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MLE-Toolbox: Training Neural Networks Like an Experimental Biologist Would

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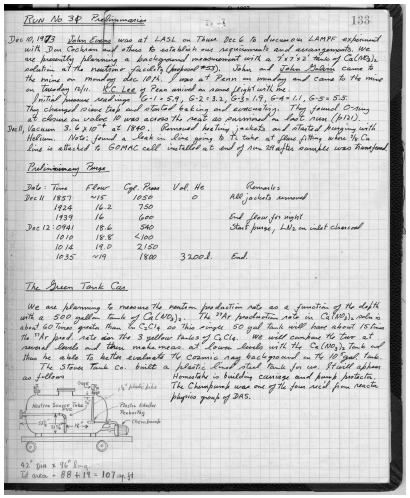
Science & Engineering - Hypothesis Formulation & Testing

400 Networks

x 5 random seeds

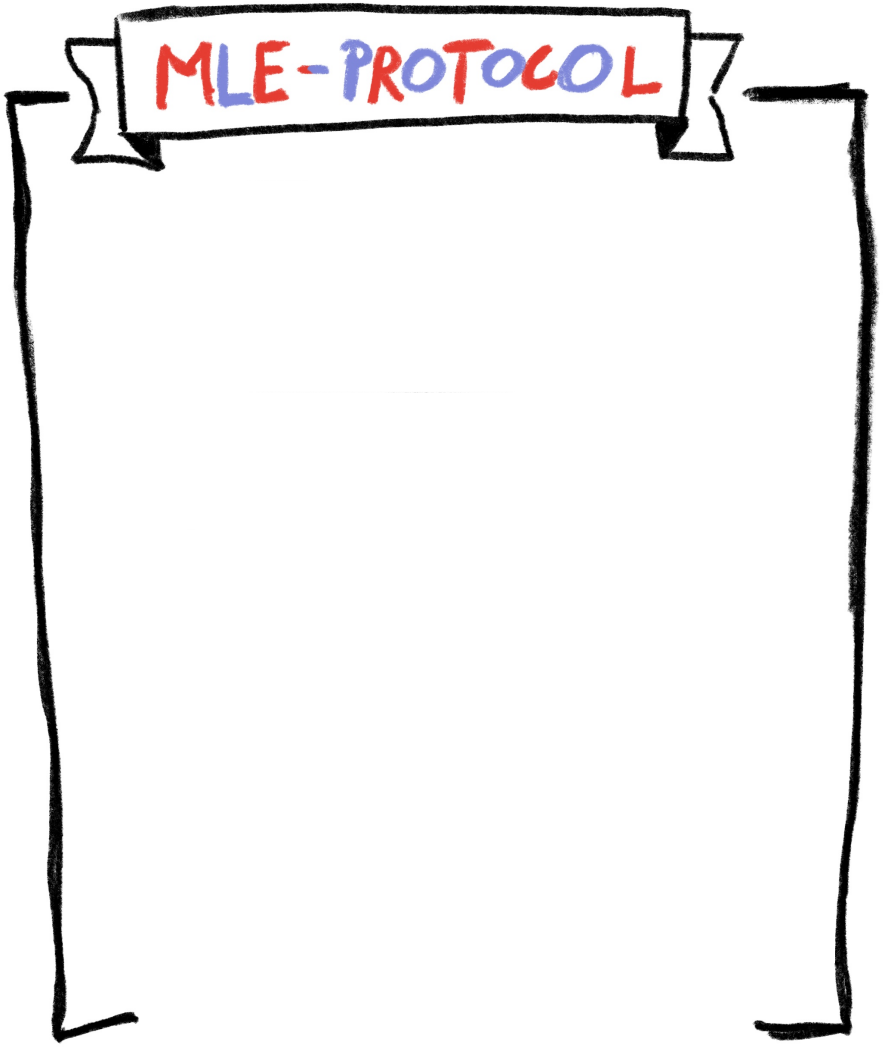
x 4 Lifetimes

+ Post-Processing

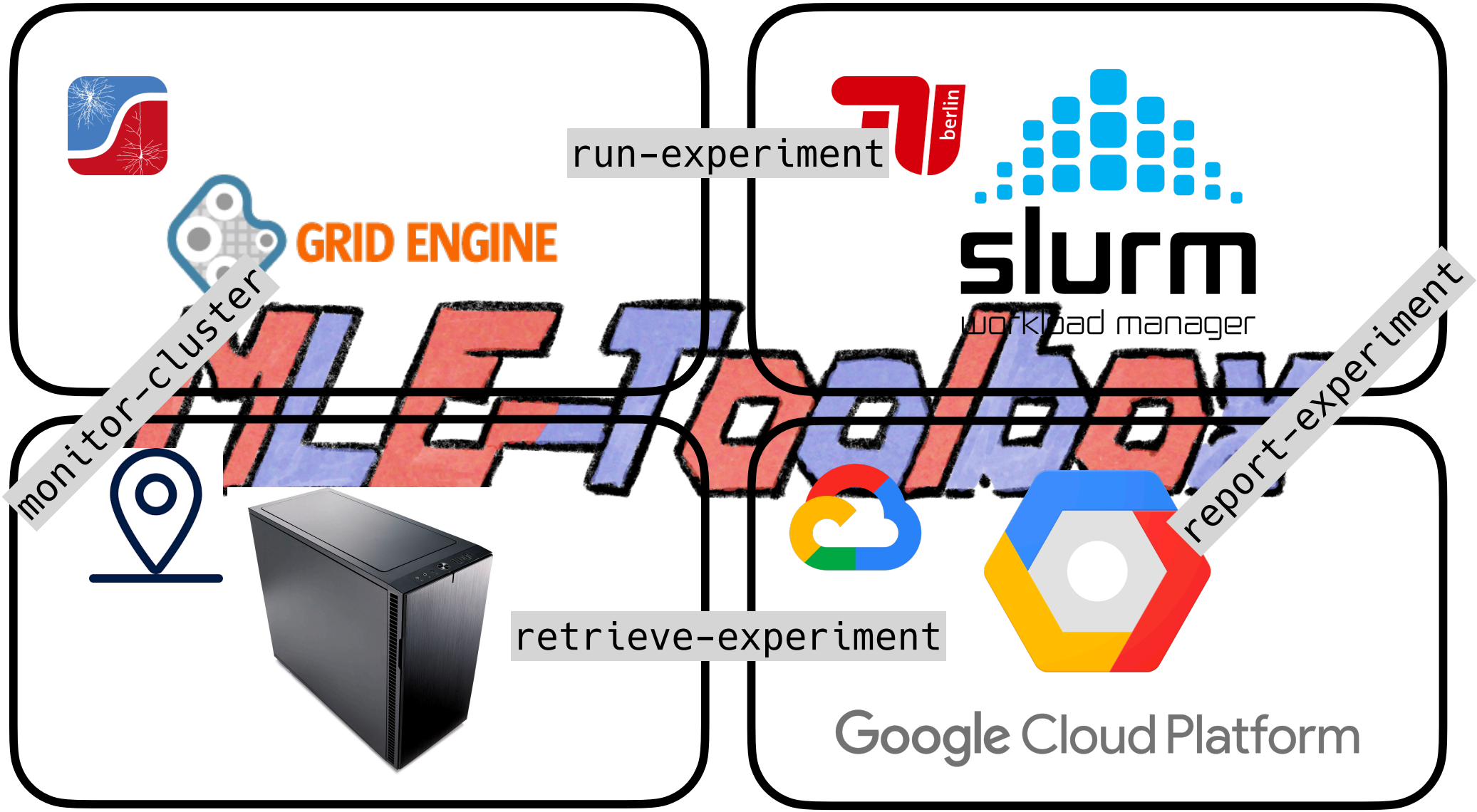


1. Experimental protocol - Efficient testing & reproducibility
2. Pipeline - Coordination of parallel scheduling across resources

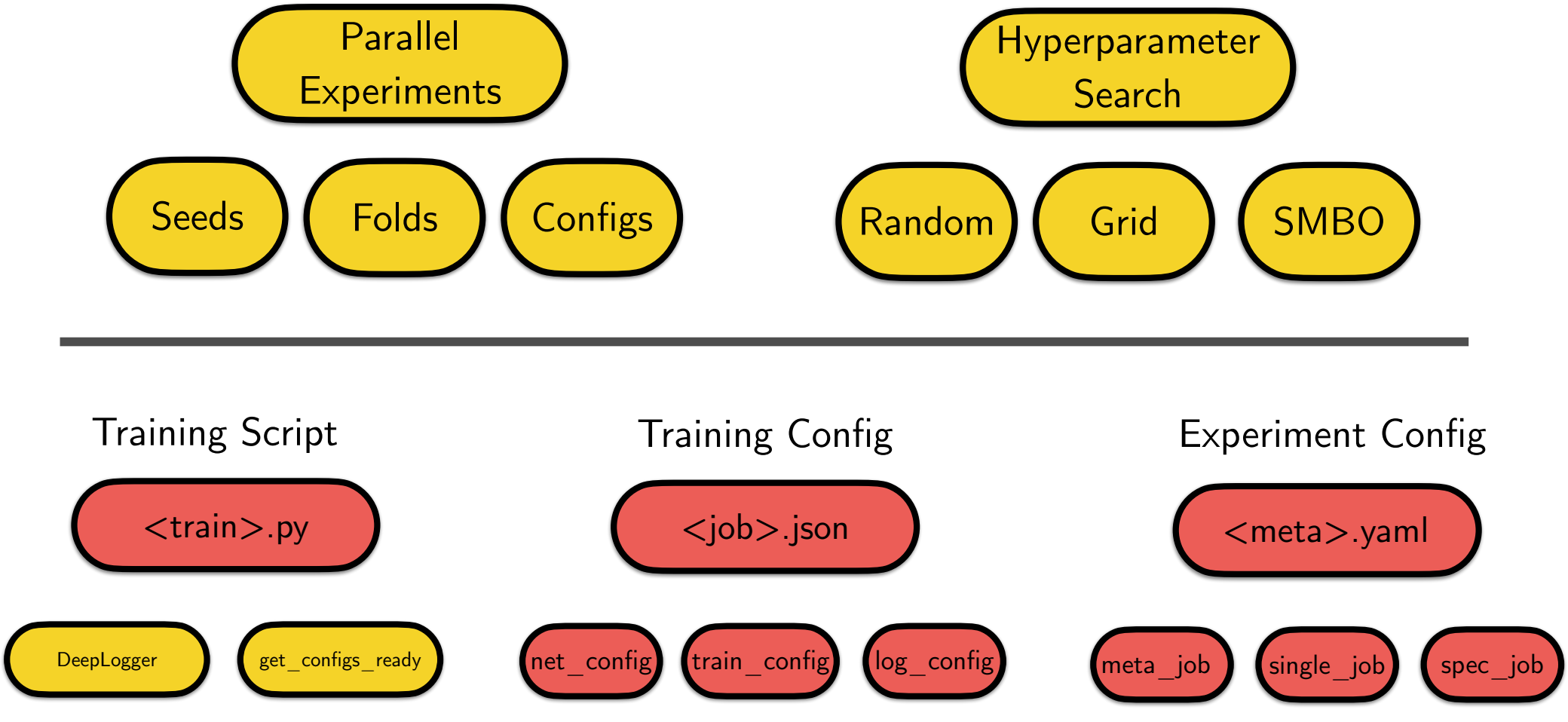
MLE-Protocol: Never run a simulation twice!



