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How to run CANDLE on Biowulf

Andrew Weisman
High Performance Computing Analyst
Strategic Data Science Initiatives

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What is CANDLE?

- CANDLE (CANcer Distributed Learning Environment) is an open-source software project built to provide this support
  - Actively developed
  - Scales very efficiently on the world's fastest supercomputers
- Our recent contributions:
  - We've set it up on Biowulf ("grid" and "bayesian" workflows)
  - Enabled R support (in addition to Python)
  - Made it easy to use, including single input file support

(Disney)

CANDLE Quick Start

- Enter a working directory on Biowulf's /data partition, e.g.,

```
mkdir /data/$USER/candle
cd /data/$USER/candle
```

- Load the CANDLE module:

```
module load candle
```

- Copy over a CANDLE template:

```
candle import-template {grid,bayesian,r}
```

- Submit the template:

```
candle submit-job XXXX_example.in
```

How do we run our own model?

Modify the template!

(Staples)

How to run your model using CANDLE

- Load the CANDLE module
- Copy over a CANDLE template
- Modify your model script in two simple ways
- Modify the settings in the input file
- Submit the CANDLE job

Prerequisites to implementing your own model in CANDLE

- Write a model script (e.g., “mnist.py”)
  - A “model script” is a program written in Python or R that employs a deep learning library (e.g., Keras, TensorFlow, PyTorch) to construct a machine or deep learning “model” and optimize its weights
  - Instead of a machine/deep learning model, your script can simply be any computational pipeline
- Make sure your model script runs as-is on Biowulf

How do I modify my model script for use with CANDLE?

1. Decide what the hyperparameters are and substitute them with a Python dictionary or R data.frame called `hyperparams`:

Python example

Change:

```
n_conv_layers = 4
batch_size = 128
```

To:

```
n_conv_layers = hyperparams['nconv_layers']
batch_size = hyperparams['batch_size']
```

R example

Change:

```
n_conv_layers <- 4
batch_size <- 128
```

To:

```
n_conv_layers <- hyperparams[["nconv_layers"]]
batch_size <- hyperparams[["batch_size"]]
```

How do I modify my model script for use with CANDLE?

2. Return a metric (call it `val_to_return`) of how well the run performed (a single number) or a dummy number
   - Instead, for Python models you may define the variable `history` as the return value of a Keras `model.fit()` method

Python example

Add:

```
score = model.evaluate(x_test, y_test)
val_to_return = score[0]
```

Or:

```
history = model.fit(x_train, y_train, ...)
```

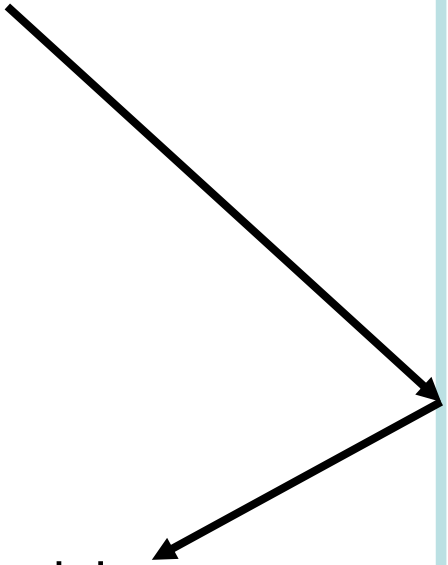
R example

Add:

```
val_to_return <- my_validation_loss
```

Modify and submit the CANDLE input file

(1) Modify the input file



(2) Submit the job:

```
candle submit-job grid_example.in
```

```
&control
  model_script="$(pwd)/mnist_mlp.py"
  workflow="grid"
  ngpus=2
  gpu_type="k80"
  walltime="00:20:00"
/

&default_model
  epochs=20
  batch_size=128
  activation='relu'
  optimizer='rmsprop'
  num_filters=32
/

&param_space
  {"id": "hpset_01", "epochs": 15, "activation": "tanh"}
  {"id": "hpset_02", "epochs": 30, "activation": "tanh"}
  {"id": "hpset_03", "epochs": 15, "activation": "relu"}
  {"id": "hpset_04", "epochs": 30, "activation": "relu"}
  {"id": "hpset_05", "epochs": 10, "batch_size": 128}
  {"id": "hpset_06", "epochs": 10, "batch_size": 256}
  {"id": "hpset_07", "epochs": 10, "batch_size": 512}
/
```

