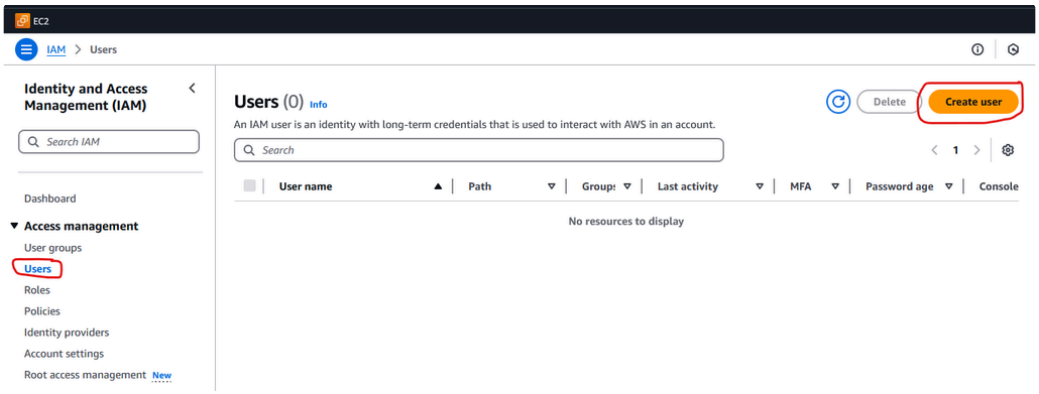
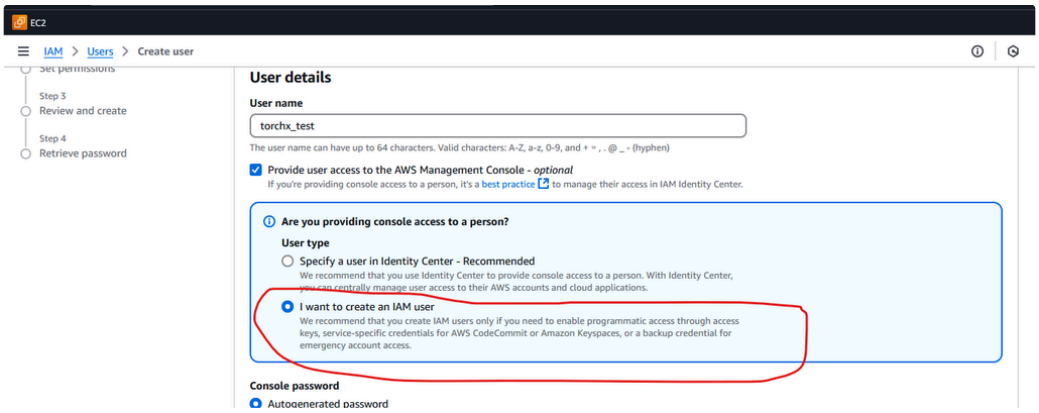
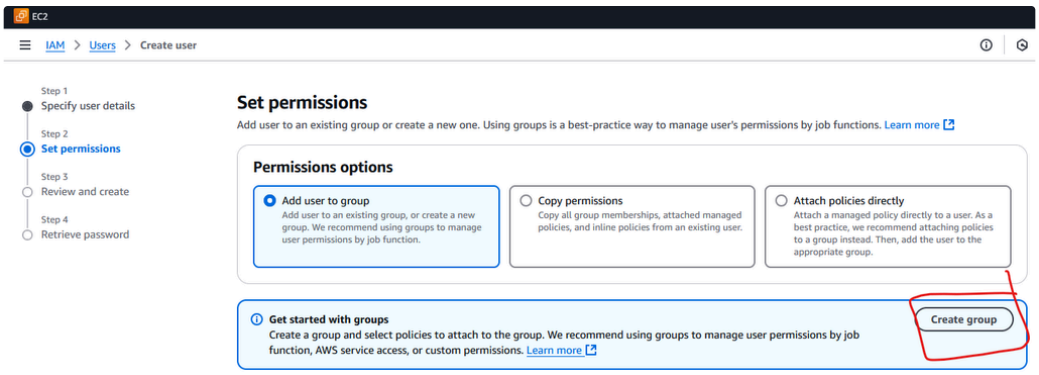
AWS training: BoTorch TorchX - Neural architecture search

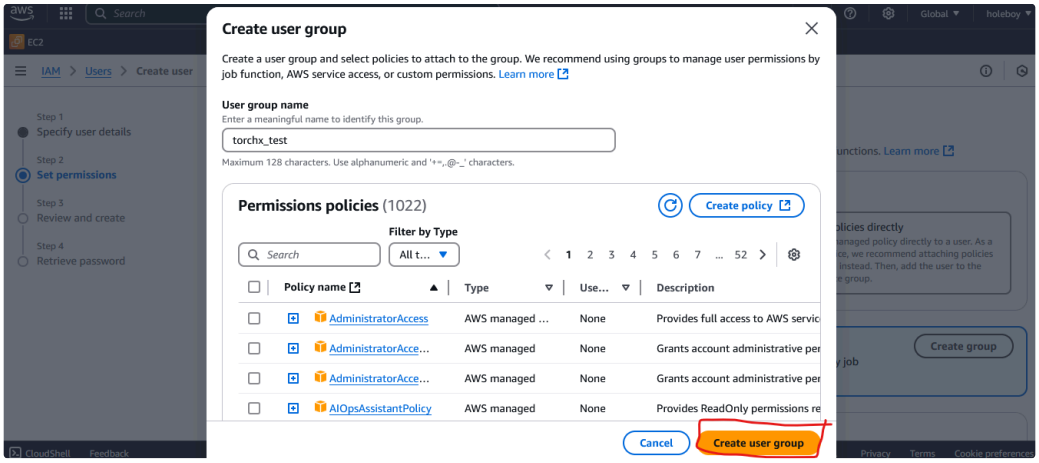
EC2 setup (free tier)

