Soopervisor

Ploomber

Feb 11, 2022

BATCH PROCESSING

Soopervisor runs Ploomber pipelines for batch processing (large-scale training or batch serving) or online inference.

```
pip install soopervisor
```

Watch our presentation at EuroPython 2021: Develop and Deploy a Machine Learning Pipeline in 30 Minutes With Ploomber.

CHAPTER

ONE

SUPPORTED PLATFORMS

- Batch serving and large-scale training:
  - *Airflow*
  - *Argo/Kubernetes*
  - *AWS Batch*
  - *Kubeflow*
  - *SLURM*
- Online inference:
  - *AWS Lambda*

CHAPTER

TWO

FROM NOTEBOOK TO A PRODUCTION PIPELINE

We also have *an example* that shows how to use our ecosystem of tools to go **from a monolithic notebook to a pipeline deployed in Kubernetes.**

CHAPTER

THREE

STANDARD LAYOUT

Soopervisor expects your Ploomber project to be in the standard project layout, which requires the following:

3.1 Dependencies file

- `requirements.lock.txt`: `pip` dependencies file

Tip: You can generate it with `pip freeze > requirements.lock.txt`

OR

- `environment.lock.yml`: conda environment with pinned dependencies

Tip: You can generate it with `conda env export --no-build --file environment.lock.yml`

3.2 Pipeline declaration

A `pipeline.yaml` file in the current working directory (or in `src/{package-name}/pipeline.yaml` if your project is a Python package).

Note: If your project is a package (i.e., it has a `src/` directory, a `setup.py` file is also required.

3.3 Scaffolding standard layout

The fastest way to get started is to scaffold a new project:

```
# install ploomber
pip install ploomber

# scaffold project
ploomber scaffold

# or to use conda (instead of pip)
```

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```
ploomber scaffold --conda

# or to use the package structure
ploomber scaffold --package

# or to use conda and the package structure
ploomber scaffold --conda --package
```

Then, configure the development environment:

```
# move to your project's root folder
cd {project-name}

# configure dev environment
ploomber install
```

Note: `ploomber install` automatically generates the `environment.lock.yml` or `requirements.lock.txt` file. If you prefer so, you may skip `ploomber install` and create the lock files yourself.

CHAPTER

FOUR

USAGE

Say that you want to train multiple models in a Kubernetes cluster, you may create a new target environment to execute your pipeline using Argo Workflows:

```
soopervisor add training --backend argo-workflows
```

After filling in some basic configuration settings, export the pipeline with:

```
soopervisor export training
```

Soopervisor will take care of packaging your code and submitting it for execution. Using Argo Workflows will create a Docker image, upload it to the configured registry, generate an Argo's YAML spec, and submit the workflow.

Depending on the selected backend (Argo, Airflow, AWS Batch, or AWS Lambda), configuration details will change, but the API remains the same: `soopervisor add`, then `soopervisor export`.

4.1 Airflow

Important: This tutorial requires soopervisor `0.6.1` or higher

Note: This tutorial exports an Airflow DAG using the `KubernetesPodOperator`, to use alternative Operators, see *Airflow cookbook*. **Got questions?** Reach out to us on Slack.

This tutorial shows you how to export a Ploomber pipeline to Airflow.

If you encounter any issues with this tutorial, let us know.

4.1.1 Pre-requisites

- docker

4.1.2 Building Docker image

We provide a Docker image so you can quickly run this example:

```
# get repository
git clone https://github.com/ploomber/soopervisor
cd soopervisor/tutorials/airflow

# create a directory to store the pipeline output
export SHARED_DIR=$HOME/ploomber-airflow
mkdir -p $SHARED_DIR

# build image
docker build --tag ploomber-airflow .

# start
docker run -i -t -p 8080:8080 --privileged=true \
    -v /var/run/docker.sock:/var/run/docker.sock \
    --volume $SHARED_DIR:/mnt/shared-folder \
    --env SHARED_DIR \
    --env PLOOMBER_STATS_ENABLED=false \
    ploomber-airflow /bin/bash
```

Note: We need to run `docker run` in privileged mode since we'll be running `docker` commands inside the container. More on that here

4.1.3 Create Kubernetes cluster

By default, the Airflow integration exports each task in your pipeline as a Airflow task using the KubernetesPodOperator, so we need to create a Kubernetes cluster to run the example:

The Docker image comes with `k3d` pre-installed; let's create a cluster:

```
# create cluster
k3d cluster create mycluster --volume $SHARED_DIR:/host

# check cluster
kubectl get nodes
```

4.1.4 Get sample Ploomber pipeline

```
# get example
ploomber examples -n templates/ml-intermediate -o ml-intermediate
cd ml-intermediate

cp requirements.txt requirements.lock.txt
# configure development environment
pip install ploomber soopervisor
pip install -r requirements.txt
```

4.1.5 Configure target platform

```
# add a new target platform
soopervisor add training --backend airflow
```

Usually, you'd manually edit `soopervisor.yaml` to configure your environment; for this example, let's use one that we already configured, which tells soopervisor to mount a local directory to every pod so we can review results later:

```
cp ../soopervisor-airflow.yaml soopervisor.yaml
```

We must configure the project to store all outputs in the shared folder so we copy the pre-configured file:

```
cp ../env-airflow.yaml env.yaml
```

4.1.6 Submit pipeline

```
soopervisor export training --skip-tests --ignore-git

# import image to the cluster
k3d image import ml-intermediate:latest --cluster mycluster
```

Note: `k3d image import` is only required if creating the cluster with `k3d`.

Once the export process finishes, you'll see a new `training/` folder with two files: `ml-intermediate.py` (Airflow DAG) and `ml-intermediate.json` (DAG structure).

4.1.7 Customizing Airflow DAG

The `.py` file generated by `soopervisor export` contains the logic to convert our pipeline into an Airflow DAG with basic defaults. However, we can further customize it. In our case, we need some initialization parameters in the generated `KubernetesPodOperator` tasks. Execute the following command to replace the generated file with one that has the appropriate settings:

```
cp ../ml-intermediate.py training/ml-intermediate.py
```

4.1.8 Submitting pipeline

To execute the pipeline, move the generated files to your `AIRFLOW_HOME`. For this example, `AIRFLOW_HOME` is `/root/airflow`:

```
mkdir -p /root/airflow/dags
cp training/ml-intermediate.py ~/airflow/dags
cp training/ml-intermediate.json ~/airflow/dags

ls /root/airflow/dags
```

If everything is working, you should see the `ml-intermediate` DAG here:

```
airflow dags list
```

Let's start the airflow UI and scheduler (this will take a few seconds):