General settings

Default hyperparameters

Workflow settings

cbiit.github.com/sdsi/candle

Sample directory structure after CANDLE job completion


```
.
├── experiments
│   └── X000
│       ├── cfg-sys-biowulf.sh
│       ├── grid_workflow-GENERATED.txt
│       ├── jobid.txt
│       ├── metadata.json
│       ├── output.txt
│       ├── run
│       │   ├── hpset_01
│       │   ├── hpset_02
│       │   ├── hpset_03
│       │   ├── hpset_04
│       │   ├── hpset_05
│       │   ├── hpset_06
│       │   └── hpset_07
│       ├── submit.sh
│       ├── turbine.log
│       ├── turbine-slurm.sh
│       ├── workflow.sh.log
│       └── workflow.tic
├── last-exp -> /gpfs/gsfs10/users/weismanal/notebook/2019-07-11/test_grid/experiments/X000
└── grid_example.in
```

Aggregating the results

- Put the hyperparameters and corresponding metrics into CSV format:

```
candle aggregate-results
 <EXPERIMENT-DIRECTORY>
```

- Example:

```
candle aggregate-results
/data/$USER/candle/experiments
/X004
```

- This will print to the file `candle_results.csv` all the hyperparameters and metrics in CSV format

Sample CSV file in Microsoft Excel

	A	B	C	D	E	F	G
1	result	dirname	id	batch_size	num_cores	use_gpu	learning_rate
2	73.26	hpset_00420	hpset_00420	1024	14	TRUE	1000
3	73.778	hpset_00415	hpset_00415	1024	14	TRUE	150
4	73.852	hpset_00416	hpset_00416	1024	14	TRUE	200
5	74.196	hpset_00401	hpset_00401	1024	8	TRUE	150
6	74.365	hpset_00418	hpset_00418	1024	14	TRUE	500
7	74.469	hpset_00414	hpset_00414	1024	14	TRUE	100
8	74.631	hpset_00404	hpset_00404	1024	8	TRUE	500
9	74.711	hpset_00417	hpset_00417	1024	14	TRUE	300
10	74.917	hpset_00400	hpset_00400	1024	8	TRUE	100
11	74.972	hpset_00406	hpset_00406	1024	8	TRUE	1000
12	75.005	hpset_00403	hpset_00403	1024	8	TRUE	300
13	75.124	hpset_00402	hpset_00402	1024	8	TRUE	200
14	75.43	hpset_00348	hpset_00348	512	14	TRUE	500
15	75.525	hpset_00350	hpset_00350	512	14	TRUE	1000
16	75.589	hpset_00419	hpset_00419	1024	14	TRUE	700
17	75.822	hpset_00349	hpset_00349	512	14	TRUE	700

Summary of how to run CANDLE on Biowulf

- Enter working directory on Biowulf's /data partition, e.g., `cd /data/$USER/candle`
- Load the CANDLE module: `module load candle`
- Copy over one of the CANDLE templates: `candle import-template {grid,bayesian,r}`
- Ensure your model script works standalone on Biowulf

- Modify your model script in two ways:
  1. Substitute the hyperparameters with a `hyperparams` dictionary/data.frame
  2. Return a single number metric of performance in `val_to_return`
- Modify the CANDLE input (.in) file
- Submit the CANDLE job: `candle submit-job XXXX.in`
- Aggregate the results to the file `candle_results.csv`: `candle aggregate-results <EXPERIMENT-DIRECTORY>`

Hands-on exercise!