1. **Purpose/Hypothesis**
   What question are you trying to answer?
2. **Materials**
   What code version? Git Commit Hash
3. **Methods**
   Which hyperparams? Hash of configs
4. **Evaluation**
   What figures shall be created?


GRID ENGINE
slurm
workload manager
MLE-Toolbox
run-experiment
monitor-cluster
report-experiment
retrieve-experiment
Google Cloud Platform

Types of Supported Jobs and Ingredients



<train>.py

MNIST-CNN (I): Training Code/Pipeline

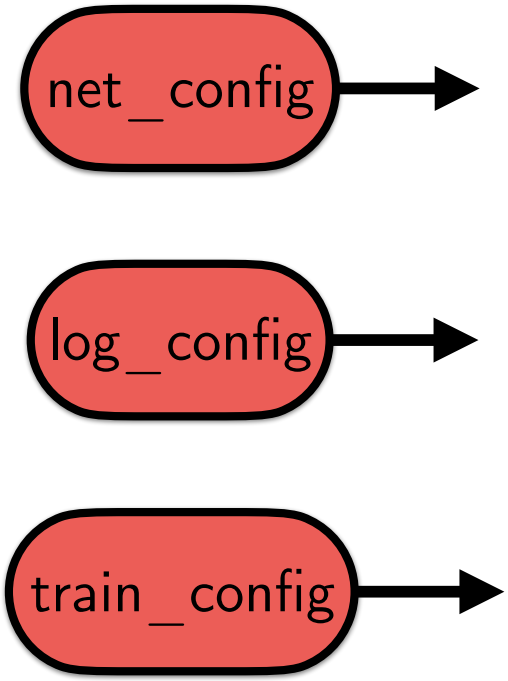
DeepLogger

get_configs_ready

```python
from mle_toolbox.utils import get_configs_ready, DeepLogger

def main(net_config, train_config, log_config):
    """ Train a network on MNIST dataset. """
    ...
    # Setup the experiment run - device/dataloader/net, etc.
    train_loader, test_loader = ..., ...
    mnist_net = MNIST_CNN(**net_config).to(device)
    nll_loss = nn.CrossEntropyLoss()
    optimizer = torch.optim.Adam(mnist_net.parameters(), lr=train_config.l_rate)
    run_log = DeepLogger(**log_config)

    # Train the MNIST Network using the training loop
    train_mnist_cnn(...)

def train_mnist_cnn(...):
    """ Run the training loop over a set of epochs. """
    for epoch in range(1, num_epochs + 1):
        # Run the training loop ...
        train_loss, test_loss = ..., ...

        # Log newest results
        time_tick = [epoch]
        stats_tick = [train_loss, test_loss]
        train_log.update_log(time_tick, stats_tick)
        train_log.save_log()
        train_log.save_network(model)
    return  model, train_log


if __name__ == "__main__":
    conf = get_configs_ready(default_config_fname="mnist_cnn_config_1.json")
    train_config, net_config, log_config = conf
    main(net_config, train_config, log_config)
```

