

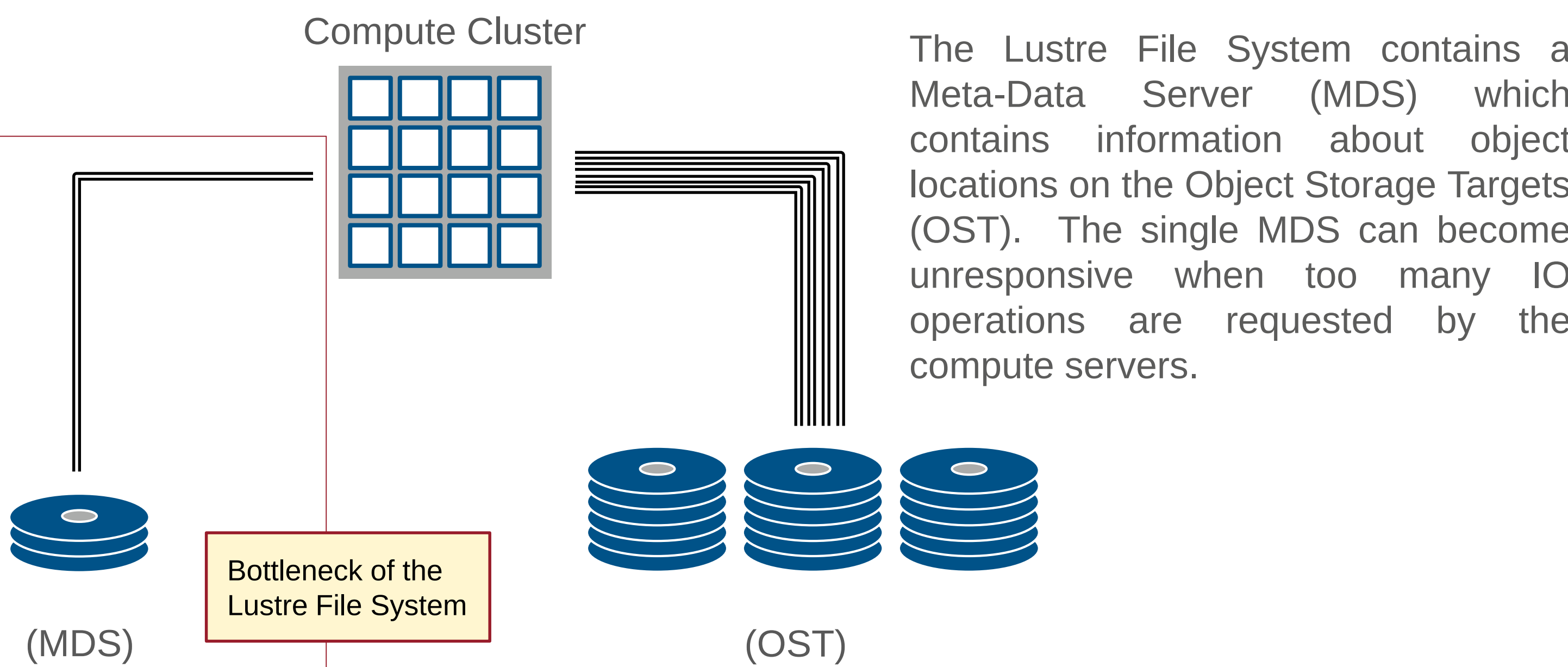
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Challenges in HPC

- Application performance is reliant on the cluster, other running jobs, and availability of *shared resources*
- The Lustre File System is a shared resource which may become unresponsive if several IO-intensive jobs are running simultaneously
- Knowing the number of *metadata operations* an application will use during its runtime allows for smarter scheduling



Goal: Leverage Neural Networks to extract features and patterns from job submissions and predict runtime and metadata operations.