```
bash /start_airflow.sh
```

Let's unpause the DAG then trigger the run:

```
airflow dags unpause ml-intermediate
```

After unpausing, you should see the following message:

> Dag: ml-intermediate, paused: False

If you don't, likely, the Airflow scheduler isn't ready yet, so wait for a few seconds and try again.

Trigger execution:

```
airflow dags trigger ml-intermediate
```

Congratulations! You just ran Ploomber on Airflow!

Note: If you encounter issues with Airflow, you can find the logs at `/airflow-scheduler.log` and `/airflow-webserver.log`.

4.1.9 Monitoring execution status

You may track execution progress from Airflow's UI by opening http://localhost:8080 (Username: `ploomber`, Password: `ploomber`)

Alternatively, with the following command:

```
airflow dags state ml-intermediate {TIMESTAMP}
```

The TIMESTAMP shows after running `airflow dags trigger ml-intermediate`, for example, once you execute the `airflow dags trigger` command, you'll see something like this in the console:

> Created <DagRun ml-intermediate @ 2022-01-02T18:05:19+00:00: manual__2022-01-02T18:05:19+00:00, externally triggered: True>

Then, you can get the execution status with:

```
airflow dags state ml-intermediate 2022-01-02T18:05:19+00:00
```

4.1.10 Incremental builds

Try exporting the pipeline again:

```
soopervisor export training --skip-tests --ignore-git
```

You'll see a message like this: `Loaded DAG in 'incremental' mode has no tasks to submit`. Soopervisor checks the status of your pipeline and only schedules tasks that have changed since the last run; since all your tasks are the same, there is nothing to run!

Let's now modify one of the tasks and submit again:

```
# modify the fit.py task, add a print statement
echo -e "\nprint('Hello from Kubernetes')" >> fit.py

# re-build docker image
soopervisor export training --skip-tests --ignore-git

# import image
k3d image import ml-intermediate:latest --cluster mycluster

# copy files to the dags directory
cp training/ml-intermediate.py ~/airflow/dags
cp training/ml-intermediate.json ~/airflow/dags

# trigger execution
airflow dags trigger ml-intermediate
```

If you open the UI, you'll see that this time, only the `fit` task ran because that's the only tasks whose source code change; we call this incremental builds, and they're a great feature for quickly running experiments in your pipeline such as changing model hyperparameters or adding new pre-processing methods; it saves a lot of time since you don't have to execute the entire pipeline every time.

4.1.11 Clean up

To delete the cluster:

```
k3d cluster delete mycluster
```

4.1.12 Using other Operator

If you want to generate Airflow DAGs using other operators, check out the *Airflow cookbook*

4.2 AWS Batch

Important: This tutorial requires soopervisor `0.6.1` or higher

Note: **Got questions?** Reach out to us on Slack.

AWS Batch is a managed service for batch computing. This tutorial shows you how to submit a Ploomber pipeline to AWS Batch.

If you encounter any issues with this tutorial, let us know.

Click here to see a recorded demo.

4.2.1 Pre-requisites

- conda
- docker
- aws cli
- git

`soopervisor` takes your pipeline, packages it, creates a Docker image, uploads it, and submits it for execution; however, you still have to configure the AWS Batch environment. Specifically, you must configure a computing environment and a job queue. Refer to this guide for instructions.

Note: Only EC2 compute environments are supported.

Once you've configured an EC2 compute environment and a job queue, continue to the next step.

4.2.2 Setting up project

First, let's install `ploomber`:

```
pip install ploomber
```

Fetch an example pipeline:

```
# get example
ploomber examples -n templates/ml-online -o ml-online
cd ml-online
```

Configure the development environment:

```
ploomber install
```

Then, activate the environment:

```
conda activate ml-online
```

4.2.3 Configure S3 client

We must configure a client to upload all generated artifacts to S3. To obtain such credentials, you may use the AWS console, ensure you give read and write S3 access. You may also create an S3 bucket or use one you already have.

Save a `credentials.json` file in the root directory (the folder that contains the `setup.py` file) with your authentication keys:

```
{
    "aws_access_key_id": "YOUR-ACCESS-KEY-ID",
    "aws_secret_access_key": "YOU-SECRET-ACCESS-KEY"
}
```

Now, configure the pipeline to upload artifacts to S3. Modify the `pipeline.yaml` file at `ml-online/src/ml_online/pipeline.yaml` so it looks like this:

```
meta:
  source_loader:
  module: ml_online

  import_tasks_from: pipeline-features.yaml

# add this
clients:
    File: ml_online.clients.get_s3

# content continues...
```

Go to the `src/ml_online/clients.py` file and edit the `get_s3` function, modifying the `bucket_name` and `parent` parameters. The latter is the folder inside the bucket to save pipeline artifacts. Ignore the second function; it's not relevant for this example.

To make sure your pipeline works, run:

```
ploomber status
```

You should see a table with a summary. If you see an error, check the traceback to see if it's an authentication problem or something else.

4.2.4 Submitting a pipeline to AWS Batch

We are almost ready to submit. To execute tasks in AWS Batch, we must create a Docker image with all our project's source code.

Create a new repository in Amazon ECR before continuing. Once you create it, authenticate with:

```
aws ecr get-login-password --region your-region | docker login --username AWS --password-
↪stdin your-repository-url/name
```

Note: Replace `your-repository-url/name` with your repository's URL and `your-region` with the corresponding ECR region

---

Let's now create the necessary files to export our Docker image:

```
# get soopervisor
pip install soopervisor

# register new environment
soopervisor add training --backend aws-batch
```

Open the `soopervisor.yaml` file and fill in the missing values in `repository`, `job_queue` and `region_name`.

```
training:
  backend: aws-batch
  repository: your-repository-url/name
  job_queue: your-job-queue
  region_name: your-region-name
  container_properties:
```

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```
  memory: 16384
  vcpus: 8
```

Submit for execution:

```
soopervisor export training --skip-tests --ignore-git
```

The previous command will take a few minutes since it has to build the Docker image from scratch. After that, subsequent runs will be much faster.

Note: if you successfully submitted tasks, but they are stuck in the console in `RUNNABLE` status. It's likely that the requested resources (the `container_properties` section in `soopervisor.yaml`) exceeded the capacity of the computing environment. Try lowering resources and submit again. If that doesn't work, check this out.

Tip: The number of concurrent jobs is limited by the resources in the Compute Environment. Increase them to run more tasks in parallel.

Congratulations! You just ran Ploomber on AWS Batch!

4.3 Kubernetes (Argo)

Note: **Got questions?** Reach out to us on Slack.