<job>.json

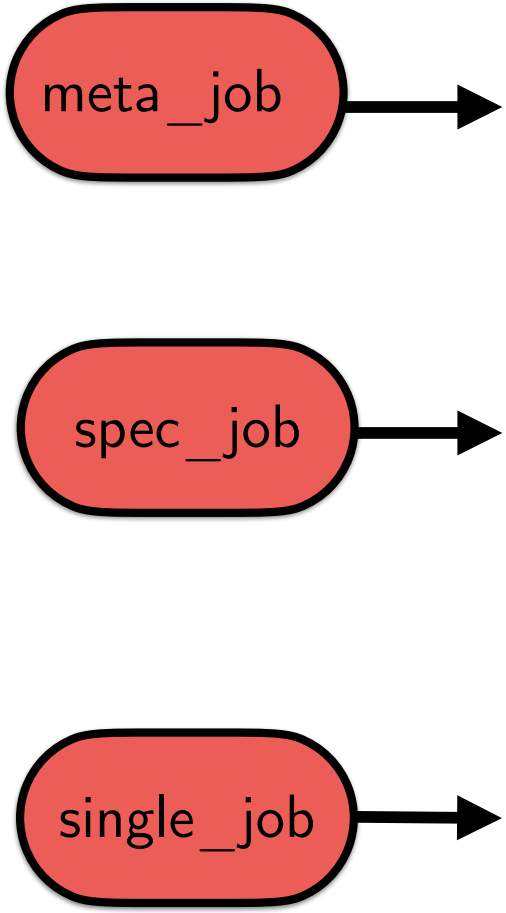
MNIST-CNN (II): Base Configuration



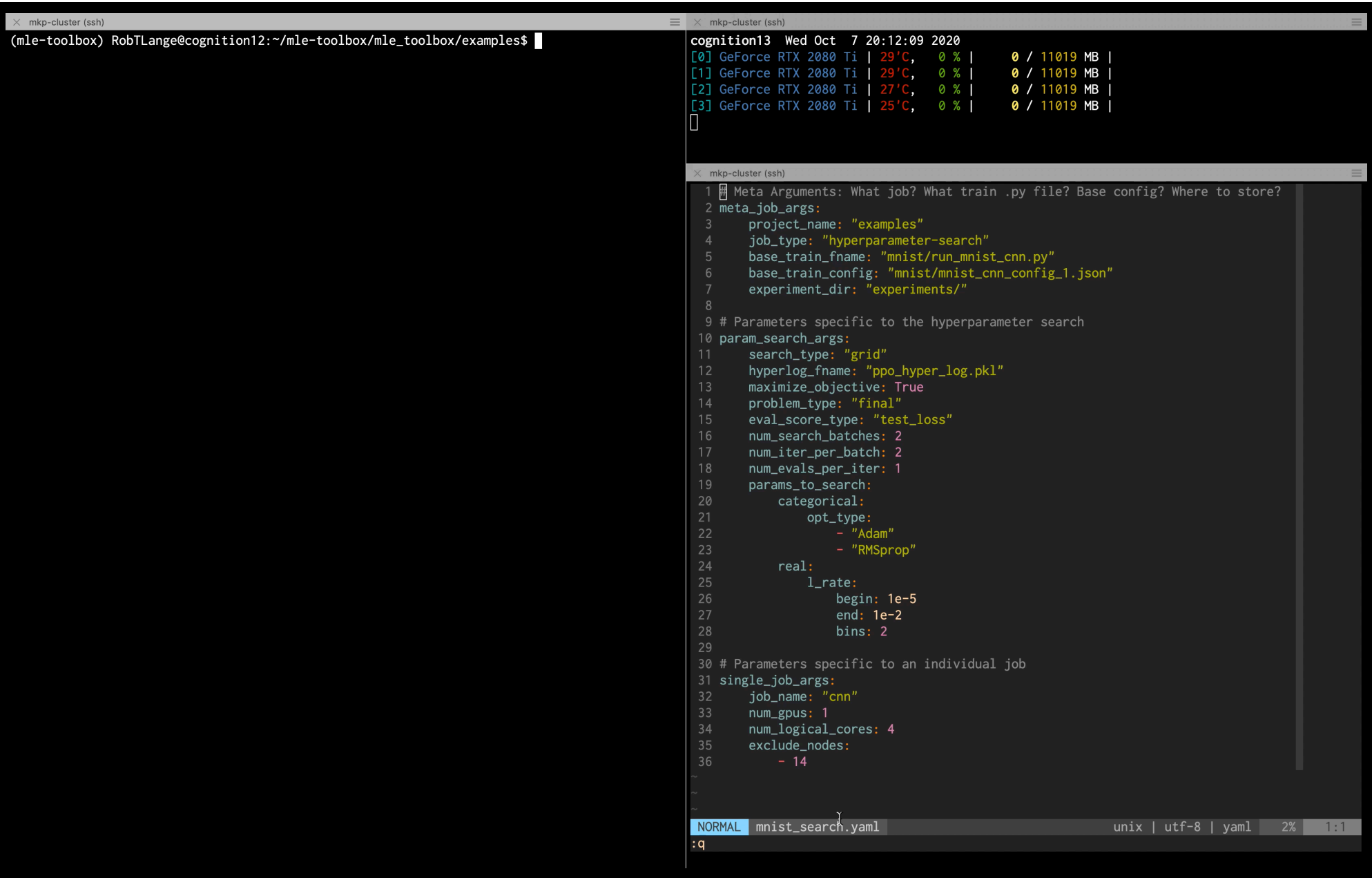

```
{
"net_config": {"dropout_prob": 0.5,
               "hidden_fc_dim": 128},
"log_config": {"time_to_track": ["epoch"],
               "what_to_track": ["train_loss", "test_loss"],
               "tboard_fname": "config_1",
               "time_to_print": ["epoch"],
               "what_to_print": ["train_loss", "test_loss"],
               "print_every_k_updates": 1,
               "overwrite_experiment_dir": 1},
"train_config": {"seed_id": 0,
                 "num_epochs": 2,
                 "net_type": "CNN",
                 "torch_num_threads": 3,
                 "train_batch_size": 256,
                 "test_batch_size": 256,
                 "l_rate": 0.001}
}
```

