

RADICAL-Learning

Radical.hpo

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What is HPO?

- Any machine learning model has some values (hyperparameters) that need to be specified a priori before the training process.
 - They help adapt the model to the data and they influence the quality of the prediction.
- Hyperparameter optimization deals with the search of the best combination of values for the given model, and there are already many methods that help us find them.

HPO Approaches

1. Grid Search: try all combinations (brute force)
2. Random Search: try as many combinations as possible (better)
3. Informed Search (Bayesian Optimization): try the most promising combinations by reevaluating where to look next (even better)
4. ...more

Background

- There already exists HyperSpace, a parallel Bayesian Model-Based Optimization (parallel Bayesian SMBO) library with one of the main goals of optimizing model performance with respect to hyperparameters. It supports Scikit-Optimize, RoBo and Hyperband
 - i.e, we can run a bag-of-tasks of optimizations where each task runs the Gaussian process that explores a search space (hyperspace)

Goal

- Since our HPO module wants to integrate HyperSpace with EnTK, the logical path to follow is to treat each hyperspace optimization as an independent task, and set up a bag (stage) of tasks inside a single pipeline
 - We take full advantage of EnTK and achieve concurrency at EnTK level, while still making use of HyperSpace's spaces creation and optimization through its supported HPO engines

Requirements

- Functional

- It must satisfy Bayesian Model-Based Optimization (SMBO) requirements:
 - Define a machine learning model (or objective function)
 - Provide with train/test datasets (if ML model selected)
 - Define a validation protocol: cross-validation (if ML model selected)
 - Define the parameter search space: upper and lower bounds for each hyperparameter
 - Define the optimization function: Gaussian process with guided sampling
- Must use RADICAL-EnTK

- Non-Functional

- The code must be simple
- The code must be easy to maintain

- Non-Functional

- It must use the maximum number of cores available on the largest XSEDE machine, without significant overhead

Execution of HyperSpace

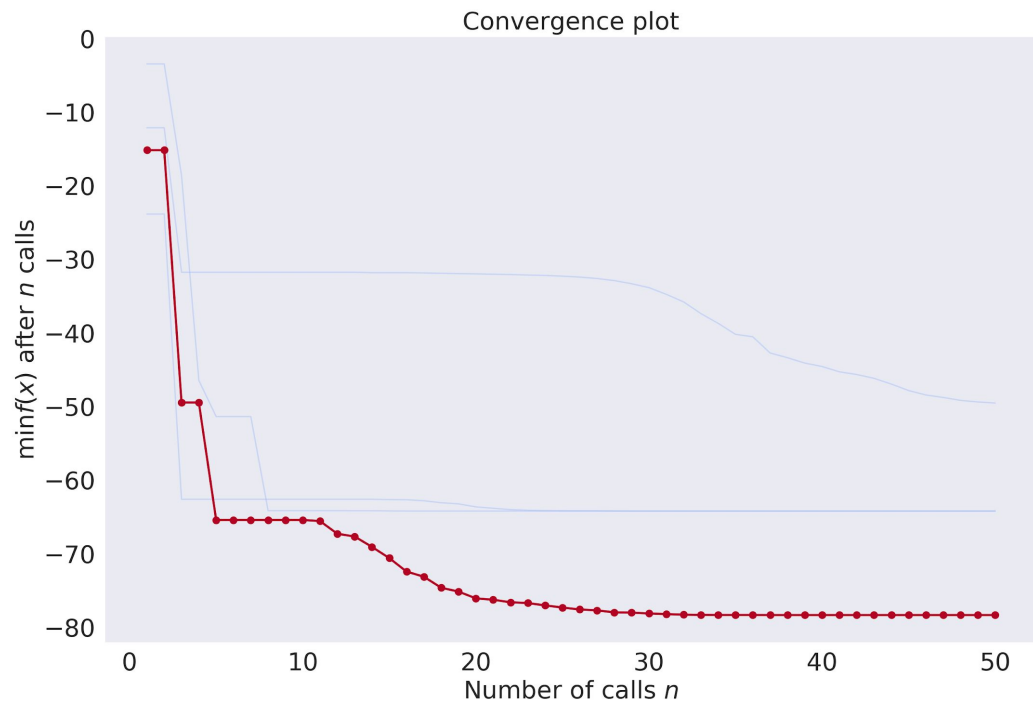
- HyperSpaces use Scikit-Optimize
- Creates combinations of hyperparameters (hyperspaces) using overlapping boundaries between hyperparameters
- Bag-of-tasks are executed with mpi4py
- Number of tasks depends on the number of hyperparameters for the model:
 - $\text{HyperSpaces} = 2^H$ where H is the number of hyperparameters
 - Avg. num of hyperparameters $\sim 7-8$ but depending on model can go up to 12
 - Each optimization runs for N -iterations, where N is ~ 100
- Tasks (Bayesian optimization step) are independent on HyperSpace, requiring each 1 MPI Rank at minimum and using 1 core each

