Clicking on the **Datasets** tab, then on the **Images** menu button under the **New Dataset** label, opens up a menu. Choosing the **Classification** menu item leads to the login page (figure 2.2). The login is carried out without authentication, for convenience. It is not a security feature.
2.6 Creating Training And Validation Datasets

After login the New Image Classification Dataset page appears (figure 2.3). The page shows several panes which group the input values for the training dataset that is about to be imported.
2.6 Creating Training And Validation Datasets

Figure 2.3: New Image Classification Dataset Dialog

For the pane starting with the Image Type field:

- The Image Type should be set to Grayscale
- The Image size should be changed to 28 x 28

For the pane starting with the Use Image Folder tab label:

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• For Training Images, the path to the MNIST training images should be entered. For the download described earlier in section 2.1 the path would be /home/tim/mnist/train.

• For the checkbox options:
  – The folder of MNIST test images can optionally also be added as a Separate validation images folder.
  – The Separate test images folder should not be used—test images are not used for anything in DIGITS yet.

For the pane starting with the DB backend field:

• The dataset should be given a name, for example mnistdataset

The Create button can then be clicked to start the job run to create the classification databases. A new screen showing the classification job status is then displayed. The screen is scrollable in the browser. The screen is shown in this manual, for printing reasons, as a top part (figure 2.4) and a bottom part (figure 2.5).

A Job Status pane at the top right hand side (figure 2.4) shows the expected job completion time if it is refreshed before the job completes, and shows the time the job took after it has completed.
2.6 Creating Training And Validation Datasets

Figure 2.4: DIGITS MNIST Job Run Screen, Top Part

The bottom section (figure 2.5) allows access to the input and log files.
After the training and validation database import run is complete, the classification spread can be visualized in the refreshed updated bottom section (figure 2.6).
2.6 Creating Training And Validation Datasets

Figure 2.6: DIGITS MNIST Job Run Screen, Bottom Part, After Run

© Bright Computing, Inc.
The corresponding training (train) and validation (val) database entries can be explored by clicking the Explore the db button.

Clicking DIGITS in the top left hand part of the web page brings up the home page again. Within the Datasets tab (figure 2.7), the name mnistdataset that was set earlier is now visible. Clicking on the name brings a screen where like in figure 2.6 the classification spread can be visualized, and the corresponding training (train) and validation (val) database entries can be explored by clicking the Explore the db button.

![Figure 2.7: Generated Dataset Tab](image)

### 2.7 Training A Model

The datasets can now be used to train the LeNet model.

Clicking on the Images button that is associated with the New Model label (figure 2.7), and then on the Classification option, opens up the New Image Classification Model page. The top part of the page is shown in figure 2.8:
New Image Classification Model

The bottom part of the page, with network and GPU options (figure 2.9) shows network and GPU options.
In the **New Image Classification Model** page the following steps can be followed to classify the data:

- **mnistdataset** is selected in the **Select Dataset** field
- The **LeNet** network can be selected from the **Standard Networks** tab
- The model is given a name, for example **Len**
- The **Create** button is clicked

If there is no GPU on the system, then the **Torch (experimental)** tab should be selected instead of Caffe.

While training the model, the expected completion time is seen on the right side (figure 2.10):
2.8 Testing A Model

The bottom of the page (figure 2.11) allows the model to be tested.

Figure 2.10: New Image Classification Model Training
Figure 2.11: New Image Classification Of One Image

- The **Browse button** in the **Upload Image field**, in the **Test a single image** can be clicked upon and a file chosen.
  - There are plenty to choose from under the `/home/username/mnist/test/` directory.
  - Alternatively an image of a digit can be created by hand in an image manipulation software such as Gimp.
  - Alternatively an image from the web can have its URL pasted into the **Image URL** field.
- The **Show visualizations and statistics** box can be checked for extra information on how the algorithm was applied.

Clicking on the **Classify One** button then displays a classified image (figure 2.12):
2.8 Testing A Model

Figure 2.12: New Image Classification Result For One Image

At the top of the page, DIGITS displays the top five classifications and corresponding confidence values. DIGITS also provides further visualizations and statistics about the weights and activations of each layer of the network.