Please go to:

https://cbiit.github.com/sdsi/vae_with_pytorch

Sample hyperparameter analysis: (2) Split up into GPU vs. CPU only

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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	result	dirname	id	batch_size	num_cores	use_gpu	learning_rate			result	dirname	id	batch_size	num_cores	use_gpu	learning_rate
2																
3	73.26	hpset_00420	hpset_00420	1024	14	TRUE	1000			104.3	hpset_00343	hpset_00343	512	14	FALSE	1000
4	73.778	hpset_00415	hpset_00415	1024	14	TRUE	150			104.873	hpset_00341	hpset_00341	512	14	FALSE	500
5	73.852	hpset_00416	hpset_00416	1024	14	TRUE	200			105.224	hpset_00339	hpset_00339	512	14	FALSE	200
6	74.196	hpset_00401	hpset_00401	1024	8	TRUE	150			105.254	hpset_00337	hpset_00337	512	14	FALSE	100
7	74.365	hpset_00418	hpset_00418	1024	14	TRUE	500			105.353	hpset_00342	hpset_00342	512	14	FALSE	700
8	74.469	hpset_00414	hpset_00414	1024	14	TRUE	100			105.71	hpset_00338	hpset_00338	512	14	FALSE	150
9	74.631	hpset_00404	hpset_00404	1024	8	TRUE	500			105.879	hpset_00408	hpset_00408	1024	14	FALSE	150
10	74.711	hpset_00417	hpset_00417	1024	14	TRUE	300			106.061	hpset_00413	hpset_00413	1024	14	FALSE	1000
11	74.917	hpset_00400	hpset_00400	1024	8	TRUE	100			106.09	hpset_00340	hpset_00340	512	14	FALSE	300
12	74.972	hpset_00406	hpset_00406	1024	8	TRUE	1000			106.843	hpset_00411	hpset_00411	1024	14	FALSE	500
13	75.005	hpset_00403	hpset_00403	1024	8	TRUE	300			107.166	hpset_00412	hpset_00412	1024	14	FALSE	700
14	75.124	hpset_00402	hpset_00402	1024	8	TRUE	200			107.46	hpset_00409	hpset_00409	1024	14	FALSE	200
15	75.43	hpset_00348	hpset_00348	512	14	TRUE	500			108.253	hpset_00323	hpset_00323	512	8	FALSE	100
16	75.525	hpset_00350	hpset_00350	512	14	TRUE	1000			108.877	hpset_00407	hpset_00407	1024	14	FALSE	100
17	75.589	hpset_00419	hpset_00419	1024	14	TRUE	700			110.057	hpset_00410	hpset_00410	1024	14	FALSE	300
18	75.822	hpset_00349	hpset_00349	512	14	TRUE	700			110.139	hpset_00268	hpset_00268	256	14	FALSE	150
19	75.833	hpset_00344	hpset_00344	512	14	TRUE	100			110.147	hpset_00273	hpset_00273	256	14	FALSE	1000
20	75.946	hpset_00345	hpset_00345	512	14	TRUE	150			110.207	hpset_00329	hpset_00329	512	8	FALSE	1000
21	76.048	hpset_00405	hpset_00405	1024	8	TRUE	700			110.332	hpset_00267	hpset_00267	256	14	FALSE	100
22	76.274	hpset_00346	hpset_00346	512	14	TRUE	200			110.341	hpset_00271	hpset_00271	256	14	FALSE	500