Minimal Example: Styblinski-Tang

```
Time taken: 0.8317
Function value obtained: -46.8635
Current minimum: -46.8635
Iteration No: 48 started. Searching for the next optimal point.
Iteration No: 48 ended. Search finished for the next optimal point.
Time taken: 0.9449
Function value obtained: -47.2895
Current minimum: -47.2895
Iteration No: 49 started. Searching for the next optimal point.
Iteration No: 49 ended. Search finished for the next optimal point.
Time taken: 0.9206
Function value obtained: -47.7904
Current minimum: -47.7904
Iteration No: 50 started. Searching for the next optimal point.
Iteration No: 50 ended. Search finished for the next optimal point.
Time taken: 1.1440
Function value obtained: -48.0842
Current minimum: -48.0842
/home/karahbit/miniconda3/envs/radical.hpo/lib/python3.6/site-packages/scikit_learn-0.21.3-py3.6-linux-x86_64.egg/sklearn/externals/joblib/__init__.py:15: DeprecationWarning:
sklearn.externals.joblib is deprecated in 0.21 and will be removed in 0.23. Please imp
ort this functionality directly from joblib, which can be installed with: pip install j
oblib. If this warning is raised when loading pickled models, you may need to re-serial
ize those models with scikit-learn 0.21+.
warnings.warn(msg, category=DeprecationWarning)
Command being timed: "mpirun -n 4 python3 benchmark.py --ndims 2 --results /hom
e/karahbit"
User time (seconds): 0.02
System time (seconds): 0.02
Percent of CPU this job got: 0%
Elapsed (wall clock) time (h:mm:ss or m:ss): 0:30:16
Average shared text size (kbytes): 0
Average unshared data size (kbytes): 0
Average stack size (kbytes): 0
Average total size (kbytes): 0
Maximum resident set size (kbytes): 5240
Average resident set size (kbytes): 0
Major (requiring I/O) page faults: 0
Minor (reclaiming a frame) page faults: 4484
Voluntary context switches: 127
Involuntary context switches: 64
Swaps: 0
File system inputs: 0
File system outputs: 0
Socket messages sent: 0
Socket messages received: 0
Signals delivered: 0
Page size (bytes): 4096
Exit status: 0
(radical.hpo) [karahbit@s08 hyperdrive]$ /usr/bin/time -v mpirun -n 4 python3 benchmar
k.py --ndims 2 --results /home/karahbit
0.01 [ 0.0%] 8 [ 0.0%] 15 [ 0.0%] 22 [ 0.0%]
2 [ 0.0%] 9 [ 0.0%] 16 [ 0.0%] 23 [ 0.0%]
3 [ 0.0%] 10 [ 0.0%] 17 [ 0.0%] 24 [ 0.0%]
4 [ 0.0%] 11 [ 0.0%] 18 [ 0.0%] 25 [ 0.0%]
5 [ 0.0%] 12 [ 0.0%] 19 [ 0.0%] 26 [ 0.0%]
6 [ 0.0%] 13 [ 0.0%] 20 [ 0.0%] 27 [ 0.0%]
7 [ 0.0%] 14 [ 0.0%] 21 [ 0.0%] 28 [ 0.0%]
Mem| 3.65G/124G Tasks: 69, 97 thr: 5 running
Swp| 60.5M/16.8G Load average: 2.55 3.80 11.29
Uptime: 21 days, 13:42:11

PID USER PRI NI VIRT RES SHR S CPU% MEM% TIME+ Command
21310 karahbit 20 0 33.0G 212M 104M R 100.0 0.2 0:17.52 python3 benchmark.py --n
21309 karahbit 20 0 33.0G 207M 104M R 99.6 0.2 0:17.55 python3 benchmark.py --n