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Running TensorFlow

This chapter goes through some example runs with TensorFlow. The INFO output messages have been removed in the runs for readability.

### 3.1 Hello World

A “Hello World” example that just shows that the software is in place for TensorFlow 0.10 can be run as follows:

**Example**

```
[root@bright80 ~]# python
Python 2.7.5 (default, Nov 20 2015, 02:00:19)
[GCC 4.8.5 20150623 (Red Hat 4.8.5-4)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import tensorflow as tf
hello = tf.constant('Hello, TensorFlow!')
>>> sess = tf.Session()
name: Tesla K40c
major: 3 minor: 5 memoryClockRate (GHz) 0.745
pciBusID 0000:05:00.0
Total memory: 11.92GiB
Free memory: 11.78GiB

> (device: 0, name: Tesla K40c, pci bus id: 0000:05:00.0)
>>> sess.run(hello)
'Hello, TensorFlow!'
>>> a = tf.constant(10)
>>> b = tf.constant(32)
>>> sess.run(a+b)
42
```
3.3 Image Recognition

The following session shows a pre-trained model recognizing a test image of a tiger:

Example

```bash
[root@bright80 ~]# python -m tensorflow.models.image.mnist.convolutional
Successfully downloaded train-images-idx3-ubyte.gz 9912422 bytes.
Successfully downloaded train-labels-idx1-ubyte.gz 28881 bytes.
Successfully downloaded t10k-images-idx3-ubyte.gz 1648877 bytes.
Successfully downloaded t10k-labels-idx1-ubyte.gz 4542 bytes.
Extracting data/train-images-idx3-ubyte.gz
Extracting data/train-labels-idx1-ubyte.gz
Extracting data/t10k-images-idx3-ubyte.gz
Extracting data/t10k-labels-idx1-ubyte.gz
name: Tesla K40c
major: 3 minor: 5 memoryClockRate (GHz) 0.745
pciBusID 0000:05:00.0
Total memory: 11.92GiB
Free memory: 11.78GiB
Initialized!
Step 0 (epoch 0.00), 36.5 ms
Minibatch loss: 12.054, learning rate: 0.010000
Minibatch error: 90.6%
Validation error: 84.6%
Step 100 (epoch 0.12), 14.2 ms
Minibatch loss: 3.301, learning rate: 0.010000
Minibatch error: 4.7%
Validation error: 7.4%
Step 200 (epoch 0.23), 14.2 ms
Minibatch loss: 3.458, learning rate: 0.010000
Minibatch error: 14.1%
... 
Step 8400 (epoch 9.77), 14.1 ms
Minibatch loss: 1.596, learning rate: 0.006302
Minibatch error: 0.0%
Validation error: 0.8%
Step 8500 (epoch 9.89), 14.1 ms
Minibatch loss: 1.626, learning rate: 0.006302
Minibatch error: 1.6%
Validation error: 0.9%
Test error: 0.8%
[root@bright80 ~]#
```

Example

```bash
[root@bright80 ~]# module load tensorflow/0.10
[root@bright80 ~]# cd /cm/shared/apps/tensorflow/0.10/lib/python2.7/site-packages/tensorflow/models/image/imagenet
[root@bright80 imagenet]# python classify_image.py --image_file=Indochinese-Tiger-Zoo.jpg
name: Tesla K40c
major: 3 minor: 5 memoryClockRate (GHz) 0.745
pciBusID 0000:05:00.0
Total memory: 11.92GiB
Free memory: 11.78GiB
W tensorflow/core/framework/op_def_util.cc:332] Op BatchNormWithGlobalNormalization is depre
```
cated. It will cease to work in GraphDef version 9. Use `tf.nn.batch_normalization()`.

- tiger, Panthera tigris (score = 0.71628)
- tiger cat (score = 0.11725)
- lynx, catamount (score = 0.00376)
- jaguar, panther, Panthera onca, Felis onca (score = 0.00371)
- cougar, puma, catamount, mountain lion, painter, panther, Felis concolor (score = 0.00218)

[root@bright80 imagenet]#
Jupyter And JupyterHub Usage

This chapter covers the usage of Jupyter and JupyterHub, as well as the possibility to integrate it alongside a Spark deployment within Bright Cluster Manager.