<meta>.yaml

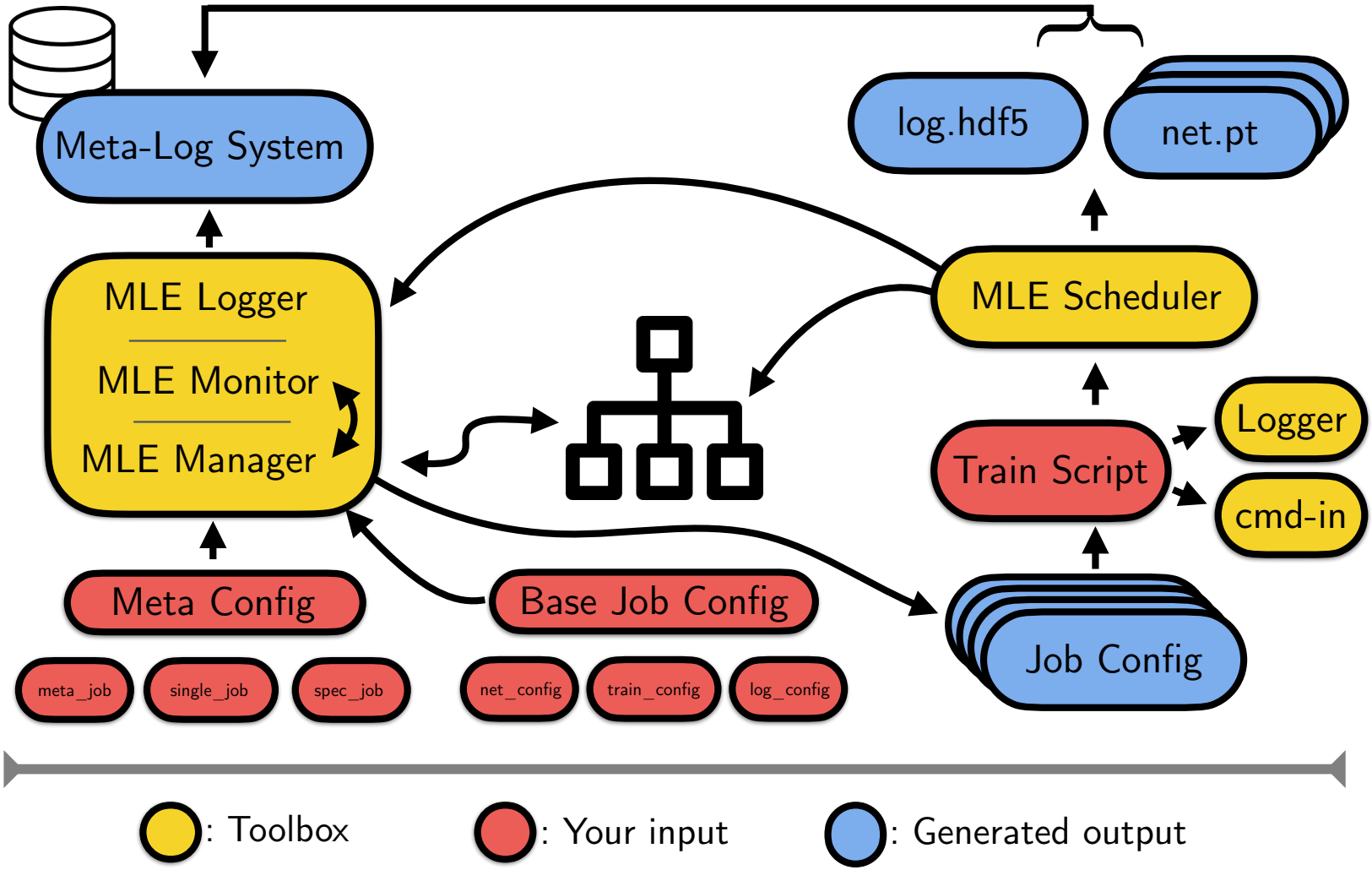
MNIST-CNN (III): Experiment Configuration




```yaml
# Meta Arguments: What job? What train .py file? Base config? Where to store?
meta_job_args:
    project_name: "examples"
    job_type: "hyperparameter-search"
    base_train_fname: "mnist/run_mnist_cnn.py"
    base_train_config: "mnist/mnist_cnn_config_1.json"
    experiment_dir: "experiments/"

# Parameters specific to the hyperparameter search
param_search_args:
    search_type: "grid"
    hyperlog_fname: "ppo_hyper_log.pkl"
    maximize_objective: True
    problem_type: "final"
    eval_score_type: "test_loss"
    num_search_batches: 1
    num_iter_per_batch: 2
    num_evals_per_iter: 3
    params_to_search:
        categorical:
            opt_type:
                - "Adam"
                - "RMSprop"
        real:
            l_rate:
                begin: 1e-5
                end: 1e-2
                bins: 2

# Parameters specific to an individual job
single_job_args:
    job_name: "cnn"
    num_gpus: 1
    num_logical_cores: 4
```