21308 karahbit 20 0 33.0G 216M 104M R 99.6 0.2 0:17.55 python3 benchmark.py --n
21311 karahbit 20 0 33.0G 208M 104M R 99.6 0.2 0:17.50 python3 benchmark.py --n
20713 karahbit 20 0 120M 2508 1464 R 0.7 0.0 0:01.80 http
24776 root 20 0 624M 503M 2328 S 0.0 0.4 1h35:29 /var/lib/pcp/pmdas/proc/
7747 pcp 20 0 106M 4884 3032 S 0.0 0.0 8:44.51 /var/lib/pcp/pmdas/perfe
7750 pcp 20 0 106M 4884 3032 S 0.0 0.0 5:30.30 /var/lib/pcp/pmdas/perfe
20180 root 20 0 334M 3524 2568 S 0.0 0.0 0:00.07 slurmstepd: [6821394.0]
2741 root 20 0 379M 74868 8644 S 0.0 0.1 2:23.25 /opt/puppetlabs/puppet/b
21296 root 20 0 204M 3436 2516 S 0.0 0.0 0:00.02 slurmstepd: [6821394.4]
2078 root 20 0 3388M 56820 10000 S 0.0 0.0 0:05.25 /opt/packages/slurm/defa
21049 nscd 20 0 1502M 2408 1404 S 0.0 0.0 0:41.38 /usr/sbin/nscd
21287 karahbit 20 0 15004 1704 1360 S 0.0 0.0 0:00.01 mpiexec.hydra -n 4 pytho
21303 karahbit 20 0 16716 1640 1280 S 0.0 0.0 0:00.01 /opt/intel/compilers_and
5820 root 20 0 561M 19652 6316 S 0.0 0.0 2:50.89 /usr/bin/python2 -Es /us
1 root 20 0 187M 4792 2616 S 0.0 0.0 8:13.33 /usr/lib/systemd/systemd
5996 root 20 0 561M 19652 6316 S 0.0 0.0 2:50.65 /usr/bin/python2 -Es /us
5341 polkitd 20 0 599M 14404 4784 S 0.0 0.0 0:13.52 /usr/lib/polkit-1/polkit
18764 root 20 0 21768 1428 996 S 0.0 0.0 6:15.24 /usr/sbin/irqbalance --f
6276 root 20 0 413M 3704 776 S 0.0 0.0 5:07.22 hpsmlited -f /dev/hpilo
5874 root 20 0 405M 124M 14652 S 0.0 0.1 1:25.33 /usr/sbin/rsyslogd -n
6754 root 20 0 10640 616 488 S 0.0 0.0 0:44.58 /opt/hp/hp-health/bin/hp
5760 munge 20 0 735M 2392 1932 S 0.0 0.0 0:12.63 /usr/sbin/munged --num-t
20177 root 20 0 267M 3204 2424 S 0.0 0.0 0:00.03 slurmstepd: [6821394.ext
6278 root 20 0 413M 3704 776 S 0.0 0.0 1:24.72 hpsmlited -f /dev/hpilo
6260 root 20 0 93536 3008 2292 S 0.0 0.0 1:44.55 /var/lib/pcp/pmdas/linux
6137 root 20 0 718M 5284 3372 S 0.0 0.0 0:46.43 /usr/sbin/automount --fo
5863 root 20 0 405M 124M 14652 S 0.0 0.1 1:37.08 /usr/sbin/rsyslogd -n
20197 karahbit 20 0 114M 2320 1672 S 0.0 0.0 0:00.06 /bin/bash
20196 root 20 0 334M 3524 2568 S 0.0 0.0 0:00.02 slurmstepd: [6821394.0]
11915 root 20 0 296M 69652 9984 S 0.0 0.1 0:23.78 /opt/puppetlabs/puppet/b
21050 nscd 20 0 1502M 2408 1404 S 0.0 0.0 0:05.70 /usr/sbin/nscd
6149 pcp 20 0 172M 3364 2224 S 0.0 0.0 0:54.45 /usr/libexec/pcp/bin/pmc
21223 postfix 20 0 91296 3908 2928 S 0.0 0.0 0:02.04 qmgr -l -t unix -u
7751 root 20 0 203M 5700 3452 S 0.0 0.0 1:04.73 perl /var/lib/pcp/pmdas/
2743 root 20 0 379M 74868 8644 S 0.0 0.1 0:00.00 /opt/puppetlabs/puppet/b
2744 root 20 0 379M 74868 8644 S 0.0 0.1 0:00.69 /opt/puppetlabs/puppet/b
2762 root 20 0 379M 74868 8644 S 0.0 0.1 0:20.78 /opt/puppetlabs/puppet/b
[0] <bi>@br018:~/hyperspace/benchmarks/styblinski_tang/hyperdrive* "two" 07:28 14-Nov-19
F1Help F2Setup F3SearchF4FilterF5Tree F6SortByF7Nice F8Nice F9Kill F10Quit
```