This tutorial shows how to run a pipeline in Kubernetes via Argo Workflows locally or in Google Cloud.

If you encounter any issues with this tutorial, let us know.

Click here to see the Argo Community Meeting talk.

We have two tutorials:

- *Local* (only requires `docker`)
- *Google Cloud*

4.3.1 Local example

Important: This tutorial requires soopervisor `0.6.1` or higher

This tutorial runs a pipeline in a local Kubernetes cluster using `k3d`.

Pre-requisites

- docker

Building Docker image

We provide a Docker image so you can quickly run this example:

```
# get repository
git clone https://github.com/ploomber/soopervisor
cd soopervisor/tutorials/kubernetes

# create a directory to store the pipeline output
export SHARED_DIR=$HOME/ploomber-k8s
mkdir -p $SHARED_DIR

# build image
docker build --tag ploomber-k8s .

# start
docker run -i -t \
    --privileged=true -v /var/run/docker.sock:/var/run/docker.sock \
    --volume $SHARED_DIR:/mnt/shared-folder \
    --env SHARED_DIR \
    --env PLOOMBER_STATS_ENABLED=false \
    -p 2746:2746 \
    ploomber-k8s /bin/bash
```

Note: We need to run `docker run` in privileged mode since we'll be running `docker` commands inside the container. More on that here

Create Kubernetes cluster

The Docker image comes with `k3d` pre-installed; let's create a cluster:

```
# create cluster
k3d cluster create mycluster --volume $SHARED_DIR:/host --port 2746:2746

# check cluster
kubectl get nodes
```

Note: If you see the error message `Bind for 0.0.0.0:2746 failed: port is already allocated`, you may drop the `--port 2746:2746` and try again: `k3d cluster create mycluster --volume $SHARED_DIR:/host` the command will work but you'll be unable to open Argo's GUI.

Install Argo

We now install argo; note that we are using a custom installation file (`argo-pns.yaml`) to ensure this works with `k3d`.

```
# install argo
kubectl create ns argo
kubectl apply -n argo -f argo-pns.yaml

# check argo pods (once they're all running, argo is ready)
kubectl get pods -n argo
```

Note: `argo-pns.yaml` is a custom file that changes the Argo executor to PNS; this is required to ensure Argo works on `k3d`; however, this change isn't required in a production environment.

Tip: Optionally, submit sample Argo workflow to ensure everything is working:

```
argo submit -n argo --watch https://raw.githubusercontent.com/argoproj/argo-workflows/
↪master/examples/hello-world.yaml
```

Get sample Ploomber pipeline

```
# get example
ploomber examples -n templates/ml-intermediate -o ml-intermediate
cd ml-intermediate

# configure development environment
cp requirements.txt requirements.lock.txt
pip install ploomber soopervisor
pip install -r requirements.txt
```

Configure target platform

Soopervisor allows you to configure the target platform using a `soopervisor.yaml` file, let's add it and set the backend to `argo-worflows`:

```
soopervisor add training --backend argo-workflows
```

Usually, you'd manually edit `soopervisor.yaml` to configure your environment; for this example, let's use one that we already configured, which tells soopervisor to mount a local directory to every pod so we can review results later:

```
cp ../soopervisor-k8s.yaml soopervisor.yaml
```

We must configure the project to store all outputs in the shared folder, so we copy the pre-configured file:

```
cp ../env-k8s.yaml env.yaml
```

Submit pipeline

We finished configuring; let's now submit the workflow:

```
# build docker image (takes a few minutes the first time) and generate an argo's yaml spec
soopervisor export training --skip-tests --ignore-git

# import image to the k8s cluster
k3d image import ml-intermediate:latest --cluster mycluster

# submit workflow
argo submit -n argo --watch training/argo.yaml
```

Congratulations! You just ran Ploomber on Kubernetes!

Note: `k3d image import` is only required if creating the cluster with `k3d`.

Once the execution finishes, take a look at the generated artifacts:

```
ls /mnt/shared-folder
```

Tip: You may also watch the progress from the UI.

```
# port forwarding to enable the UI
kubectl -n argo port-forward svc/argo-server 2746:2746
```

Then, open: https://127.0.0.1:2746

Incremental builds

Try exporting the pipeline again:

```
soopervisor export training --skip-tests --ignore-git
```

You'll see a message like this: `Loaded DAG in 'incremental' mode has no tasks to submit`. Soopervisor checks the status of your pipeline and only schedules tasks that have changed since the last run; since all your tasks are the same, there is nothing to run!

Let's now modify one of the tasks and submit it again:

```
# modify the fit.py task, add a print statement
echo -e "\nprint('Hello from Kubernetes')" >> fit.py

# re-build docker image and submit
soopervisor export training --skip-tests --ignore-git
k3d image import ml-intermediate:latest --cluster mycluster
argo submit -n argo --watch training/argo.yaml
```

You'll see that this time, only the `fit` task ran because that's the only tasks whose source code change, we call this incremental builds, and they're a a great feature for quickly running experiments in your pipeline, such as changing model hyperparameters or adding new pre-processing methods; it saves a lot of time since you don't have to execute the entire pipeline every time.

Clean up

To delete the cluster:

```
k3d cluster delete mycluster
```

4.3.2 Google Cloud

Important: This tutorial requires soopervisor `0.6.1` or higher

This second tutorial runs a pipeline in a local Kubernetes cluster using Google Cloud.

Note: You may use or create a new Google Cloud project to follow this tutorial.

Pre-requisites

- `kubectl`
- Google Cloud SDK
- conda instructions
- git
- Install Ploomber with `pip install ploomber`

Instructions

Create a cluster and install Argo:

```
# create cluster
gcloud container clusters create my-cluster --num-nodes=1 --zone us-east1-b

# install argo
kubectl create ns argo
kubectl apply -n argo -f https://raw.githubusercontent.com/argoproj/argo-workflows/
↪stable/manifests/quick-start-postgres.yaml

# create storage bucket (choose whatever name you want)
gsutil mb gs://YOUR-BUCKET-NAME
```

Submit a sample workflow to make sure Argo is working:

```
argo submit -n argo --watch https://raw.githubusercontent.com/argoproj/argo/master/
↪examples/hello-world.yaml
```

Tip: Enable Argo's UI:

```
# port forwarding to enable the UI
kubectl -n argo port-forward svc/argo-server 2746:2746
```

Then, open: https://127.0.0.1:2746

Install `ploomber`:

```
pip install ploomber
```

Let's now run a Ploomber sample Machine Learning pipeline:

```
# get example
ploomber examples -n templates/ml-online -o ml-online
cd ml-online

# configure development environment
ploomber install

# activate environment
conda activate ml-online

# add a new target platform
soopervisor add training --backend argo-workflows
```

The previous command creates a `soopervisor.yaml` file where we can configure the container registry to upload our Docker image:

```
training:
  backend: argo-workflows
  repository: gcr.io/PROJECT-ID/my-ploomber-pipeline
```

Replace `PROJECT-ID` with your actual project ID.