Limits of Prior Techniques

- Standard machine learning algorithms use simple features extracted from job scripts with regular expressions
 - Fail to utilize features embedded in irregular patterns
- A Neural Network is able to detect features in irregular patterns

```
#!/bin/bash
#PBS -S /bin/bash
#PBS -l partition=cab
#PBS -W x=partition:cab
#PBS -N EX_nu
##
#PBS -q pbatch
#PBS -e run.err
##
#PBS -A mixapp
#PBS -l nodes=1:ppn=8
#PBS -l walltime=02:55:00

##pdebug
PBS_PWD=$(pwd)
cd "${PBS_O_WORKDIR}"

#run_mpirun()
#{
    . /usr/local/tools/dotkit/init.sh
    use openmpi-intel
    mpirun -np 8 /k/k22/frdo1/bin/mpl_misc < big_bird.in >>
    cookiemonster.out
#}
```

```
#!/bin/bash
#PSUB -r R2D2-C3PO-B88
#PSUB -eo
#PSUB -o psub.out
#PSUB -ro
#PSUB -d 0
#PSUB -th 9h
#PSUB -ln 12
#PSUB -b gsmisc
#PSUB -c cab
#PSUB -me # send email when job completes
#PSUB -x # pass-through environment variables
#PSUB # no more embedded options

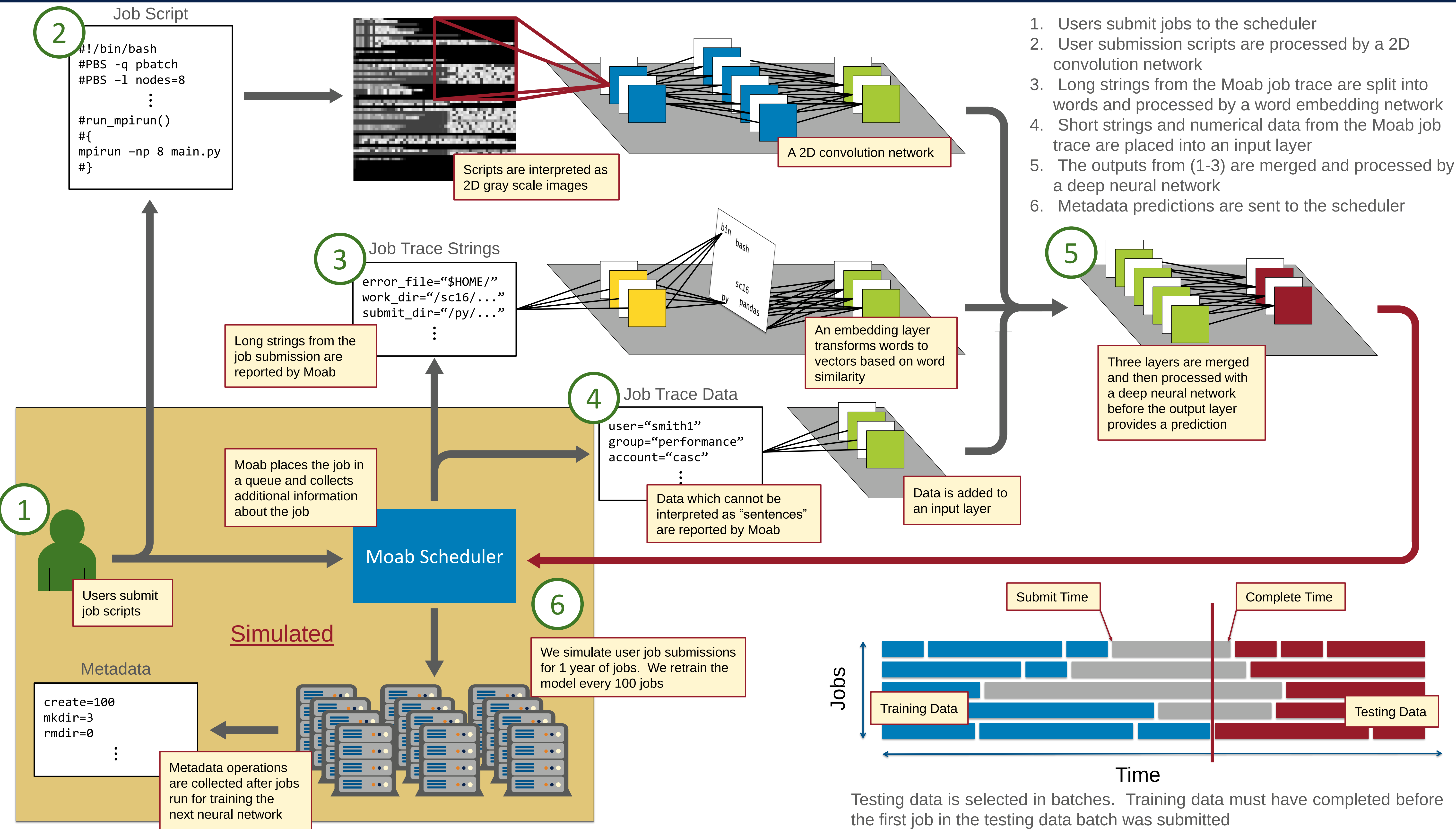
echo job ID = $PSUB_JOBID
date
echo
let echo

#cd /p/lscatche/boots99/onerig/Eyes_Wide/shut+0
cp INCAR1 INCAR
srn -N12 -n192 /usr/tools/space/2001
cp INCAR2 INCAR
/usr/tools/drinks/martini -d #check
srn -N12 -n192 /usr/tools/drinks/mix --shake --no-stir

wait
exit
```