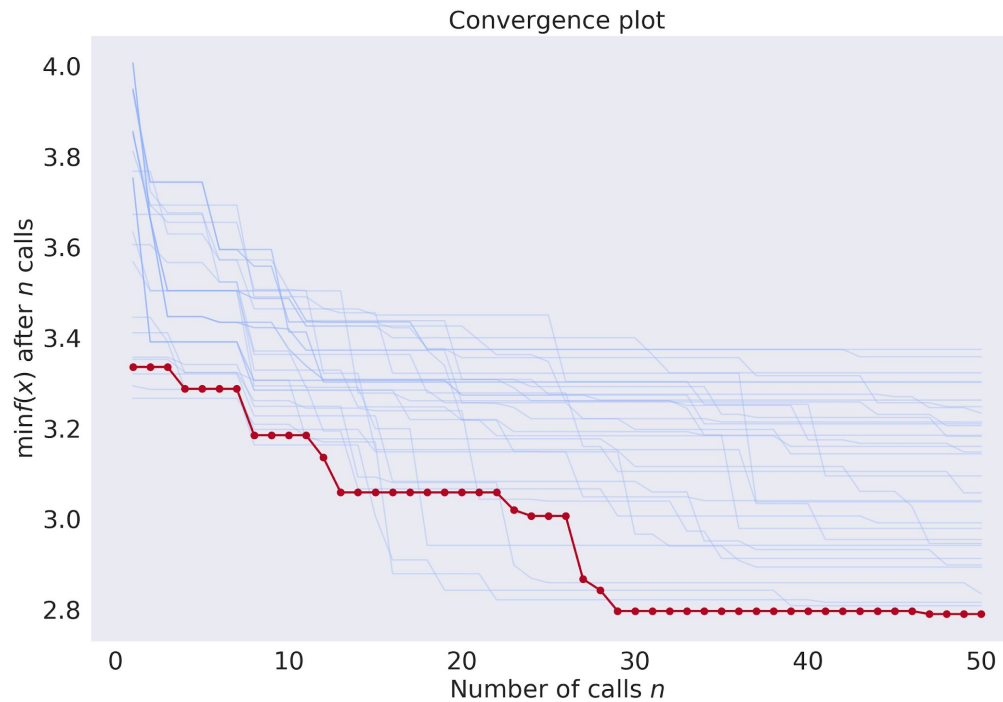

Minimal Example: Styblinski-Tang



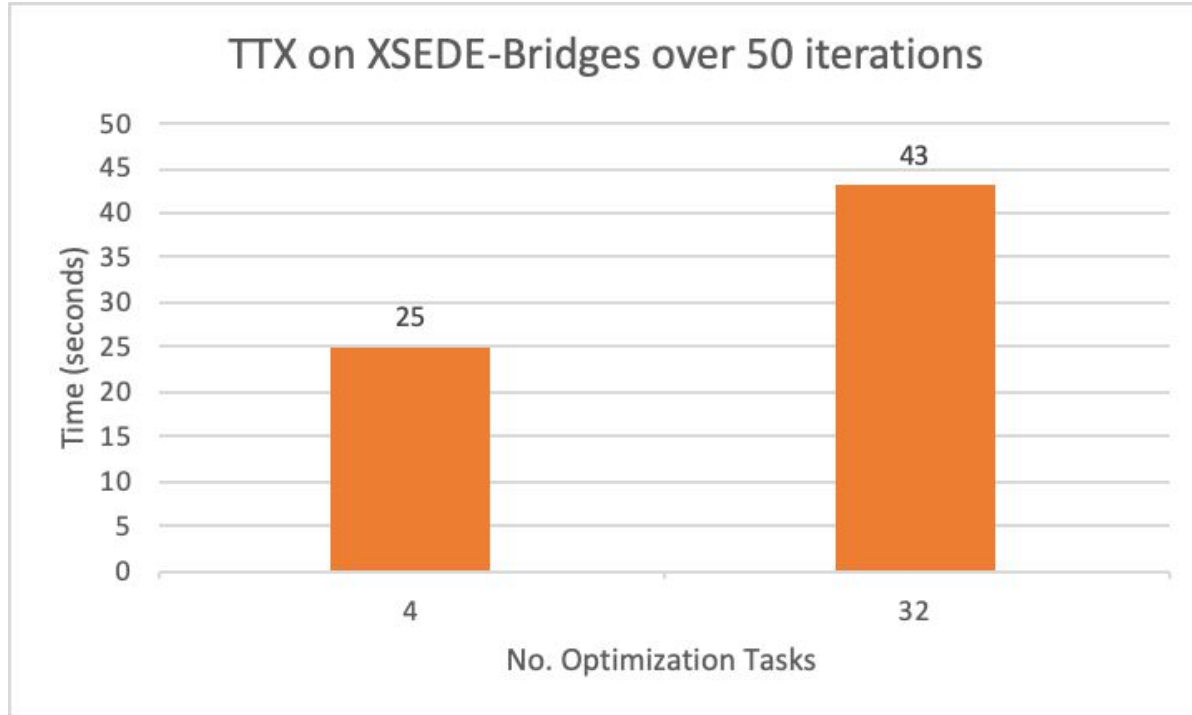
ML Example: Gradient Boosted Trees

ite-packages/scikit_optimize-0.5.2-py3.6.egg/skopt/optimizer/optimizer.py:399: UserWarning: The objective has been evaluated at this point before. warnings.warn("The objective has been evaluated " /home/karahbit/miniconda3/envs/radical.hpo/lib/python3.6/s ite-packages/scikit_optimize-0.5.2-py3.6.egg/skopt/optimizer/optimizer.py:399: UserWarning: The objective has been evaluated at this point before. warnings.warn("The objective has been evaluated " /home/karahbit/miniconda3/envs/radical.hpo/lib/python3.6/s ite-packages/scikit_learn-0.21.3-py3.6-linux-x86_64.egg/sklearn/externals/joblib/_init_.py:15: DeprecationWarning: sklearn.externals.joblib is deprecated in 0.21 and will be removed in 0.23. Please import this functionality directly from joblib, which can be installed with: pip install joblib. If this warning is raised when loading pickled models, you may need to re-serialize those models with skkit-learn 0.21+. warnings.warn(msg, category=DeprecationWarning) /home/karahbit/miniconda3/envs/radical.hpo/lib/python3.6/s ite-packages/hyperspaces-0.3.0-py3.6.egg/hyperspace/space/skopt/space.py:173: UserWarning: Each hyperspace contains a single value. Command being timed: "mpirun -n 32 python3 gbm.py --results /home/karahbit/results/gbm" User time (seconds): 0.01 System time (seconds): 0.03 Percent of CPU this job got: 0% Elapsed (wall clock) time (h:mm:ss or m:ss): 0:42. 