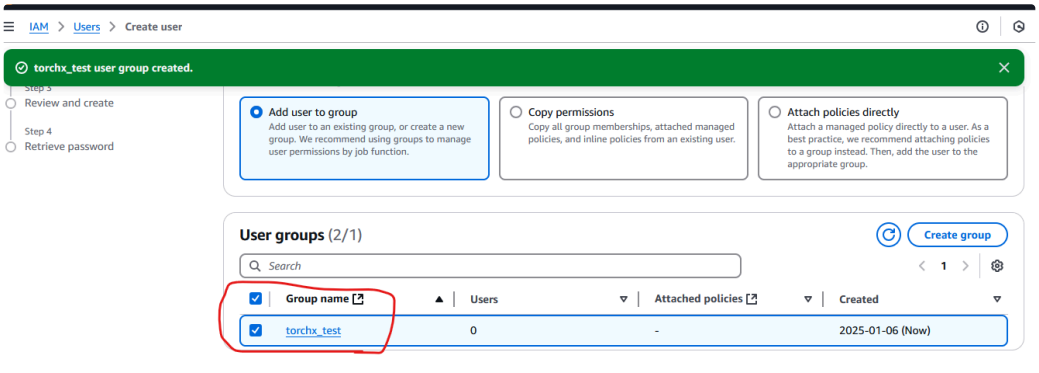
Credentials






EC2
IAM > Users > Create user
Step 1
Specify user details
Step 2
Set permissions
Step 3
Review and create
Step 4
Retrieve password
Set permissions
Add user to an existing group or create a new one. Using groups is a best-practice way to manage user's permissions by job functions. Learn more
Permissions options
Add user to group
Add user to an existing group, or create a new group. We recommend using groups to manage user permissions by job function.
Copy permissions
Copy all group memberships, attached managed policies, and inline policies from an existing user.
Attach policies directly
Attach a managed policy directly to a user. As a best practice, we recommend attaching policies to a group instead. Then, add the user to the appropriate group.
Get started with groups
Create a group and select policies to attach to the group. We recommend using groups to manage user permissions by job function, AWS service access, or custom permissions. Learn more
Create group


Create user group
Create a user group and select policies to attach to the group. We recommend using groups to manage user permissions by job function, AWS service access, or custom permissions. Learn more
User group name
Enter a meaningful name to identify this group.
torchx_test
Maximum 128 characters. Use alphanumeric and '+=,.@-_' characters.
Permissions policies (1022)
Create policy
Filter by Type
Search
All t...
Policy name
Type
Use...
Description
AdministratorAccess
AWS managed ...
None
Provides full access to AWS servic
AdministratorAcce...
AWS managed
None
Grants account administrative per
AdministratorAcce...
AWS managed
None
Grants account administrative per
AIOpsAssistantPolicy
AWS managed
None
Provides ReadOnly permissions re
Cancel
Create user group