mkp-cluster (ssh)
(mle-toolbox) RobTLange@cognition12:~/mle-toolbox/mle_toolbox/examples$
mkp-cluster (ssh)
cognition13 Wed Oct 7 20:12:09 2020
[0] GeForce RTX 2080 Ti | 29'C, 0 % | 0 / 11019 MB |
[1] GeForce RTX 2080 Ti | 29'C, 0 % | 0 / 11019 MB |
[2] GeForce RTX 2080 Ti | 27'C, 0 % | 0 / 11019 MB |
[3] GeForce RTX 2080 Ti | 25'C, 0 % | 0 / 11019 MB |
mkp-cluster (ssh)
Meta Arguments: What job? What train .py file? Base config? Where to store?
meta_job_args:
project_name: "examples"
job_type: "hyperparameter-search"
base_train_fname: "mnist/run_mnist_cnn.py"
base_train_config: "mnist/mnist_cnn_config_1.json"
experiment_dir: "experiments/"
Parameters specific to the hyperparameter search
param_search_args:
search_type: "grid"
hyperlog_fname: "ppo_hyper_log.pkl"
maximize_objective: True
problem_type: "final"
eval_score_type: "test_loss"
num_search_batches: 2
num_iter_per_batch: 2
num_evals_per_iter: 1
params_to_search:
categorical:
opt_type:
- "Adam"
- "RMSprop"
real:
l_rate:
begin: 1e-5
end: 1e-2
bins: 2
Parameters specific to an individual job
single_job_args:
job_name: "cnn"
num_gpus: 1
num_logical_cores: 4
exclude_nodes:
- 14
NORMAL mnist_search.yaml unix | utf-8 | yaml 2% 1:1
:q