49 Average shared text size (kbytes): 0 Average unshared data size (kbytes): 0 Average stack size (kbytes): 0 Average total size (kbytes): 0 Maximum resident set size (kbytes): 5260 Average resident set size (kbytes): 0 Major (requiring I/O) page faults: 0 Minor (reclaiming a frame) page faults: 4487 Voluntary context switches: 248 Involuntary context switches: 64 Swaps: 0 File system inputs: 0 File system outputs: 0 Socket messages sent: 0 Socket messages received: 0 Signals delivered: 0 Page size (bytes): 4096 Exit status: 0 (radical.hpo) [karahbit@r507 examples]\$ /usr/bin/time -v mpirun -n 32 python3 gbm.py --results /home/karahbit/results/gbm	1 [100.0] 8 [100.0] 15 [100.0] 22 [100.0] 2 [100.0] 9 [100.0] 16 [100.0] 23 [0.0] 3 [100.0] 10 [100.0] 17 [0.0] 24 [0.0] 4 [100.0] 11 [100.0] 18 [0.0] 25 [0.0] 5 [100.0] 12 [100.0] 19 [0.0] 26 [0.0] 6 [100.0] 13 [100.0] 20 [0.0] 27 [0.0] 7 [100.0] 14 [100.0] 21 [0.0] 28 [0.0] Mem[] 5.12G/126G Tasks: 78, 113 thr: 17 running Swp[] 114M/16.8G Load average: 5.42 9.04 10.71 Uptime: 21 days, 14:28:17	1 [100.0] 8 [100.0] 15 [100.0] 22 [100.0] 2 [100.0] 9 [100.0] 16 [100.0] 23 [0.0] 3 [100.0] 10 [100.0] 17 [0.0] 24 [0.0] 4 [100.0] 11 [100.0] 18 [0.0] 25 [0.0] 5 [100.0] 12 [100.0] 19 [0.0] 26 [0.0] 6 [100.0] 13 [100.0] 20 [0.0] 27 [0.0] 7 [100.0] 14 [100.0] 21 [0.0] 28 [0.0] Mem[] 4.99G/126G Tasks: 74, 100 thr: 18 running Swp[] 60.5M/16.8G Load average: 5.45 9.04 11.07 Uptime: 21 days, 14:28:16
PID USER PRI NI VIRT RES SHR S CPU% MEM% TI	PID USER PRI NI VIRT RES SHR S CPU% MEM% TI	PID USER PRI NI VIRT RES SHR S CPU% MEM% TI
21005 karahbit 20 0 33.4G 152M 41760 R 100.0 0.1 0.0	27859 karahbit 20 0 33.4G 153M 41760 R 100.0 0.1 0.0	27859 karahbit 20 0 33.4G 153M 41760 R 100.0 0.1 0.0
21008 karahbit 20 0 33.4G 153M 41772 R 100.0 0.1 0.0	27870 karahbit 20 0 33.4G 146M 41724 R 100.0 0.1 0.0	27870 karahbit 20 0 33.4G 146M 41724 R 100.0 0.1 0.0
20999 karahbit 20 0 33.4G 149M 41772 R 100.0 0.1 0.0	27866 karahbit 20 0 33.4G 148M 41716 R 100.0 0.1 0.0	27866 karahbit 20 0 33.4G 148M 41716 R 100.0 0.1 0.0