IAM > Users > Create user
torchx_test user group created.
Step 3
Review and create
Step 4
Retrieve password
Add user to group
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Copy permissions
Copy all group memberships, attached managed policies, and inline policies from an existing user.
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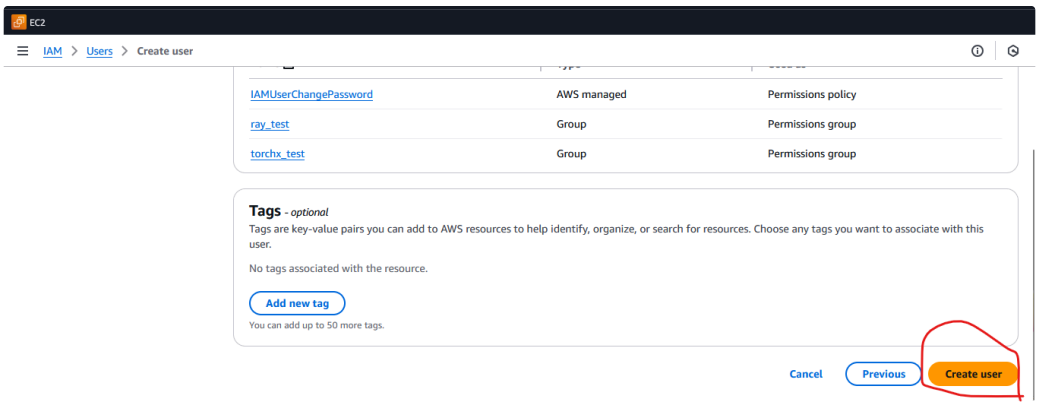
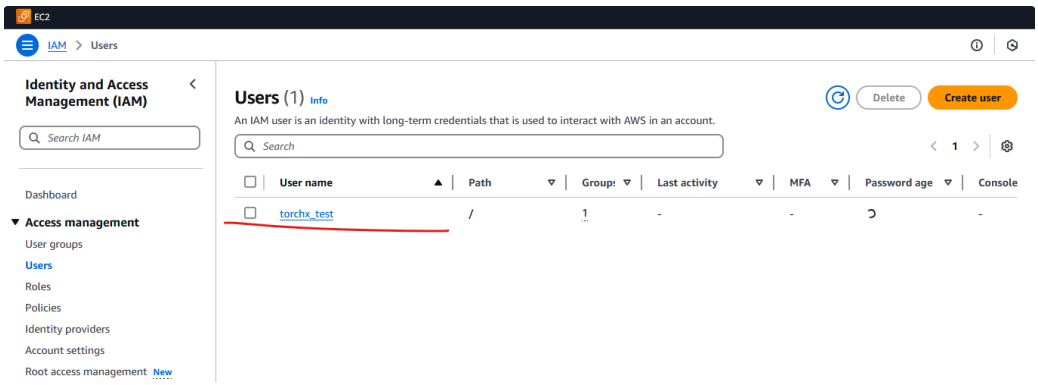
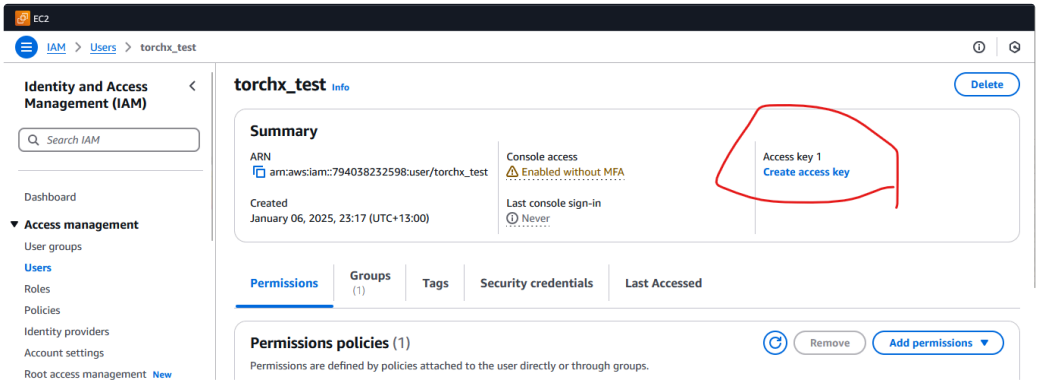
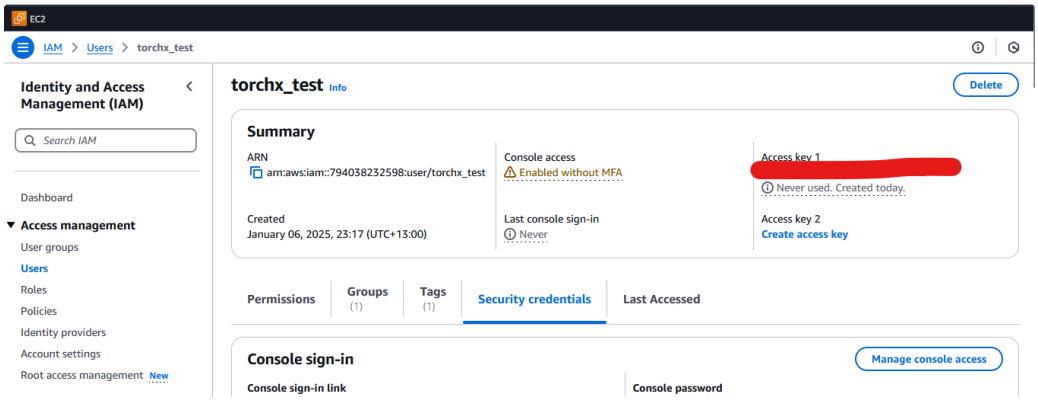
Attach a managed policy directly to a user. As a best practice, we recommend attaching policies to a group instead. Then, add the user to the appropriate group.
User groups (2/1)
Create group
Search
Group name
Users
Attached policies
Created
torchx_test
0
-
2025-01-06 (Now)

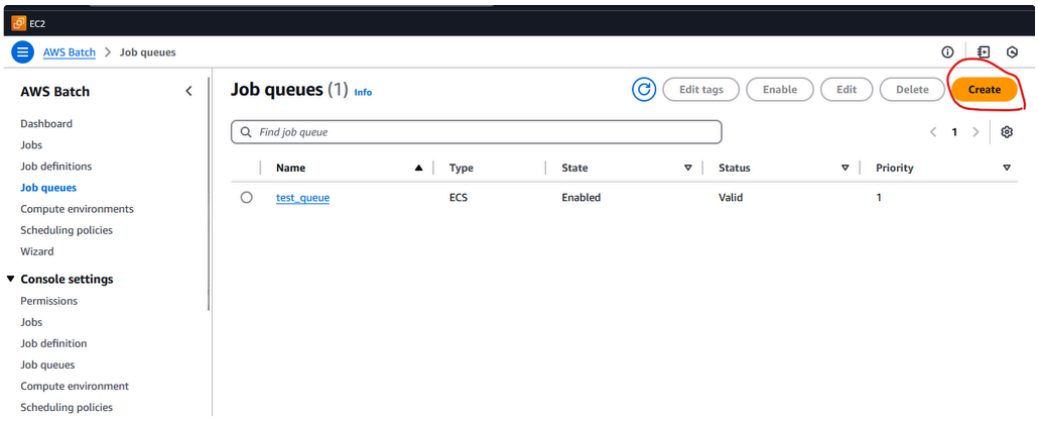

EC2
IAM > Users > Create user
IAMUserChangePassword
AWS managed
Permissions policy
ray_test
Group
Permissions group
torchx_test
Group
Permissions group
Tags - optional
Tags are key-value pairs you can add to AWS resources to help identify, organize, or search for resources. Choose any tags you want to associate with this user.
No tags associated with the resource.
Add new tag
You can add up to 50 more tags.
Cancel
Previous
Create user