Each task will run in isolation, we must ensure that products generated by a given task are available to its corresponding downstream tasks. Ww can use Google Cloud Storage for that, add the following to the `src/ml_online/pipeline.yaml` file:

```
# more content above...

serializer: ml_online.io.serialize
unserializer: ml_online.io.unserialize

# add these two lines
clients:
  File: ml_online.clients.get_gcloud

# content continues...
```

The previous change tells Ploomber to call the function `get_gcloud` defined in module `src/ml_online/clients.py` to get the client. Edit the `clients.py` to add your bucket name:

```
from ploomber.clients import GCloudStorageClient

def get_gcloud():
    # edit YOUR-BUCKET-NAME
    return GCloudStorageClient(bucket_name='YOUR-BUCKET-NAME',
                               parent='ml-online',
                               json_credentials_path='credentials.json')
```

You can ignore the rest of the file. Finally, we add service account credentials to upload to Google Cloud Storage. To learn more about service accounts, click here.

Store the service account details in a `credentials.json` in the root project directory (same folder as `setup.py`):

We are ready to execute the workflow:

```
# authenticate to push docker image
gcloud auth configure-docker

# packages code, create docker image and upload it (takes a few mins)
soopervisor export training

# submit workflow
argo submit -n argo training/argo.yaml
```

You may keep track of execution by opening the UI. Check out the bucket to see output.

Congratulations! You just ran Ploomber on Kubernetes!

Attention: Make sure you delete your cluster, bucket, and image after running this example!

```
# delete cluster
gcloud container clusters delete my-cluster --zone us-east1-b

# delete bucket
gsutil rm -r gs://my-sample-ploomber-bucket

# delete image (you can get the image id from the google cloud console)
gcloud container images delete IMAGE-ID
```

Optional: Mounting a shared disk

Note: If you use a shared disk instead of storing artifacts in S3 or Google Cloud Storage, you must execute the pipeline with the `--skip-tests` flag. e.g., `soopervisor export training --skip-tests`, otherwise the command will fail if your project does not have a remote storage client configured.

In the example, we configured the `pipeline.yaml` file to use Google Cloud Storage to store artifacts, this serves two purposes: 1) Make artifacts available to us upon execution, and 2) Make artifacts available to dowstream tasks.

This happens because pods run in isolation, if task B depends on task A, it will fetch A's output from cloud storage before execution. We can save dowload time (and cut costs) by mounting a shared volume so that B doesn't have to download A's output. Ploomber automatically detects this change and only calls the cloud storage API for uploading.

Here's how to configure a shared disk:

```
# create disk. make sure the zone matches your cluster
gcloud compute disks create --size=10GB --zone=us-east1-b gce-nfs-disk

# configure the nfs server
curl -O https://raw.githubusercontent.com/ploomber/soopervisor/master/doc/assets/01-nfs-
↪server.yaml
kubectl apply -f 01-nfs-server.yaml
```

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```
# create service
curl -O https://raw.githubusercontent.com/ploomber/soopervisor/master/doc/assets/02-nfs-
↪service.yaml
kubectl apply -f 02-nfs-service.yaml

# check service
kubectl get svc nfs-server

# create persistent volume claim
curl -O https://raw.githubusercontent.com/ploomber/soopervisor/master/doc/assets/03-nfs-
↪pv-pvc.yaml
kubectl apply -f 03-nfs-pv-pvc.yaml
```

Optionally, you can check that the disk is properly configured by running this sample workflow:

```
# run sample workflow (uses nfs and creates an empty file on it)
curl -O https://raw.githubusercontent.com/ploomber/soopervisor/master/doc/assets/dag.yaml
argo submit -n argo --watch dag.yaml
```

Check the output:

```
# get nfs-server pod name
kubectl get pod

# replace with the name of the pod
kubectl exec --stdin --tty {nfs-server-pod-name} -- /bin/bash
```

Once inside the Pod, run:

```
ls /exports/
```

You should see files A, B, C, D. Generated by the previous workflow.

Let's now run the Machine Learning workflow. Since we configured a shared disk, artifacts from upstream tasks will be available to downstream ones (no need to download them from Cloud Storage anymore); the Cloud Storage client is only used to upload artifacts for us to review later.

To make the shared disk available to the pods that run each task, we have to modify `soopervisor.yaml`:

```
training:
  backend: argo-workflows
  repository: gcr.io/your-project/your-repository
  mounted_volumes:
    - name: nfs
      sub_path: my-shared-folder
      spec:
        persistentVolumeClaim:
          claimName: nfs
```

This exposes `/my-shared-folder` sub directory in our shared disk in `/mnt/nfs/` on each pod. Now, we must configure the pipeline to store all products in `/mnt/nfs/`. Create an `env.yaml` file in the root folder (same folder that contains the `setup.py` file) with this content:

```
sample: False
# this configures the pipeline to store all outputs in the shared disk
product_root: /mnt/nfs
```

4.4 Kubeflow

Important: The kubeflow integration requires `soopervvisor>=0.7`

Important: **The Kubeflow tutorial is in beta! Got questions or found issues?** Reach out to us on Slack.

This tutorial shows you how to export a Ploomber pipeline to Kubeflow.

If you encounter any issues with this tutorial, let us know.

Note: This tutorial uses cloud storage (S3 or Google Cloud Storage). In addition, it runs on the local cluster local storage for faster data fetch.

4.4.1 Pre-requisites

- Kubeflow
- `conda` See instructions here
- docker
- git
- Install Ploomber with `pip install ploomber`

Note: When installing Kubeflow, you must use a strong enough VM to meet the basic requirements. This tutorial assumes the Kubeflow is configured and you're running within this cluster. Another option is to run the tutorial locally and upload the final `ploomber_pipeline.yaml` to Kubeflow.

Instructions

First, let's install `ploomber`:

```
pip install ploomber
```

Let's now pull some sample code:

```
# get example
ploomber examples -n templates/ml-intermediate -o ml-intermediate
cd ml-intermediate
```

Since each task executes in a different Docker container, we have to configure cloud storage for tasks to share data. Modify the `environment.yml` file and add the appropriate dependency:

```
# content...
- pip:
  # dependencies...