Jupyter on its own is single user. However JupyterHub allows it to provide a multi-user service, and is therefore commonly installed with Jupyter. In any case, in Bright Cluster Manager, the package cm-jupyter depends upon cm-jupyterhub, and so in this chapter, Jupyter and JupyterHub will be referred by only JupyterHub.

To be able to use it as multi-user, it is necessary to have JupyterHub. It is possible to install and use Jupyter alone. The package cm-jupyter won’t trigger the installation of cm-jupyterhub. However, this chapter covers the most common case, which is to have them working together. Indeed, the Bright Cluster Manager package cm-jupyter is a dependence of cm-jupyterhub. Therefore, in this chapter, the combination of Jupyter and JupyterHub are conveniently referred to as JupyterHub.

4.1 Installation Options

There are two ways in which JupyterHub can be installed in Bright Cluster Manager: manual installation, or integrated installation with Spark.

1. Manual installation: This installs only the default Jupyter kernels, normally python3 and whichever others are found in the package. It can be installed on any node, independently of any Spark deployment.

2. Integrated installation: This is associated with a Spark deployment. The Spark deployment can be standalone or YARN. Besides providing the default kernels, custom kernels are provided for Python 2 and 3, Scala, R (if R is installed on the system), and SQL interpreters. These are for the associated Spark deployment. The advantage of an integrated installation, in practice, is being able to access the Spark context that is automatically set by Toree, by using the variable sc.

4.1.1 Requirements

Python 3.3 and higher are recommended, although older versions of Python can be used. Using an older version however results in restricted functionality. Incidentally, Python 2 can be installed alongside Python 3, and users can run kernels normally with any version.

Most administrators should simply install python with:

Example

```
[root@bright80 ~]# (yum install -y python3) || (yum install -y python34)
```

At the time of writing of this section of text (October 2017), there is a minor bug open for CentOS 7.3, at https://bugzilla.redhat.com/show_bug.cgi?id=1481008. The bug affects the installation of the nodejs package. JupyterHub requires nodejs indirectly. If needed, the installation can be carried out manually with the following workaround:

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Example
[root@bright80 ~]# rpm -ivh https://kojipkgs.fedoraproject.org//packages/http-parser/2.7.1/3.e17/x86_64/http-parser-2.7.1-3.e17.x86_64.rpm && yum -y install nodejs

For an integrated deployment, the SparkR kernel is only available if the R package is installed on the cluster:

Example
[root@bright80 ~]# yum install R

4.1.2 Manual Installation
A manual installation of JupyterHub consists of the following steps:

- Installation of the cm-jupyterhub package to each software image that is to be used
- Re-provisioning of the active nodes that are using these software images, and waiting for the re-provisioning to finish
- Starting the cm-jupyterhub service on each of the re-provisioned nodes, and waiting for the services to come up on those nodes

The cm-jupyter and cm-jupyterhub service should then be ready for use as a systemd static unit file, and can be added as a service. In Bright Cluster Manager the service can be added within the device mode of cmsh, within the services submode.

For example, if the administrator would like to run JupyterHub on the head node and on node001, and if node001 has /cm/images/default-image/ as its path for its software image, then it can be configured as follows:

Example
[root@bright80 ~]# yum install -y cm-jupyterhub ... Complete!
[root@bright80 ~]# yum install -y cm-jupyterhub --installroot=/cm/images/default-image ... Complete!
[root@bright80 ~]# cmsh -c "device; imageupdate -w -c default"
[root@bright80 ~]# cmsh -c "device use master; services; add cm-jupyterhub; commit"
[root@bright80 ~]# cmsh -c "device use node001; services; add cm-jupyterhub; commit"

4.1.3 Integrated Installation
Integrated installation is only supported for Spark versions starting from 2.0.0.

There are two ways to set up an integrated installation of JupyterHub with Spark in Bright Cluster Manager:

1. alongside the Spark installation itself (section 4.1.4)
   or
2. carrying it out as a Spark maintenance option (section 4.1.5)
4.1.4 Integrated Installation Alongside Spark Installation

If setting up an integrated installation alongside a Spark installation, then the extra option
--connect-jupyter is used with cm-spark-setup (section 5.1.2 of the Big Data Deployment Manual). The option takes a list of nodes as argument. The installation works with deployments of Spark YARN, as well as with deployments of Spark standalone.