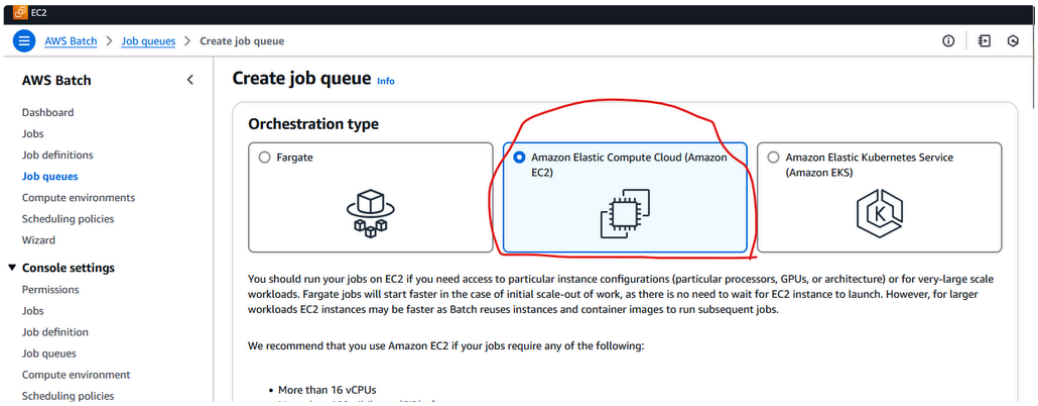


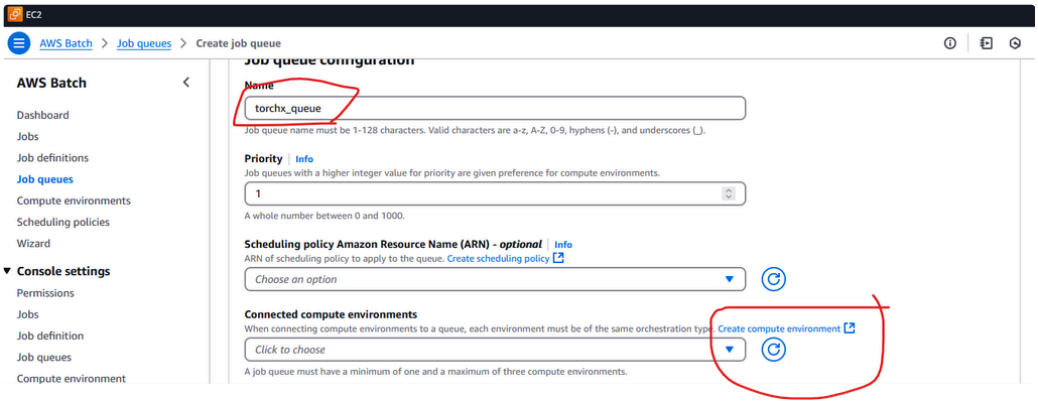




Create job queue




EC2
AWS Batch > Job queues > Create job queue
AWS Batch
Dashboard
Jobs
Job definitions
Job queues
Compute environments
Scheduling policies
Wizard
Console settings
Permissions
Jobs
Job definition
Job queues
Compute environment
Scheduling policies
Create job queue Info
Orchestration type
Fargate
Amazon Elastic Compute Cloud (Amazon EC2)
Amazon Elastic Kubernetes Service (Amazon EKS)
You should run your jobs on EC2 if you need access to particular instance configurations (particular processors, GPUs, or architecture) or for very-large scale workloads. Fargate jobs will start faster in the case of initial scale-out of work, as there is no need to wait for EC2 instance to launch. However, for larger workloads EC2 instances may be faster as Batch reuses instances and container images to run subsequent jobs.
We recommend that you use Amazon EC2 if your jobs require any of the following:
More than 16 vCPUs