  # add your dependency here
  - boto3 # if you want to use S3
  - google-cloud-storage # if you want to use Google Cloud Storage
```

We also need to configure the pipeline to use cloud storage, open the `pipeline.yaml` file, and add the following next to the `meta` section.

```
meta:
    # some content...

clients:
    File: clients.get_s3
```

```
meta:
    # some content...

clients:
    File: clients.get_gcloud
```

Now, edit the `clients.py` file, you only need to change the `bucket_name` parameter for the corresponding function. For example, if using a bucket with the name `bucket-name` and S3, `clients.py` should look like this:

```
from ploomber.clients import S3Client

def get_s3():
    return S3Client(bucket_name='bucket-name',
                    parent='ml-intermediate',
                    json_credentials_path='credentials.json')
```

```
from ploomber.clients import GCloudStorageClient

def get_gcloud():
    return GCloudStorageClient(bucket_name='bucket-name',
                               parent='ml-online',
                               json_credentials_path='credentials.json')
```

To authenticate to the cloud storage service, add a `credentials.json` file in the project root (the same folder that has the `environment.yml` file.

```
{
    "aws_access_key_id": "YOUR-ACCESS-KEY-ID",
    "aws_secret_access_key": "YOU-SECRET-ACCESS-KEY"
}
```

```
{
    "type": "service_account",
    "project_id": "project-id",
    "private_key_id": "private-key-id",
```

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```
    "private_key": "private-key",
    "client_email": "client-email",
    "client_id": "client-id",
    "auth_uri": "https://accounts.google.com/o/oauth2/auth",
    "token_uri": "https://oauth2.googleapis.com/token",
    "auth_provider_x509_cert_url": "https://www.googleapis.com/oauth2/v1/certs",
    "client_x509_cert_url": "https://www.googleapis.com/robot/v1/metadata/x509/service-
↪account.iam.gserviceaccount.com"
}
```

Note: When running with local storage, Kubeflow takes the product path and name and stores it accordingly to its temporary outputs folder. You will need to set the path of the products in the `pipeline.yaml` (the file that defines the pipeline - above) to: `product: '{{root}}/product/data/get.parquet'` note how the product name appears in the path (mandatory). In addition we can see below that for the nb and model products we set the path according to their names.

This is how your `pipeline.yaml` file should look like if you're using GCP:

```
meta:
  jupyter_functions_as_notebooks: True
  import_tasks_from: partial.features.yaml

clients:
  File: clients.get_gcloud

tasks:
  - source: tasks.get.fn
    name: get
    product: '{{root}}/product/data/get.parquet'
    params:
      sample: '{{sample}}'

  - source: fit.py
    name: fit
    product:
        nb: '{{root}}/nb/data/nb.html'
        model: '{{root}}/model/data/model.pickle'
```

Important: Make sure to adjust those files to have the same output structure: `partial.features.yaml` and `pipeline.serve.yaml`.

In addition, we also need to configure the env files to the right root location. Make sure in these files `env.local.yaml`, `env.serve.yaml` and `env.yaml` the root is set to `'outputs'` in a similar fashion to the `env.yaml` below:

```
root: 'outputs'
sample: False
```

Let's now create the virtual environment:

```
# configure environment
conda env create --file environment.yml

# activate environment
conda activate ml-intermediate

# generate lock file
conda env export --no-build --file environment.lock.yml
```

Let's now verify that everything is configured correctly:

```
ploomber status
```

We now export the pipeline to Kubeflow:

```
soopervisor add train --backend kubeflow
```

Note: You don't have to install `soopervisor` manually; it should've been installed when running `ploomber install`. If missing, install it with `pip install soopervisor`.

`soopervisor add` creates a few new files. Let's configure `soopervisor.yaml` which controls some settings:

```
train:
  backend: kubeflow
  # we will be using a remote docker hub, we'll set this image name
  repository: idomic/general:kubeflow1
  # make sure our credentials are included when building the image
  include: [credentials.json]
```

Note: See how the repository is configured to the docker hub `idomic/general` and the image within it `kubeflow1` (: separated)

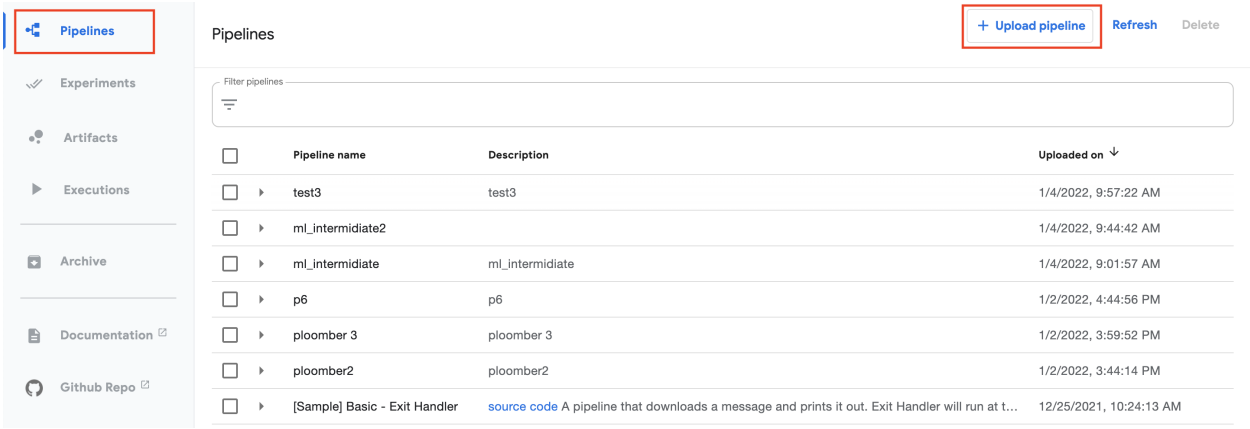
Build the Docker image (takes a few minutes the first time):

```
soopervisor export train
```