So, for example, if there is a Hadoop instance hdfs1 with YARN already deployed, and the administrator wishes to install Spark and JupyterHub on the head node and have node001 connected to it, then the command to install Jupyter with Spark can be run as:

Example

[root@bright80 ~]# cm-spark-setup -i hdfs1 -t spark-2.2.0-bin-hadoop2.7.tgz --connect-jupyter $(hostname),node001
Java home not specified, using: /usr/lib/jvm/jre-1.8.0-openjdk/
Spark release '2.2.0-bin-hadoop2.7'
Found Hadoop instance 'hdfs1', release: 2.7.4
Spark will be installed in YARN (client/cluster) mode.
Spark is already installed in /cm/shared/apps/hadoop/Apache/spark-2.2.0-bin-hadoop2.7/
Creating module file for Spark... done.
Creating configuration files for Spark... done.
Updating images... done.
Waiting for NameNode to be ready... done.
Initializing Spark YARN role... done.
Updating configuration in CMDaemon... done.
Doing Jupyter, JupyterHub and Toree packages installation and integration... done.
Waiting for NameNode to be ready... done.
Validating Spark setup...
-- testing '--master yarn --deploy-mode client' mode...
-- testing '--master yarn --deploy-mode cluster' mode...
Validating Spark setup... done.
Installation successfully completed.
Finished.

The Spark standalone installation (section 5.3 of the Big Data Deployment Manual) has an XML template at /cm/local/apps/cluster-tools/hadoop/conf/sparkconf.xml. Instead of using an existing instance as in the preceding example, a Spark standalone can be set up instead using an XML file based on that template. If the instance is called spark1, as defined in an XML file spark1.xml, and JupyterHub is to be installed on the head node with node001 connected to it, then the command to install Jupyter with Spark can be run as:

Example

[root@bright80 ~]# cm-spark-setup -c "spark1.xml" --connect-jupyter $(hostname),node001
Reading config from file '/tmp/spark1.xml'... done.
Spark release '2.2.0-bin-hadoop2.7'
Creating Spark instance 'spark1'... done.
Spark will be installed in Standalone mode.
Spark Master service will be run on: node001
Spark Worker service will be run on: node002,node003,node004
Spark is already installed in /cm/shared/apps/hadoop/Apache/spark-2.2.0-bin-hadoop2.7/
Creating directories for Spark... done.
Creating module file for Spark... done.
Creating configuration files for Spark... done.
Updating images... done.
Initializing Spark Master service... done.

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Initializing Spark Worker services... done.
Updating configuration in CMDaemon... done.
Doing Jupyter, JupyterHub and Toree packages installation and integration... done.
Validating Spark setup...
-- testing Python application...
-- testing Java application...
-- testing Scala application...
Validating Spark setup... done.
Installation successfully completed.
Finished.

4.1.5 Integrated Installation Using cm-spark-maint

If setting up an integrated installation using cm-spark-maint (section 5.7 of the Big Data Deployment Manual), then the extra option --connect-jupyter is used. A list of nodes is used as the input to the option.

The method can be carried out for both Spark YARN and Spark standalone. Its API is identical to the previous method.

So, for example, if there is a Spark deployment of a Hadoop instance hdfs1, and the administrator would like to connect JupyterHub on the head node with node001, then the command that can be used is:

Example

[root@bright80 ~]# cm-spark-maint -i hdfs1 --connect-jupyter $(hostname),node001
Doing Jupyter, JupyterHub and Toree integration... done.

Alternatively, if installing to an already-installed Spark standalone called spark1, and the administrator would like to connect JupyterHub on the head node with node001, then the command that can be used is:

Example

[root@bright80 ~]# cm-spark-maint -i spark1 --connect-jupyter $(hostname),node001
Doing Jupyter, JupyterHub and Toree integration... done.