EC2
AWS Batch > Job queues > Create job queue
AWS Batch
Dashboard
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Job queues
Compute environments
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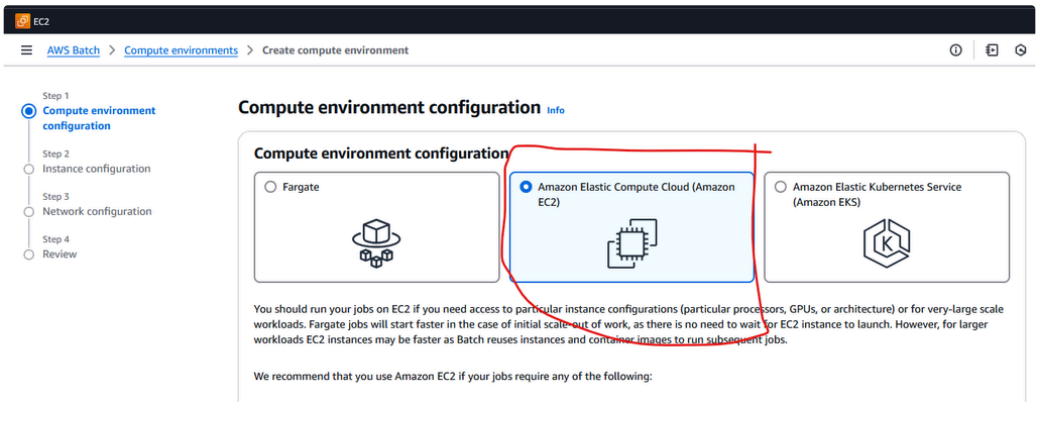
Wizard
Console settings
Permissions
Jobs
Job definition
Job queues
Compute environment
Name
torchx_queue
Job queue name must be 1-128 characters. Valid characters are a-z, A-Z, 0-9, hyphens (-), and underscores (_).
Priority Info
Job queues with a higher integer value for priority are given preference for compute environments.
1
A whole number between 0 and 1000.
Scheduling policy Amazon Resource Name (ARN) - optional Info
ARN of scheduling policy to apply to the queue. Create scheduling policy
Choose an option
Connected compute environments