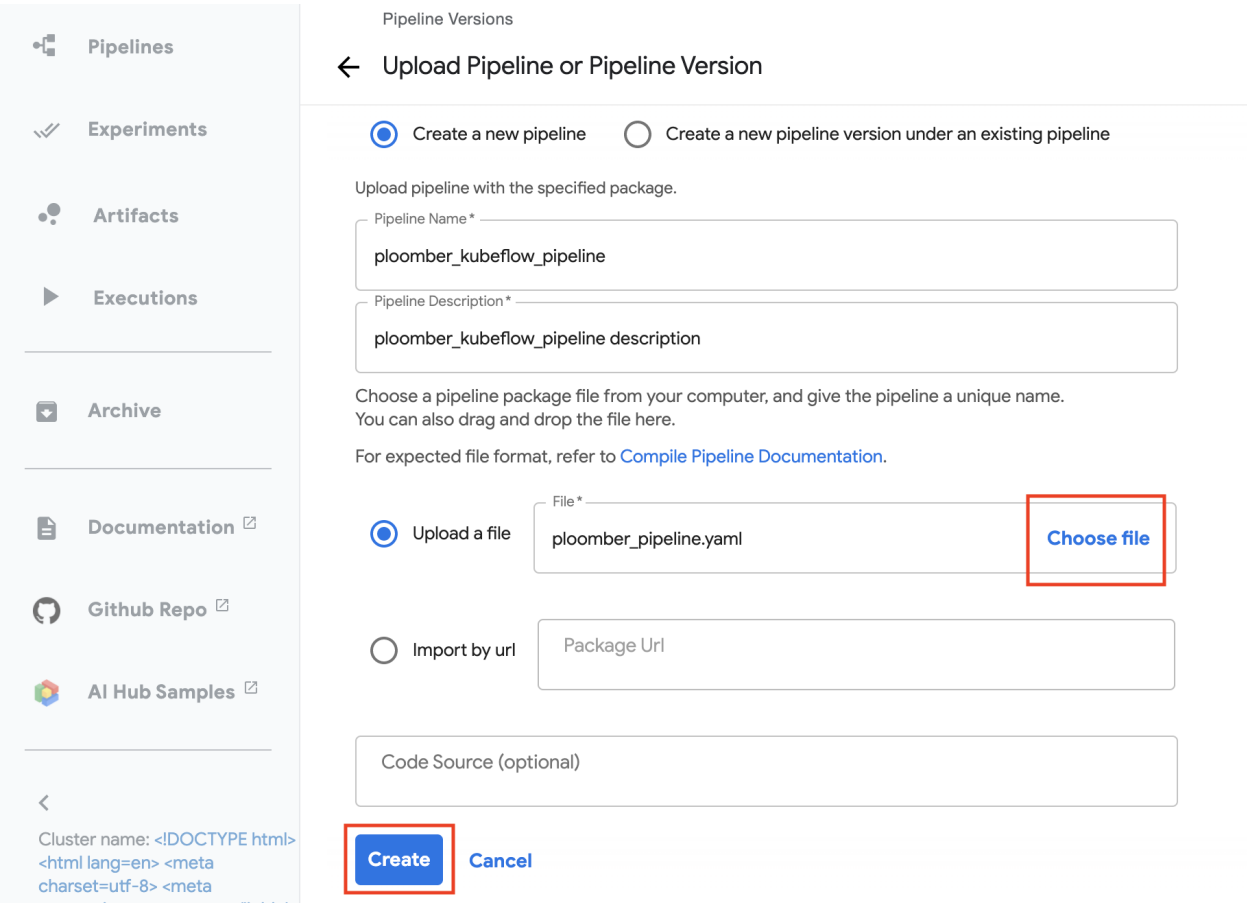
Once the export process finishes, you'll see a new `train/` folder with three files: `Dockerfile` which is the file used to build the docker image, a `kubeflow_pipeline.py` which is the pythonic version of the pipeline (you can run it directly on a notebook instance within the cluster) and the file `ploomber_pipeline.yaml` which contains the kubeflow pipeline to run. To deploy, go to your cluster and upload the `.yaml` file as a new pipeline (you can also use the CLI directly (we'll cover both options).

Option 1: UI upload of a Kubeflow pipeline

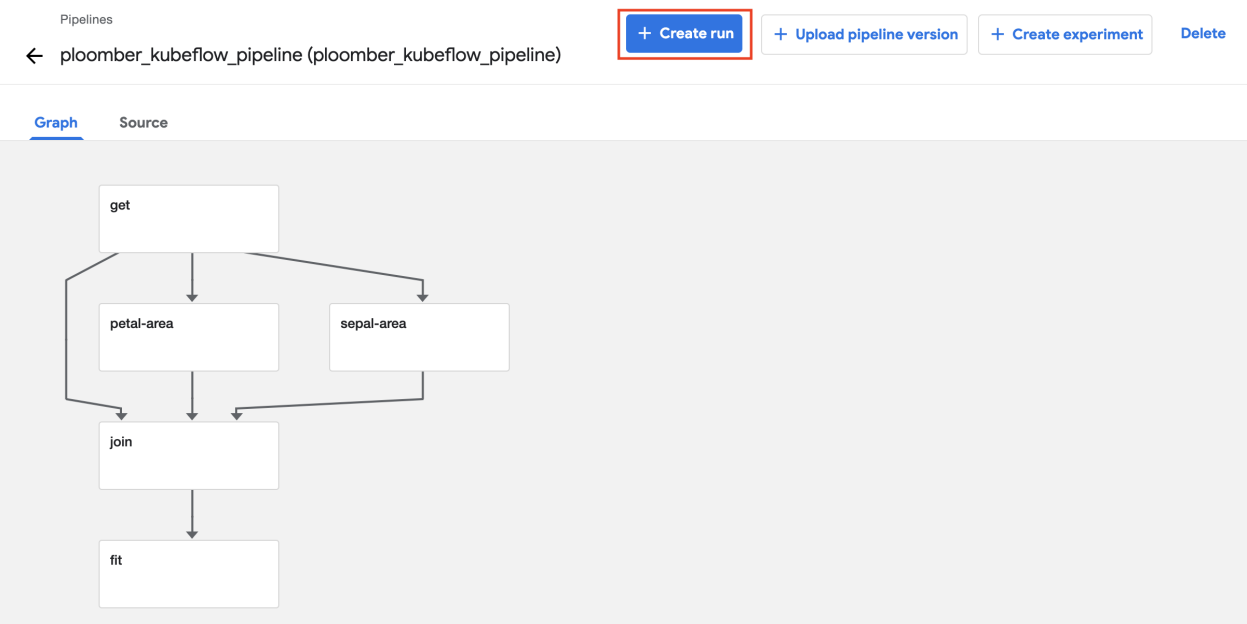
Let's go to the cluster and click on `Pipelines` (top left) and then on the top right on `+ Upload pipeline`. (see image below)