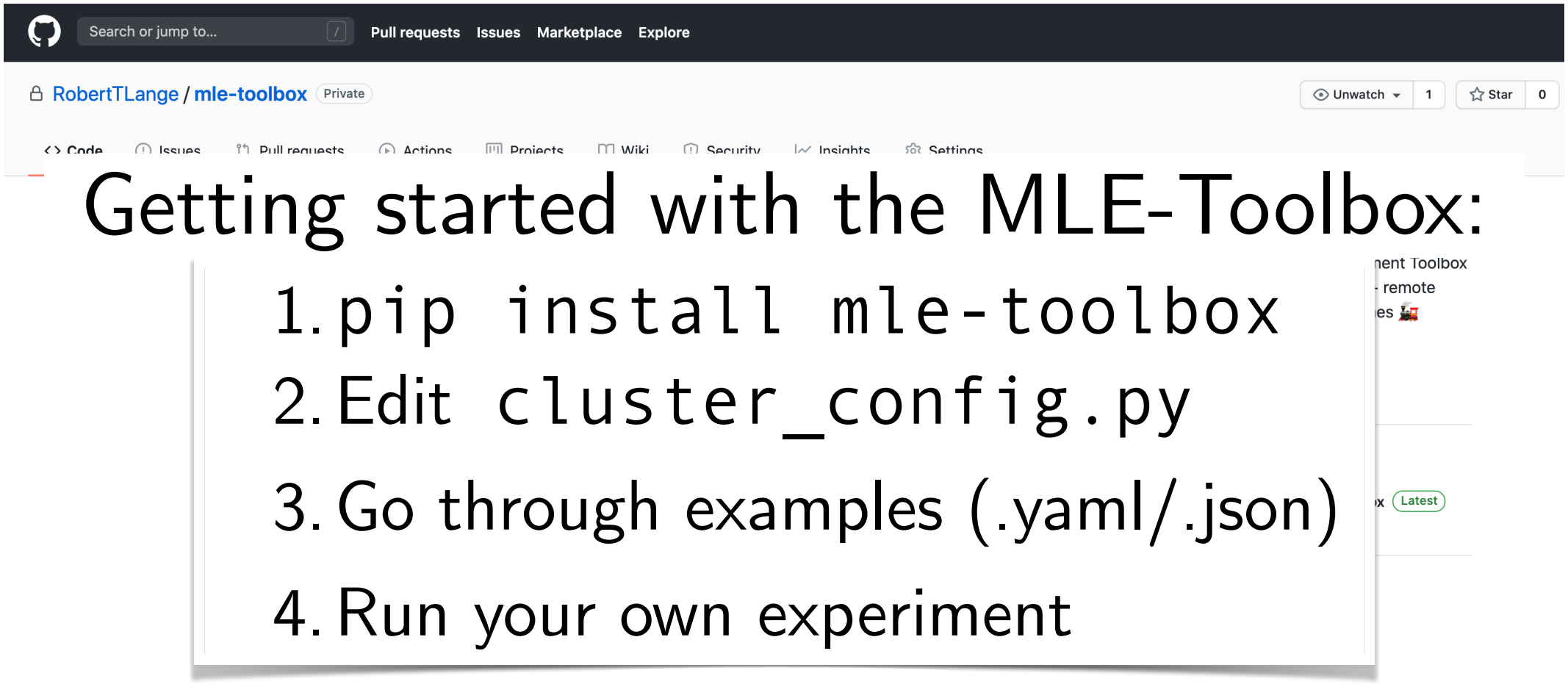
The MLE-Toolbox Experiment Workflow



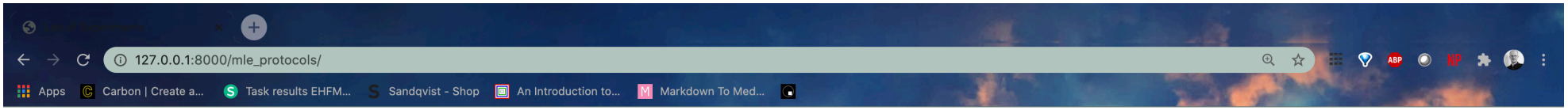
Post-Processing Pipelines: Automatic Figure Generation

```yaml
meta_job_args: ...
param_search_args: ...
single_job_args: ...

# Parameters for the post processing job
post_process_args:
  process_fname: "get_bandit_stats.py"
  process_job_args:
    num_logical_cores: 10
    time_per_job: "00:15:00"
  extra_cmd_line_input:
    life_t: 100
    num_episodes: 100
    num_seeds: 5
```