21006 karahbit 20 0 33.4G 149M 41760 R 100.0 0.1 0.0	27861 karahbit 20 0 33.4G 155M 41760 R 100.0 0.1 0.0	27861 karahbit 20 0 33.4G 155M 41760 R 100.0 0.1 0.0
21009 karahbit 20 0 33.4G 155M 41764 R 100.0 0.1 0.0	27865 karahbit 20 0 33.4G 153M 41760 R 100.0 0.1 0.0	27865 karahbit 20 0 33.4G 153M 41760 R 100.0 0.1 0.0
21000 karahbit 20 0 33.4G 149M 41760 R 100.0 0.1 0.0	27874 karahbit 20 0 33.4G 148M 41716 R 100.0 0.1 0.0	27874 karahbit 20 0 33.4G 148M 41716 R 100.0 0.1 0.0
21010 karahbit 20 0 33.4G 149M 41760 R 100.0 0.1 0.0	27862 karahbit 20 0 33.4G 148M 41728 R 100.0 0.1 0.0	27862 karahbit 20 0 33.4G 148M 41728 R 100.0 0.1 0.0
21001 karahbit 20 0 33.4G 149M 41760 R 99.6 0.1 0.0	27869 karahbit 20 0 33.4G 155M 41760 R 100.0 0.1 0.0	27869 karahbit 20 0 33.4G 155M 41760 R 100.0 0.1 0.0
21011 karahbit 20 0 33.4G 149M 41768 R 99.6 0.1 0.0	27871 karahbit 20 0 33.4G 150M 41620 R 100.0 0.1 0.0	27871 karahbit 20 0 33.4G 150M 41620 R 100.0 0.1 0.0
20996 karahbit 20 0 33.4G 149M 41764 R 99.6 0.1 0.0	27864 karahbit 20 0 33.4G 146M 41716 R 99.5 0.1 0.0	27864 karahbit 20 0 33.4G 146M 41716 R 99.5 0.1 0.0
20997 karahbit 20 0 33.4G 148M 41728 R 99.6 0.1 0.0	27863 karahbit 20 0 33.4G 153M 41760 R 99.5 0.1 0.0	27863 karahbit 20 0 33.4G 153M 41760 R 99.5 0.1 0.0
21002 karahbit 20 0 33.4G 149M 41764 R 99.6 0.1 0.0	27857 karahbit 20 0 33.4G 146M 41692 R 99.5 0.1 0.0	27857 karahbit 20 0 33.4G 146M 41692 R 99.5 0.1 0.0
21003 karahbit 20 0 33.4G 149M 41764 R 99.6 0.1 0.0	27872 karahbit 20 0 33.4G 148M 41628 R 99.5 0.1 0.0	27872 karahbit 20 0 33.4G 148M 41628 R 99.5 0.1 0.0
21004 karahbit 20 0 33.4G 149M 41728 R 99.6 0.1 0.0	27868 karahbit 20 0 33.4G 147M 41764 R 99.5 0.1 0.0	27868 karahbit 20 0 33.4G 147M 41764 R 99.5 0.1 0.0