4.1.6 Verifying Jupyter And JupyterHub Installation

After the cm-jupyterhub service is started, it can take some time until the service is fully up and running. Even if systemctl status cm-jupyterhub -l shows that the service is already running, it can still take some seconds longer start functioning.

At this point, whatever the method that was used to install JupyterHub, the cm-jupyterhub service should be running on the nodes. Each node should be accessible via a web browser on port 8000 (figure 4.1):
4.2 Creating And Running A Notebook

Any user registered in the Linux-PAM system can log in to JupyterHub. For example, a test user `jupyterhubuser` with password `pw1` can be created with:

**Example**

```
[root@bright80 ~]# cmsh -c "user ; add jupyteruser ; set password pw1 ; commit "
```

To be able to access the HDFS in the case of integrated deployment with Spark Yarn, this user has to be granted access. Access can be granted with the `cm-hadoop-user` utility, for a given instance `hdfs1`, with:

**Example**

```
[root@bright80 ~]# cd /cm/local/apps/cluster-tools/hadoop
[root@bright80 hadoop]# cm-hadoop-user --grant jupyteruser=hdfs1
```

A login can then be carried out for the test user in the JupyterHub screen. The user is forwarded to a Jupyter instance (figure 4.2):

![JupyterHub login screen](image)

Figure 4.1: JupyterHub login screen
Clicking on the New button of figure 4.2 displays a list of kernels (figure 4.3):

The two first kernels in figure 4.3, Python 2 and Python 3, are default kernels. At least one of them will be present.

The remaining ones in the example were installed using the integration methods. If Python 3 is chosen, then a notebook can be created for it (figure 4.4):
A simple Python 3 code, such as `print('Hello')` can be typed in the text entry box and run (figure 4.5):

It is not possible to import `pyspark` here, because the kernel does not know about the Spark deployment location:
The notebook can be closed by clicking on File and Close and Halt.

If the user has any kernel for a Spark deployment, then a notebook can be created for it. In this case, no error is shown after importing `pyspark`, or even accessing the Spark context automatically created by Spark directly (figure 4.7):

```python
In [1]: import pyspark

ImportError: No module named 'pyspark'
```

Figure 4.6: Sample Python 3 notebook: PySpark import not possible

That same context is available in all Toree kernels, such as the Scala one:

```scala
In [1]: sc
```

```
Out[1]: pyspark.context.SparkContext object at 0xb2a316>
```

Figure 4.7: Sample integrated Spark notebook: successful import PySpark/access Spark context

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Extra caution is required with the SQL Toree kernel, as of the writing of this chapter. The kernel hang if given invalid SQL queries. This is an open issue at https://issues.apache.org/jira/browse/TOREE-419 at the time of writing of this section (October 2017).

Also at the time of writing, the R kernel suffers from instabilities. These may prevent the kernel from running. There is an open issue for this at https://issues.apache.org/jira/browse/TOREE-396, and for which Bright Computing has proposed a patch.

4.3 An Example Of A Notebook Connecting To Spark: Word2Vec

If JupyterHub deployment has been carried out as in the preceding sections, and it has been verified and its notebook creation capability checked, then it should be ready for use. An example run is now carried out in this section.

The machine learning library code Word2Vec at https://spark.apache.org/docs/latest/mllib-feature-extraction.html#word2vec takes a dataset of words, and outputs a set of words that can be used in similar contexts. All that is needed is to place the sample data file in a location that both jupyteruser and Spark users can access.

To run the example, a Python programming language, and a Spark standalone deployment, are chose. The kernel PySpark for Spark standalone is an appropriate choice. The preparation can be carried out as follows:

Example

```
[root@bright80 ~]# su - jupyteruser
[root@bright80 ~]# wget http://mattmahoney.net/dc/text8.zip
[root@bright80 ~]# unzip text8.zip
[root@bright80 ~]# truncate -s 10000000 text8 # truncate to 9.6 MB file
[root@bright80 ~]# sudo su - spark ls $PWD/text8 # ensure spark user can access it
```

The truncate step ensures the file is small enough to run in a cluster with few resources. Truncation can be skipped for clusters that can run large enough instances.