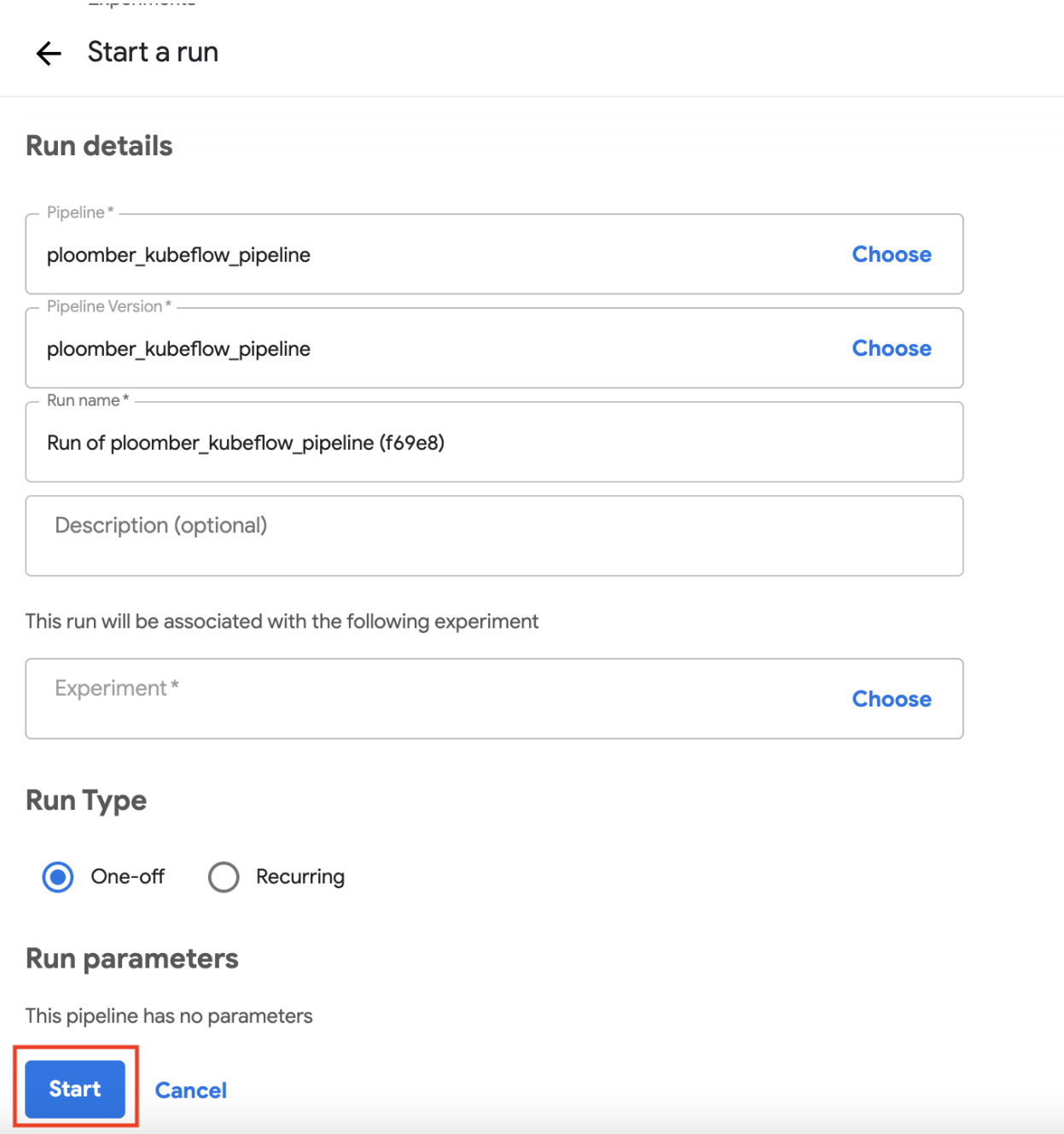
We now can name our pipeline `ml_intermidiate`, describe it (or copy the name to it), click on upload file and `choose file`, pick the `ploomber_pipeline.yaml` we just created. On the bottom click on `Create`. (see image below)



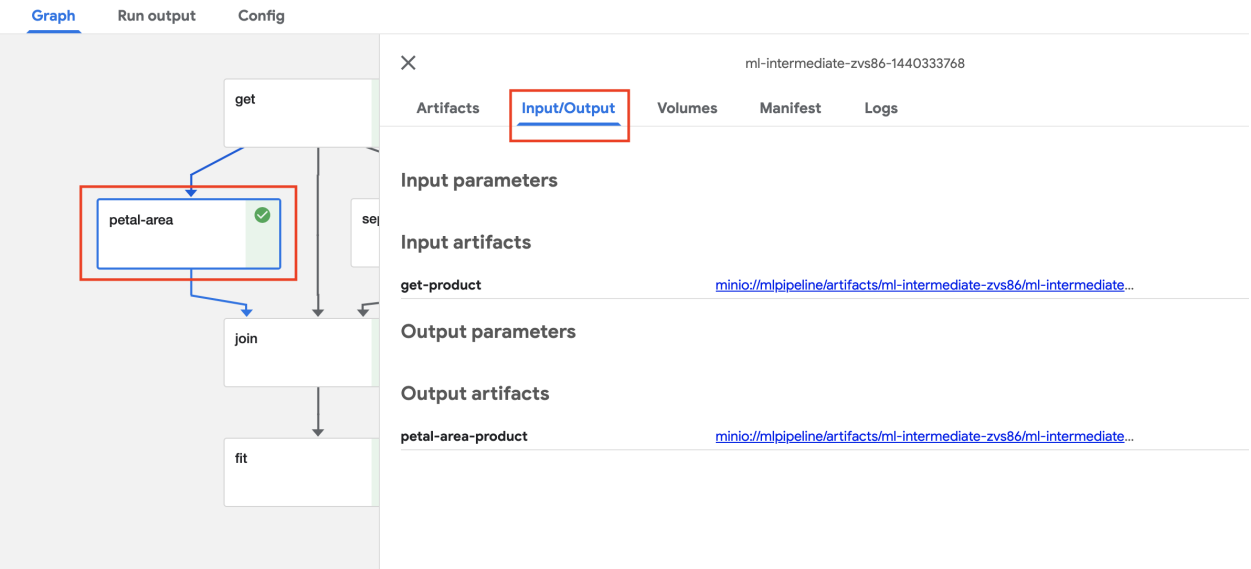
Now we can see that the pipeline is configured, we can see each step and the dependencies, we'll need to submit our first pipeline run. To do that, click on `+ Create run`



The run details should be filled automatically, if not give a run name and the other missing details. On the bottom, click on `Start`.



Now you can watch the pipeline execution by clicking on the run you've created. When the tasks are ready, you can view each task's inputs and outputs, click on the task, and then on the `Input/Output` tab. The links contain the raw files.