21007 karahbit 20 0 33.4G 149M 41760 R 99.6 0.1 0.0	27873 karahbit 20 0 33.4G 148M 41716 R 99.5 0.1 0.0	27873 karahbit 20 0 33.4G 148M 41716 R 99.5 0.1 0.0
20998 karahbit 20 0 33.4G 151M 41760 R 99.6 0.1 0.0	27860 karahbit 20 0 33.4G 148M 41748 R 98.8 0.1 0.0	27860 karahbit 20 0 33.4G 148M 41748 R 98.8 0.1 0.0
14714 karahbit 20 0 120M 2532 1464 R 1.3 0.0 0.2	21111 karahbit 20 0 120M 2396 1460 R 2.0 0.0 0.2	21111 karahbit 20 0 120M 2396 1460 R 2.0 0.0 0.2
20984 root 20 0 203M 3436 2516 S 0.0 0.0 0.0	7750 pcp 20 0 106M 4884 3032 S 0.7 0.0 5.3	7750 pcp 20 0 106M 4884 3032 S 0.7 0.0 5.3
20991 karahbit 20 0 16716 1688 1336 S 0.0 0.0 0.0	27847 root 20 0 204M 3440 2516 S 0.0 0.0 0.0	27847 root 20 0 204M 3440 2516 S 0.0 0.0 0.0
5799 munge 20 0 734M 1876 1524 S 0.0 0.0 0.1	7747 pcp 20 0 106M 4884 3032 S 0.0 0.0 8.4	7747 pcp 20 0 106M 4884 3032 S 0.0 0.0 8.4
20974 karahbit 20 0 14964 1736 1388 S 0.0 0.0 0.0	2078 root 20 0 3388M 56860 10000 S 0.0 0.0 0.0	2078 root 20 0 3388M 56860 10000 S 0.0 0.0 0.0
20975 karahbit 20 0 308M 5124 2072 S 0.0 0.0 0.0	27853 karahbit 20 0 16716 1644 1284 S 0.0 0.0 0.0	27853 karahbit 20 0 16716 1644 1284 S 0.0 0.0 0.0
6139 root 20 0 1198M 968M 3020 S 0.0 0.0 4.0	24776 root 20 0 624M 503M 2328 S 0.0 0.4 1.0	24776 root 20 0 624M 503M 2328 S 0.0 0.4 1.0
14429 root 20 0 266M 3224 2428 S 0.0 0.0 0.0	2741 root 20 0 379M 74868 8644 S 0.0 0.1 2.2	2741 root 20 0 379M 74868 8644 S 0.0 0.1 2.2
28231 root 20 0 378M 75424 8636 S 0.0 0.1 2.2	21839 root 20 0 267M 3224 2428 S 0.0 0.0 0.0	21839 root 20 0 267M 3224 2428 S 0.0 0.0 0.0
26260 pcp 20 0 94916 4348 2436 S 0.0 0.0 0.0	1 root 20 0 187M 4792 2616 S 0.0 0.0 8.1	1 root 20 0 187M 4792 2616 S 0.0 0.0 8.1
14430 root 20 0 266M 3224 2428 S 0.0 0.0 0.0	18764 root 20 0 21768 1428 996 S 0.0 0.0 6.1	18764 root 20 0 21768 1428 996 S 0.0 0.0 6.1