When connecting compute environments to a queue, each environment must be of the same orchestration type. Create compute environment
Click to choose
A job queue must have a minimum of one and a maximum of three compute environments.


EC2
AWS Batch > Compute environments > Create compute environment
Step 1
Compute environment configuration
Step 2
Instance configuration
Step 3
Network configuration
Step 4
Review
Compute environment configuration Info
Compute environment configuration
Fargate
Amazon Elastic Compute Cloud (Amazon EC2)
Amazon Elastic Kubernetes Service (Amazon EKS)
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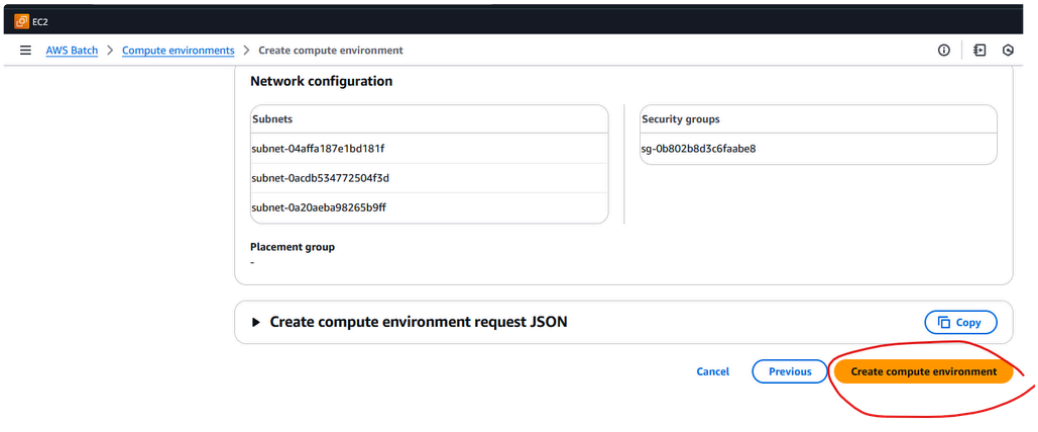
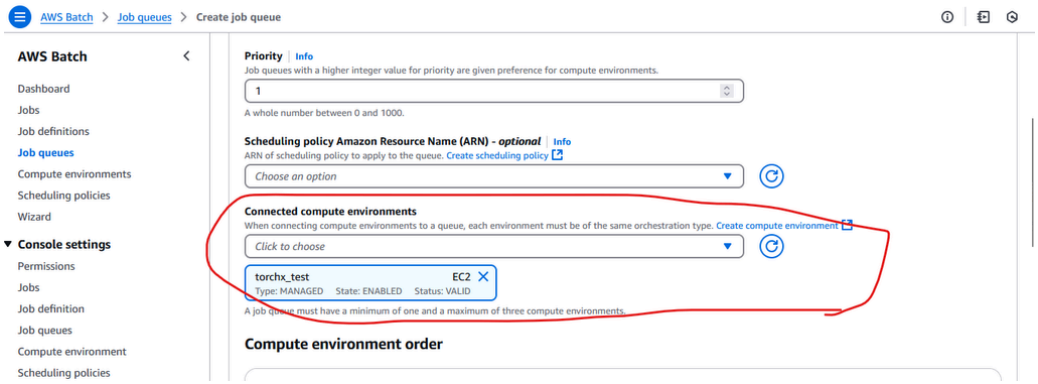
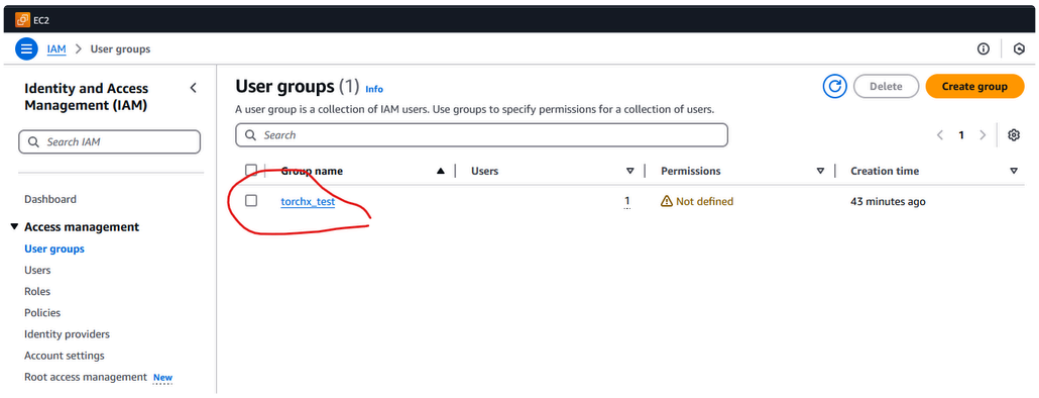
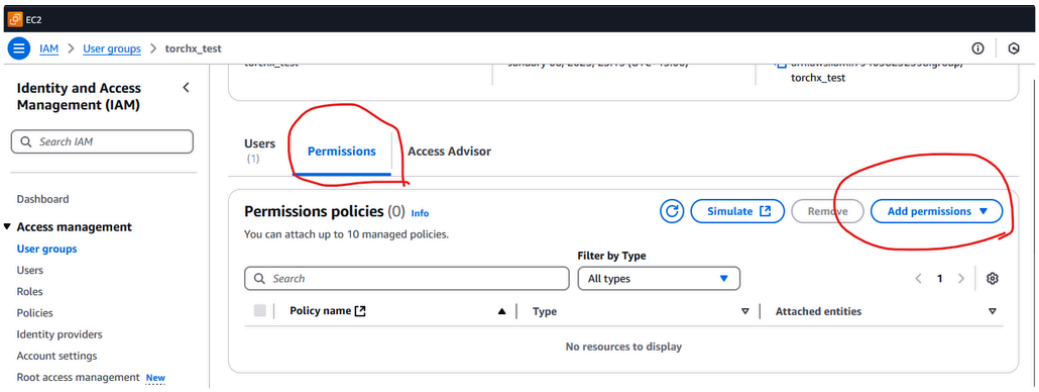
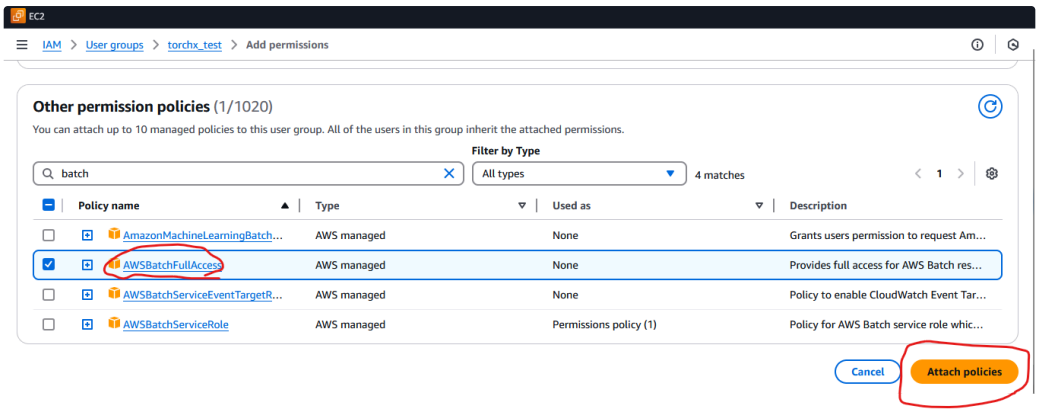