Sample hyperparameter analysis: (3) Run Pearson correlation

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	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	result	dirname	id	batch_size	num_cores	use_gpu	learning_rate			result	dirname	id	batch_size	num_cores	use_gpu	learning_rate
2	1			-0.65	-0.10		0.00			1			-0.21	-0.66		0.00
3	73.26	hpset_00420	hpset_00420	1024	14	TRUE	1000			104.3	hpset_00343	hpset_00343	512	14	FALSE	1000
4	73.778	hpset_00415	hpset_00415	1024	14	TRUE	150			104.873	hpset_00341	hpset_00341	512	14	FALSE	500
5	73.852	hpset_00416	hpset_00416	1024	14	TRUE	200			105.224	hpset_00339	hpset_00339	512	14	FALSE	200
6	74.196	hpset_00401	hpset_00401	1024	8	TRUE	150			105.254	hpset_00337	hpset_00337	512	14	FALSE	100
7	74.365	hpset_00418	hpset_00418	1024	14	TRUE	500			105.353	hpset_00342	hpset_00342	512	14	FALSE	700
8	74.469	hpset_00414	hpset_00414	1024	14	TRUE	100			105.71	hpset_00338	hpset_00338	512	14	FALSE	150
9	74.631	hpset_00404	hpset_00404	1024	8	TRUE	500			105.879	hpset_00408	hpset_00408	1024	14	FALSE	150
10	74.711	hpset_00417	hpset_00417	1024	14	TRUE	300			106.061	hpset_00413	hpset_00413	1024	14	FALSE	1000
11	74.917	hpset_00400	hpset_00400	1024	8	TRUE	100			106.09	hpset_00340	hpset_00340	512	14	FALSE	300
12	74.972	hpset_00406	hpset_00406	1024	8	TRUE	1000			106.843	hpset_00411	hpset_00411	1024	14	FALSE	500
13	75.005	hpset_00403	hpset_00403	1024	8	TRUE	300			107.166	hpset_00412	hpset_00412	1024	14	FALSE	700
14	75.124	hpset_00402	hpset_00402	1024	8	TRUE	200			107.46	hpset_00409	hpset_00409	1024	14	FALSE	200
15	75.43	hpset_00348	hpset_00348	512	14	TRUE	500			108.253	hpset_00323	hpset_00323	512	8	FALSE	100
16	75.525	hpset_00350	hpset_00350	512	14	TRUE	1000			108.877	hpset_00407	hpset_00407	1024	14	FALSE	100
17	75.589	hpset_00419	hpset_00419	1024	14	TRUE	700			110.057	hpset_00410	hpset_00410	1024	14	FALSE	300
18	75.822	hpset_00349	hpset_00349	512	14	TRUE	700			110.139	hpset_00268	hpset_00268	256	14	FALSE	150
19	75.833	hpset_00344	hpset_00344	512	14	TRUE	100			110.147	hpset_00273	hpset_00273	256	14	FALSE	1000
20	75.946	hpset_00345	hpset_00345	512	14	TRUE	150			110.207	hpset_00329	hpset_00329	512	8	FALSE	1000
21	76.048	hpset_00405	hpset_00405	1024	8	TRUE	700			110.332	hpset_00267	hpset_00267	256	14	FALSE	100
22	76.274	hpset_00346	hpset_00346	512	14	TRUE	200			110.341	hpset_00271	hpset_00271	256	14	FALSE	500

How to generate the grid of hyperparameters automatically

- You can generate a grid of hyperparameters automatically by running

```
candle generate-grid <PYTHON-LIST-1> <PYTHON-LIST-2> …
```

- For example, running

```
candle generate-grid "['nlayers',np.arange(5,15,2)]" "['dir',['x','y','z']]"
```

would output to the file `grid_workflow-XXXX.txt`:

```
{"id": "hpset_00001", "nlayers": 5, "dir": "x"}
{"id": "hpset_00002", "nlayers": 5, "dir": "y"}
{"id": "hpset_00003", "nlayers": 5, "dir": "z"}
{"id": "hpset_00004", "nlayers": 7, "dir": "x"}
{"id": "hpset_00005", "nlayers": 7, "dir": "y"}
{"id": "hpset_00006", "nlayers": 7, "dir": "z"}
{"id": "hpset_00007", "nlayers": 9, "dir": "x"}

                                    etc.
```

Sample &param_space section – “bayesian" example


```
makeDiscreteParam("batch_size", values = c(16, 32))
makeIntegerParam("epochs", lower = 2, upper = 5)
makeDiscreteParam("activation", values = c("softmax", "softplus", "relu"))
makeNumericParam("drop", lower = 0, upper = 0.9)
```

Section Title

Presenter

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Secondary Slide Title

- Bullet point
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