Examples of two job submission scripts. There exist regular (top half) and irregular (lower half) patterns in the scripts. The irregular patterns cannot be reliably parsed with regular expressions.

Neural Network Workflow for IO Prediction



Predictions and Observed Accuracy

Accuracy Metric:

$$1 - \frac{|true - pred|}{\max(true, pred)}$$

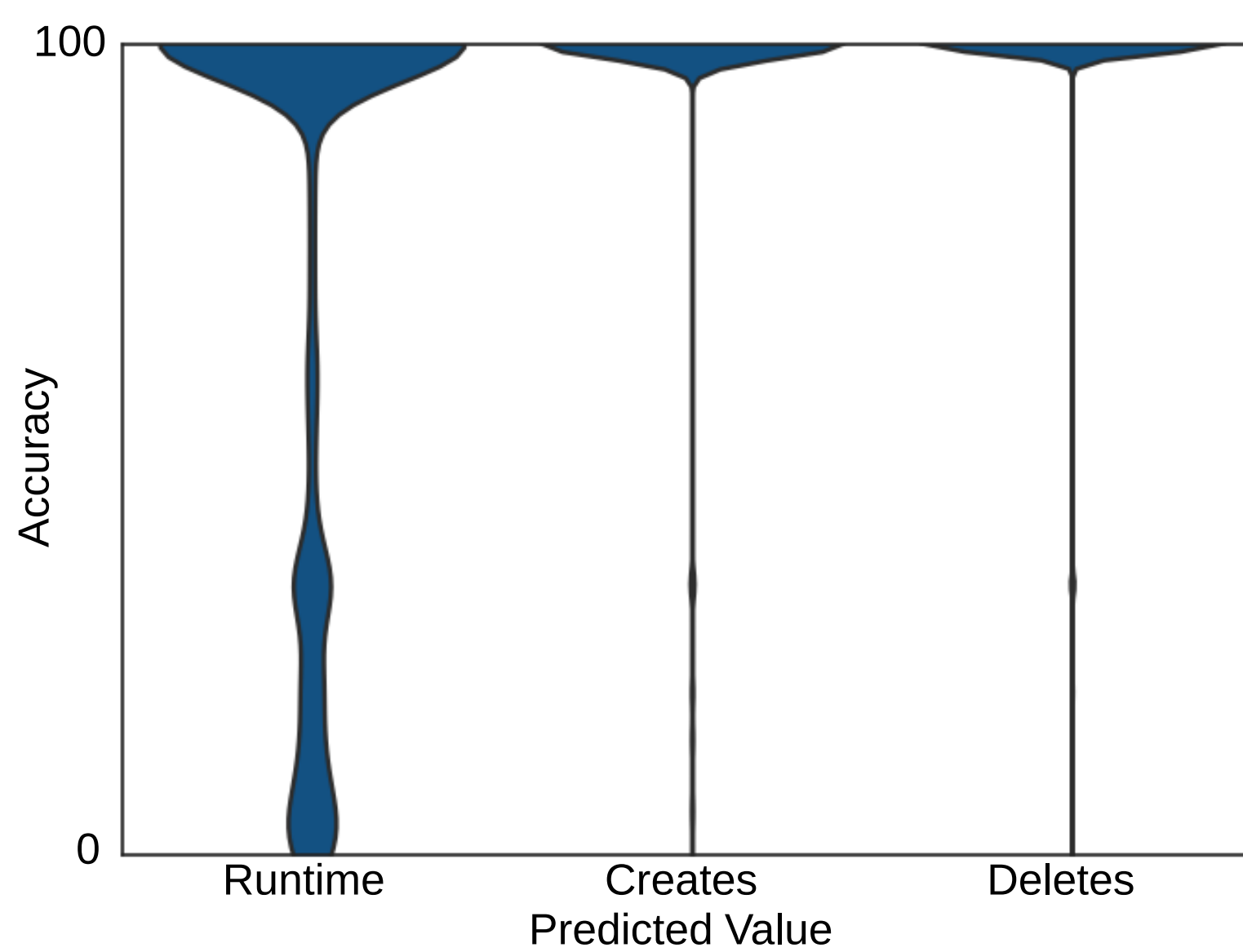
Batch Parameters:

- 100 Testing Samples
- 500 Training Samples

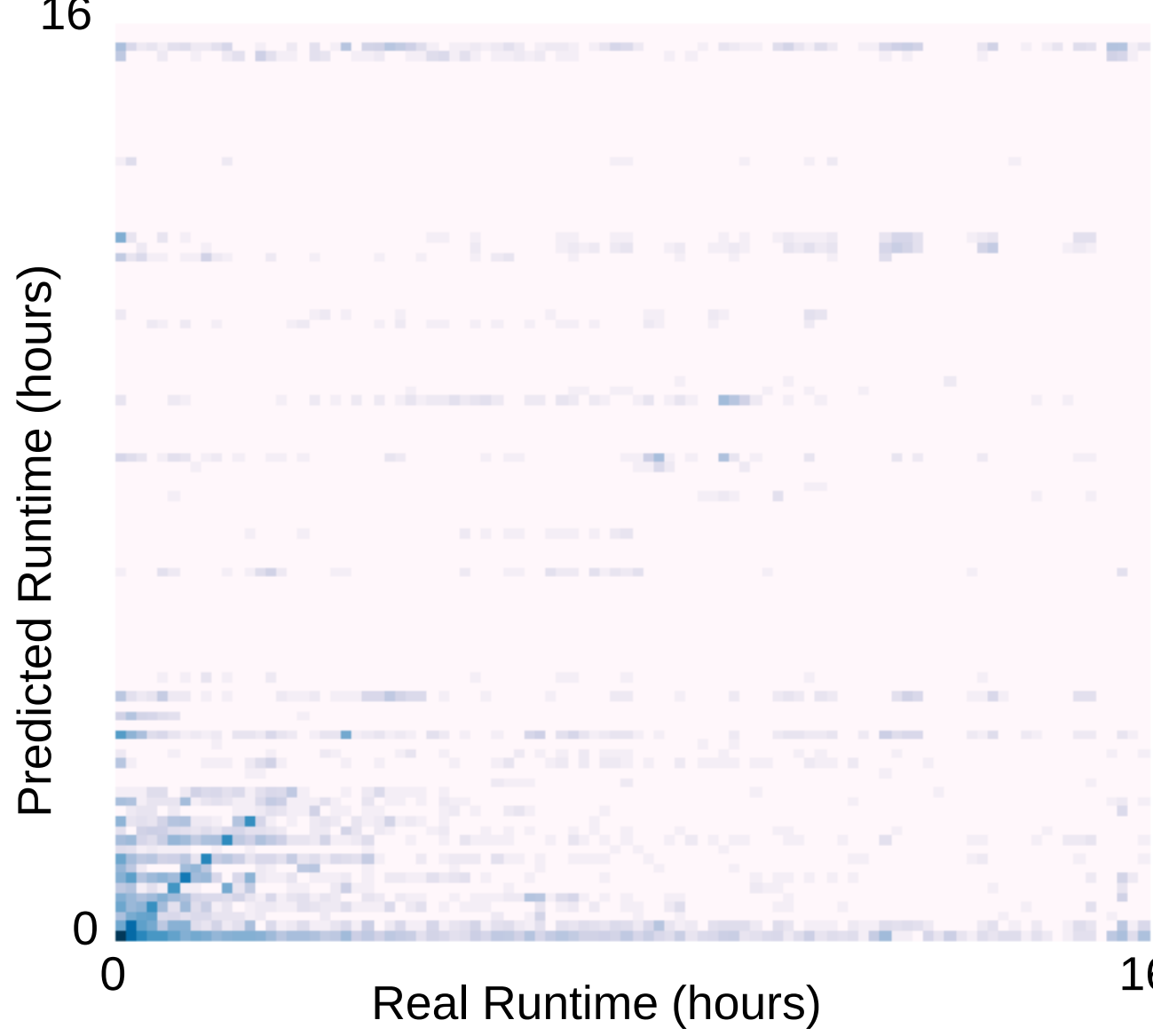
Job Feature Accuracy:

- Runtime: 75%
- Creates: 96%
- Deletes: 96%

Accuracy distributions for predicted features



Predicted runtime versus real runtime



Neural network performance over training size