EC2
AWS Batch > Compute environments > Create compute environment
Network configuration
Subnets
subnet-04affa187e1bd181f
subnet-0acdb534772504f3d
subnet-0a20aeba98265b9ff
Security groups
sg-0b802b8d3c6faabe8
Placement group
-
Create compute environment request JSON
Copy
Cancel
Previous
Create compute environment



Set user permissions







Add AWSBatchFullAccess

Python code

Installation

```
poetry add torchx[kubernetes] botorch gpytorch ax-platform tensorboard pytorch-lightning torchvision boto3
botocore torch
```

mnist.py

mnist.py

```

"""
Example training code for ``ax_multiobjective_nas_tutorial.py``
"""

import argparse
import logging
import os
import sys
import time
import warnings

import torch
from IPython.utils import io
from pytorch_lightning import LightningModule, Trainer
from pytorch_lightning import loggers as pl_loggers
from torch import nn
from torch.nn import functional as F
from torch.utils.data import DataLoader
from torchmetrics.functional.classification.accuracy import multiclass_accuracy
from torchvision import transforms
from torchvision.datasets import MNIST

warnings.filterwarnings("ignore")  # Disable data logger warnings
logging.getLogger("pytorch_lightning").setLevel(logging.ERROR)  # Disable GPU/TPU prints

def parse_args():
    parser = argparse.ArgumentParser(description="train mnist")
    parser.add_argument(
        "--log_path", type=str, required=False,
        help="dir to place tensorboard logs from all trials",
        default="/tmp/mnist"
    )
    parser.add_argument(
        "--hidden_size_1", type=int, required=False,
        help="hidden size layer 1", default=16
    )
    parser.add_argument(
        "--hidden_size_2", type=int, required=False,
        help="hidden size layer 2", default=16
    )
    parser.add_argument(
        "--learning_rate", type=float, required=False,
        help="learning rate", default=1e-2
    )
    parser.add_argument(
```

```
        "--epochs", type=int, required=False,
        help="number of epochs", default=1
    )
    parser.add_argument(
        "--dropout", type=float, required=False,
        help="dropout probability", default=0.0
    )
    parser.add_argument(
        "--batch_size", type=int, required=False,
        help="batch size", default=32
    )
    return parser.parse_args()

args = parse_args()

PATH_DATASETS = os.environ.get("PATH_DATASETS", ".")


class MnistModel(LightningModule):
    def __init__(self):
        super().__init__()

        # Tunable parameters
        self.hidden_size_1 = args.hidden_size_1
        self.hidden_size_2 = args.hidden_size_2
        self.learning_rate = args.learning_rate
        self.dropout = args.dropout
        self.batch_size = args.batch_size

        # Set class attributes
        self.data_dir = PATH_DATASETS

        # Hardcode some dataset specific attributes
        self.num_classes = 10
        self.dims = (1, 28, 28)
        channels, width, height = self.dims
        self.transform = transforms.Compose(
            [
                transforms.ToTensor(),
                transforms.Normalize((0.1307,), (0.3081,)),
            ]
        )

        # Create a PyTorch model
        layers = [nn.Flatten()]
        width = channels * width * height
        hidden_layers = [self.hidden_size_1, self.hidden_size_2]
        num_params = 0
        for hidden_size in hidden_layers:
            if hidden_size > 0:
                layers.append(nn.Linear(width, hidden_size))
                layers.append(nn.ReLU())
                layers.append(nn.Dropout(self.dropout))
                num_params += width * hidden_size
                width = hidden_size
        layers.append(nn.Linear(width, self.num_classes))
        num_params += width * self.num_classes

```

```
        # Save the model and parameter counts
        self.num_params = num_params
        self.model = nn.Sequential(*layers)  # No need to use Relu for the last layer

    def forward(self, x):
        x = self.model(x)
        return F.log_softmax(x, dim=1)

    def training_step(self, batch, batch_idx):
        x, y = batch
        logits = self(x)
        loss = F.nll_loss(logits, y)
        return loss

    def validation_step(self, batch, batch_idx):
        x, y = batch
        logits = self(x)
        loss = F.nll_loss(logits, y)
        preds = torch.argmax(logits, dim=1)
        acc = multiclass_accuracy(preds, y, num_classes=self.num_classes)
        self.log("val_acc", acc, prog_bar=False)
        return loss

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.parameters(), lr=self.learning_rate)
        return optimizer

    def prepare_data(self):
        MNIST(self.data_dir, train=True, download=True)
        MNIST(self.data_dir, train=False, download=True)

    def setup(self, stage=None):
        self.mnist_train = MNIST(self.data_dir, train=True, transform=self.transform)
        self.mnist_val = MNIST(self.data_dir, train=False, transform=self.transform)

    def train_dataloader(self):
        return DataLoader(self.mnist_train, batch_size=self.batch_size)

    def val_dataloader(self):
        return DataLoader(self.mnist_val, batch_size=self.batch_size)


def run_training_job():

    mnist_model = MnistModel()

    # Initialize a trainer (don't log anything since things get so slow...)
    trainer = Trainer(
        logger=False,
        max_epochs=args.epochs,
        enable_progress_bar=False,
        deterministic=True,  # Do we want a bit of noise?
        default_root_dir=args.log_path,
    )

    logger = pl_loggers.TensorBoardLogger(args.log_path)

    print(f"Logging to path: {args.log_path}.")
```

```
    # Train the model and log time ⚡
    start = time.time()
    trainer.fit(model=mnist_model)
    end = time.time()
    train_time = end - start
    logger.log_metrics({"train_time": end - start})

    # Compute the validation accuracy once and log the score
    with io.capture_output() as captured:
        val_accuracy = trainer.validate()[0]["val_acc"]
    logger.log_metrics({"val_acc": val_accuracy})

    # Log the number of model parameters
    num_params = trainer.model.num_params
    logger.log_metrics({"num_params": num_params})

    logger.save()

    # Print outputs
    print(f"train time: {train_time}, val acc: {val_accuracy}, num_params: {num_params}")


if __name__ == "__main__":
    run_training_job()
```

Jupyter notebook

AWS credentials

AWS credentials

```
import os

os.environ["AWS_ACCESS_KEY_ID"] = "foo"
os.environ["AWS_SECRET_ACCESS_KEY"] = "bar"
os.environ["AWS_DEFAULT_REGION"] = "ap-southeast-2"
```