6225 root 20 0 413M 3560 720 S 0.0 0.0 1.1	5820 root 20 0 561M 19652 6316 S 0.0 0.0 2.5	5820 root 20 0 561M 19652 6316 S 0.0 0.0 2.5
6223 root 20 0 413M 3560 720 S 0.0 0.0 4.1	7751 root 20 0 203M 5700 3452 S 0.0 0.0 1.0	7751 root 20 0 203M 5700 3452 S 0.0 0.0 1.0
8553 root 20 0 21768 1412 992 S 0.0 0.0 6.1	6276 root 20 0 413M 3704 776 S 0.0 0.0 5.0	6276 root 20 0 413M 3704 776 S 0.0 0.0 5.0
6146 root 20 0 93532 1792 1428 S 0.0 0.0 1.4	5996 root 20 0 561M 19652 6316 S 0.0 0.0 2.5	5996 root 20 0 561M 19652 6316 S 0.0 0.0 2.5
14436 root 20 0 333M 572 2612 S 0.0 0.0 0.0	5233 root 20 0 27656 1972 1484 S 0.0 0.0 0.3	5233 root 20 0 27656 1972 1484 S 0.0 0.0 0.3
1 root 20 0 187M 4228 2408 S 0.0 0.0 7.4	5740 munge 20 0 735M 2392 1922 S 0.0 0.0 0.1	5740 munge 20 0 735M 2392 1922 S 0.0 0.0 0.1
32413 root 20 0 295M 69428 9084 S 0.0 0.1 0.2	24019 root 16 -0 51972 8512 2966 S 0.0 0.0 0.1	24019 root 16 -0 51972 8512 2966 S 0.0 0.0 0.1
5749 root 20 0 560M 12028 2152 S 0.0 0.0 2.4	2823 root 20 0 63768 25712 25366 S 0.0 0.0 0.5	2823 root 20 0 63768 25712 25366 S 0.0 0.0 0.5
26222 root 20 0 3379M 56300 8920 S 0.0 0.0 0.0	5863 root 20 0 405M 124M 14848 S 0.0 0.1 1.3	5863 root 20 0 405M 124M 14848 S 0.0 0.1 1.3
5802 munge 20 0 734M 1876 1524 S 0.0 0.0 0.0	16228 nsld 20 0 449M 6080 3492 S 0.0 0.0 0.3	16228 nsld 20 0 449M 6080 3492 S 0.0 0.0 0.3
5811 munge 20 0 734M 1876 1524 S 0.0 0.0 0.0	4754 root 20 0 10644 616 488 S 0.0 0.0 0.4	4754 root 20 0 10644 616 488 S 0.0 0.0 0.4
2830 root 20 0 71952 28108 27760 S 0.0 0.0 0.5	21841 root 20 0 267M 3224 2428 S 0.0 0.0 0.0	21841 root 20 0 267M 3224 2428 S 0.0 0.0 0.0

ML Example: Gradient Boosted Trees



TTX on XSEDE-Bridges over 50 iterations



References

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