Instead of PySpark and Spark standalone, Scala and Spark YARN could have been chosen instead. In this case, the file should be uploaded to the HDFS. To use a bare Python 2 or Python 3 kernel, the user must also take care to obtaining the context `sc`, which is set automatically by the integrated kernels.
Cell 1 shows that the `sc` context is properly set. The Spark RDD is created in cell 3 using the source file as input.

Cell 2 shows the Word2Vec model factory being imported. It takes the Spark RDD to create `Word2VecModel` in cell 5. This is where intensive computation is carried out, and the user may expect significant latency, as indicated by an asterisk [*], depending on the cluster and RDD size. If no errors as cell 2 to 5 are processed, then no output is expected.

Cell 6 shows the output of `model`, and ensures all is well.

Cell 7 shows the already-computed model is queried to fetch 5 synonyms for the word `one`. Synonyms in the context of Word2Vec can differ from the concept as understood by humans.

In cell 8 the synonym output is shown, along with correlation coefficients. The synonyms are `nine`, `eight`, `seven`, `six`, and `three`.

### 4.4 Removal Of JupyterHub

Before removing JupyterHub, the administrator should ensure that all kernels have been halted and that no user is still logged onto `cm-jupyterhub`. Stopping `cm-jupyterhub` services with users that are still logged in, or with running kernels, has undefined behavior.

To remove the connection between a Spark deployment and a JupyterHub installation, `cm-spark-setup` offers the option `--disconnect-jupyter`. This option takes a list of nodes as argument.
Example

[root@bright80 ~]# cm-spark-maint -i hdfs1 --disconnect-jupyter $({hostname}),node001
Undoing Jupyter, JupyterHub and Toree packages installation and integration... done.

The connection of a Spark deployment with JupyterHub is removed alongside a Spark deployment, without the need of extra parameters:

Example

[root@bright80 ~]# cm-spark-setup -u hdfs1
Undoing Jupyter, JupyterHub and Toree packages installation and integration... done.
Stopping/removing services... done.
Removing module file... done.
Removing configuration directory... done.
Cleaning ZooKeeper... done.
Removing additional Spark directories... done.
Removing Spark-related metrics... done.
Removal successfully completed.
Finished.

Both of the preceding methods do not remove the packages from the nodes. This is to avoid clashes with manual installations that are not managed by Bright Cluster Manager utilities.

The packages can still be manually uninstalled by reversing the steps of a manual installation by:

- Stopping the cm-jupyterhub service on each one of the nodes.
- Removing the package cm-jupyterhub for each desired software image.
- Reprovisioning the active nodes that have those software images, and waiting for the reprovisioning to finish.

After reprovisioning, cm-jupyterhub is no longer installed.

Thus, for example, if the administrator would like to remove JupyterHub on the headnode and node001, and node001 has /cm/images/default-image/ as the path for its software image, then the removal can be carried out with:

Example

[root@bright80 ~]# ssh node001 service cm-jupyterhub stop
[root@bright80 ~]# service cm-jupyterhub stop
[root@bright80 ~]# yum remove -y cm-jupyterhub --installroot=/cm/images/default-image
[root@bright80 ~]# yum remove -y cm-jupyterhub
[root@bright80 ~]# cmsh -c "use device ; imageupdate -w -c default"

Removing cm-jupyterhub with yum does not remove the dependent packages that were installed with it. The resolution of the dependencies may spawn a whole tree of package changes, and is outside the scope of this chapter. However, the direct dependent packages for the package cm-jupyterhub in Bright Cluster Manager are as follows:

- cm-jupyterhub depends on:
  - cm-jupyter
  - cm-npm-configurable-http-proxy depends on:
    * npm

Finally, the testing user created earlier to verify the installation of JupyterHub can be removed with:

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Example

cmsh -c "user ; remove jupyteruser ; commit "
Successfully removed 1 Users
Successfully committed 0 Users