TorchXRunner

TorchXRunner

```
from pathlib import Path

import torchx

from torchx import specs
from torchx.components import utils


def trainer(
    log_path: str,
    hidden_size_1: int,
    hidden_size_2: int,
    learning_rate: float,
    epochs: int,
```

```
    dropout: float,
    batch_size: int,
    trial_idx: int = -1,
) -> specs.AppDef:

    # define the log path so we can pass it to the TorchX ``AppDef``
    if trial_idx >= 0:
        log_path = Path(log_path).joinpath(str(trial_idx)).absolute().as_posix()

    return utils.python(
        # command line arguments to the training script
        "--log_path",
        log_path,
        "--hidden_size_1",
        str(hidden_size_1),
        "--hidden_size_2",
        str(hidden_size_2),
        "--learning_rate",
        str(learning_rate),
        "--epochs",
        str(epochs),
        "--dropout",
        str(dropout),
        "--batch_size",
        str(batch_size),
        # other config options
        name="trainer",
        script="/opt/mnist.py",
        image="ghcr.io/jbris/torchx-aws-test:1.0.0",
    )

import tempfile
from ax.runners.torchx import TorchXRunner

# Make a temporary dir to log our results into
log_dir = tempfile.mkdtemp()

scheduler = "aws_batch"
# scheduler="local_cwd"

ax_runner = TorchXRunner(
    tracker_base="/tmp/",
    component=trainer,
    # NOTE: To launch this job on a cluster instead of locally you can
    # specify a different scheduler and adjust arguments appropriately.
    scheduler=scheduler,
    component_const_params={"log_path": log_dir},
    cfg={"queue": "torchx_queue"},
)
```

Parameter ranges

Parameter ranges

```
from ax.core import (
    ChoiceParameter,
    ParameterType,
    RangeParameter,
```

```
    SearchSpace,
)

parameters = [
    # NOTE: In a real-world setting, hidden_size_1 and hidden_size_2
    # should probably be powers of 2, but in our simple example this
    # would mean that ``num_params`` can't take on that many values, which
    # in turn makes the Pareto frontier look pretty weird.
    RangeParameter(
        name="hidden_size_1",
        lower=16,
        upper=128,
        parameter_type=ParameterType.INT,
        log_scale=True,
    ),
    RangeParameter(
        name="hidden_size_2",
        lower=16,
        upper=128,
        parameter_type=ParameterType.INT,
        log_scale=True,
    ),
    RangeParameter(
        name="learning_rate",
        lower=1e-4,
        upper=1e-2,
        parameter_type=ParameterType.FLOAT,
        log_scale=True,
    ),
    RangeParameter(
        name="epochs",
        lower=1,
        upper=4,
        parameter_type=ParameterType.INT,
    ),
    RangeParameter(
        name="dropout",
        lower=0.0,
        upper=0.5,
        parameter_type=ParameterType.FLOAT,
    ),
    ChoiceParameter(  # NOTE: ``ChoiceParameters`` don't require log-scale
        name="batch_size",
        values=[32, 64, 128, 256],
        parameter_type=ParameterType.INT,
        is_ordered=True,
        sort_values=True,
    ),
]

search_space = SearchSpace(
    parameters=parameters,
    # NOTE: In practice, it may make sense to add a constraint
    # hidden_size_2 <= hidden_size_1
    parameter_constraints=[],
)

from ax.metrics.tensorboard import TensorboardMetric
```

```
from tensorboard.backend.event_processing import plugin_event_multiplexer as event_multiplexer

class MyTensorboardMetric(TensorboardMetric):

    # NOTE: We need to tell the new TensorBoard metric how to get the id /
    # file handle for the TensorBoard logs from a trial. In this case
    # our convention is to just save a separate file per trial in
    # the prespecified log dir.
    def _get_event_multiplexer_for_trial(self, trial):
        mul = event_multiplexer.EventMultiplexer(max_reload_threads=20)
        mul.AddRunsFromDirectory(Path(log_dir).joinpath(str(trial.index)).as_posix(), None)
        mul.Reload()

        return mul

    # This indicates whether the metric is queryable while the trial is
    # still running. We don't use this in the current tutorial, but Ax
    # utilizes this to implement trial-level early-stopping functionality.
    @classmethod
    def is_available_while_running(cls):
        return False

val_acc = MyTensorboardMetric(
    name="val_acc",
    tag="val_acc",
    lower_is_better=False,
)
model_num_params = MyTensorboardMetric(
    name="num_params",
    tag="num_params",
    lower_is_better=True,
)
```

Run trials

Run trials

```
from ax.core import MultiObjective, Objective, ObjectiveThreshold
from ax.core.optimization_config import MultiObjectiveOptimizationConfig


opt_config = MultiObjectiveOptimizationConfig(
    objective=MultiObjective(
        objectives=[
            Objective(metric=val_acc, minimize=False),
            Objective(metric=model_num_params, minimize=True),
        ],
    ),
    objective_thresholds=[
        ObjectiveThreshold(metric=val_acc, bound=0.94, relative=False),
        ObjectiveThreshold(metric=model_num_params, bound=80_000, relative=False),
    ],
)

from ax.core import Experiment

experiment = Experiment(
    name="torchx_mnist",
```

```
    search_space=search_space,
    optimization_config=opt_config,
    runner=ax_runner,
)

total_trials = 48  # total evaluation budget

from ax.modelbridge.dispatch_utils import choose_generation_strategy

gs = choose_generation_strategy(
    search_space=experiment.search_space,
    optimization_config=experiment.optimization_config,
    num_trials=total_trials,
  )

from ax.service.scheduler import Scheduler, SchedulerOptions

scheduler = Scheduler(
    experiment=experiment,
    generation_strategy=gs,
    options=SchedulerOptions(
        total_trials=total_trials, max_pending_trials=4
    ),
)

scheduler.run_n_trials(3)
```

Results

Results

```

from ax.service.utils.report_utils import exp_to_df

df = exp_to_df(experiment)
df.head(10)

from ax.service.utils.report_utils import _pareto_frontier_scatter_2d_plotly

_pareto_frontier_scatter_2d_plotly(experiment)
```