PyPI & Manual Installation from GitHub Repository

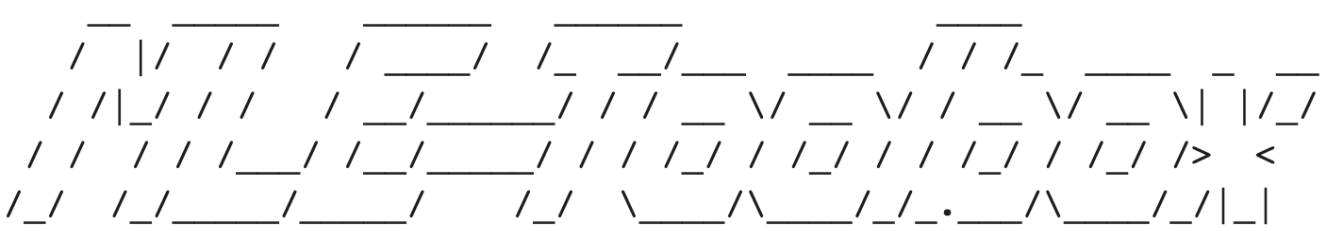


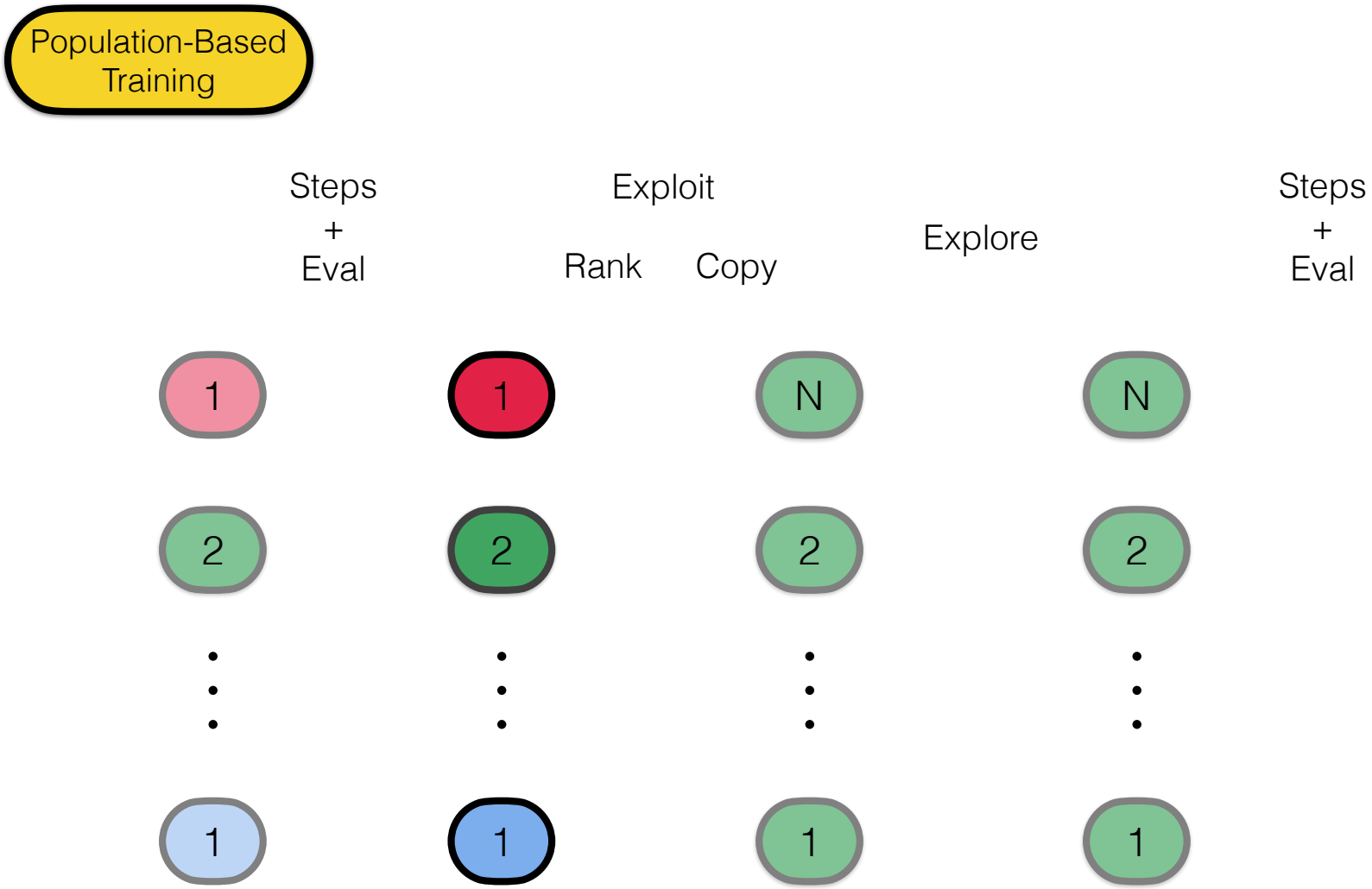
To Be Continued: The MLE-Laboratory



ID	Date	Project	Purpose	Status	Resource	Seeds	Hash	Retrieved	GCS
95	10/06/2020 12:51:51	sfa-rl	SHow off before joram	running	sge-cluster	5	ee72a0c2ec468f86f12d1dbe0f150dad	False	False
94	10/06/2020 08:10:03	crit-rnn	Small grid 1-4, 1-3	running	sge-cluster	3	87115139a1e92d24a5e0742cc7065db7	False	False
93	10/05/2020 15:18:19	sfa-rl	Random SFA-basis	completed	sge-cluster	5	3b05aa1757b293c3304075bc85130731	False	False
91	10/04/2020 15:55:41	sfa-rl	Expert SFA-basis	completed	sge-cluster	5	ee72a0c2ec468f86f12d1dbe0f150dad	False	False
90	10/03/2020 12:34:25	crit-rnn	Small grid 1-4, 1-3	completed	sge-cluster	1	d2ae209926f7cef5cd1d39dd12cae332	False	False
89	10/01/2020 23:42:09	meta-grid	And 5 more	running	sge-cluster	5	66e1af0505aad3893e4a407169009e94	False	False
88	09/30/2020 18:52:03	meta-grid	More seeds as before	completed	sge-cluster	10	3e7dee7e156f0b6e75c59a018b53ad73	True	False
87	09/29/2020 17:54:47	meta-grid	10 seeds 6x6 r=1,3,6 + no anneal	completed	sge-cluster	-	3e7dee7e156f0b6e75c59a018b53ad73	True	-
86	09/28/2020 18:26:04	meta-grid	5 seeds 6x6 r=1,3,6 + anneal + orthog	completed	sge-cluster	-	4766ca79d3c262b860a6bd027440c6fb	True	-
85	09/28/2020 18:22:39	meta-grid	5 seeds 6x6 r=1,3,5 + no anneal + orthog	completed	sge-cluster	-	874b0473fa68c7bfdcc053737ddd91cd	True	-
84	09/27/2020 17:17:35	meta-grid	r=1,3,6 + no anneal	completed	sge-cluster	-	cfda3b2f7956c51acd9bfd905f865c21	True	-
83	09/27/2020 17:15:20	meta-grid	r=1,3,6 + anneal	completed	sge-cluster	-	d659d9ed8a8cd6c0121b97bf8f736570	True	-
82	09/26/2020 17:03:35	meta-grid	10 seeds 6x6 r=1,2.5,5	completed	sge-cluster	-	7ce1032a5476b4d8120c122028ef9829	True	-
81	09/25/2020 11:56:48	meta-grid	10 seeds 6x6 r=1,3,6	completed	sge-cluster	-	198cffe8a538615f787dbd05e425af30	True	-
80	09/24/2020 12:41:33	meta-grid	6x6 r=1,3,6 discount anneal	completed	sge-cluster	-	c716134bbc529ea30c75ee6c6b4dd2f4	True	-

Backup Slides




Population-Based Training
Steps + Eval
Exploit
Rank
Copy
Explore
Steps + Eval
1
1
N
N
2
2
2
2
1
1
1
1