Option 2: CLI upload of a Kubeflow pipeline

We need to make sure we have a working notebook on the cluster, we can open it and upload/copy the content of the `kubeflow_pipeline.py` file. Make sure to uncomment the client rows below (6, 7, 10, 135). We'll also need to update the `kfp endpoint` to your cluster and port. Once set we can run the notebook and click on the run link below to get to the pipeline and its run details.

```
kfp_endpoint="YOUR_KFP_ENDPOINT"
client = kfp.Client(kfp_endpoint)

# This is a sanity check to make sure your notebook and cluster can communicate
print(client.list_experiments())from ploomber.clients import S3Client
client.create_run_from_pipeline_func(ml_intermediate, arguments={})
```

4.5 Slurm

Tip: Got questions? Reach out to us on Slack.

This tutorial shows you how to export a Ploomber pipeline to SLURM.

If you encounter any issues with this tutorial, let us know.

4.5.1 Pre-requisites

Important: This integration requires ploomber 0.13.7 or higher and soopervisor 0.6 or higher (To upgrade: `pip install ploomber soopervisor --upgrade`)

- docker and docker-compose

4.5.2 Setting up the project

Note: These instructions are based on this article.

First, let's create a SLURM cluster for testing. Create the following `docker-compose.yml` file:

```
services:
  slurmjupyter:
        image: rancavil/slurm-jupyter:19.05.5-1
        hostname: slurmjupyter
        user: admin
        volumes:
                - shared-vol:/home/admin
        ports:
                - 8888:8888
  slurmmaster:
        image: rancavil/slurm-master:19.05.5-1
        hostname: slurmmaster
        user: admin
        volumes:
                - shared-vol:/home/admin
        ports:
                - 6817:6817
                - 6818:6818
                - 6819:6819
  slurmnode1:
        image: rancavil/slurm-node:19.05.5-1
        hostname: slurmnode1
        user: admin
        volumes:
                - shared-vol:/home/admin
        environment:
                - SLURM_NODENAME=slurmnode1
        links:
                - slurmmaster
  slurmnode2:
        image: rancavil/slurm-node:19.05.5-1
        hostname: slurmnode2
        user: admin
        volumes:
                - shared-vol:/home/admin
        environment:
```

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```
                - SLURM_NODENAME=slurmnode2
        links:
                - slurmmaster
  slurmnode3:
        image: rancavil/slurm-node:19.05.5-1
        hostname: slurmnode3
        user: admin
        volumes:
                - shared-vol:/home/admin
        environment:
                - SLURM_NODENAME=slurmnode3
        links:
                - slurmmaster
volumes:
        shared-vol:
```

Now, start the cluster:

```
docker-compose up -d
```

Important: Ensure you're running a recent version of `docker-compose`, older versions may throw an error like this:

```
Unsupported config option for volumes: 'shared-vol'
Unsupported config option for services: 'slurmmaster'
```

Tip: Once the cluster is up, go http://localhost:8888 to open JupyterLab, where you can edit files, open terminals, and monitor Slurm jobs (Click on Slurm Queue under HPC Tools in the Launcher menu) from your browser.

Let's connect to the cluster to submit the jobs:

```
docker-compose exec slurmjupyter /bin/bash
```

Configure the environment:

```
# Install miniconda (to get a Python environment ready, not needed if
# There's already a Python environment up and running)
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash ~/Miniconda3-latest-Linux-x86_64.sh -b -p $HOME/miniconda

# Init conda
eval "$($HOME/miniconda/bin/conda shell.bash hook)"

# Create and activate env
conda env create --name myenv
conda activate myenv

# install ploomber and soopervisor in the base environment
pip install ploomber soopervisor
```

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```
# Download sample pipeline to example/
ploomber examples -n templates/ml-basic -o example
cd example

# Install project dependencies
pip install -r requirements.txt

# Register a soopervisor environment with the SLURM backend
soopervisor add cluster --backend slurm
```

The `soopervisor add` creates a `cluster/` directory with a `template.sh` file, this is a template that Soopervisor uses to submit the tasks in your pipeline. If should contain the placeholders `{{name}}`, and `{{command}}`, which Soopervisor will replace by the task name and the command to execute such a task, respectively. You can customize it to suit your needs.

For example, since we want the tasks to run in the `conda` environment we created, edit the `template.sh` so it looks like this:

```
#!/bin/bash
#SBATCH --job-name={{name}}
#SBATCH --output=result.out
#

# Activate myenv
conda activate myenv
srun {{command}}
```

We can now submit the tasks:

```
soopervisor export cluster
```

Once jobs finish execution, you'll see the outputs in the `output` directory.

Tip: If you execute `soopervisor export cluster`, only tasks whose source code has changed will be executed again, to force the execution of all tasks, run `soopervisor export cluster --mode force`

Note: When scheduling jobs, `soopervisor` calls the `sbatch` command and passes the `--kill-on-invalid-dep=yes`, this causes tasks to abort if any of its dependencies fails. For example, if you have a `load -> clean` pipeline and `load` fails, `clean` is aborted.

Important: For Ploomber to determine which tasks to schedule, it needs to parse your pipeline and check each task's status. **If your pipeline has functions as tasks**, the Python environment where you execute `soopervisor export` must have all dependencies required to import those functions. e.g., if a function `train_model` uses `sklearn`, then `sklearn` must be installed. If your pipeline only contains scripts/notebooks, this is not required.

Stop the cluster:

```
docker-compose stop
```

4.6 Full workflow

Important: This tutorial requires `soopervisor 0.6.2` or higher, and `soorgeon 0.0.10` or higher.

This tutorial shows how to go from a monolithic Jupyter notebook to a modular, production-ready pipeline deployed in workflow by using the tools in our ecosystem:

1. soorgeon
2. ploomber
3. soopervisor

4.6.1 Pre-requisites

- docker

4.6.2 Building Docker image

We provide a Docker image so you can quickly run this example:

```
# get repository
git clone https://github.com/ploomber/soopervisor
cd soopervisor/tutorials/workflow

# build image
docker build --tag ploomber-workflow .

# create a directory to store the pipeline output
export SHARED_DIR=$HOME/ploomber-workflow
rm -rf $SHARED_DIR
mkdir -p $SHARED_DIR

# start (takes ~1 minute to be ready)
docker run -i -t \
    --privileged=true -v /var/run/docker.sock:/var/run/docker.sock \
    --volume $SHARED_DIR:/mnt/project \
    --env SHARED_DIR \
    --env PLOOMBER_STATS_ENABLED=false \
    -p 2746:2746 \
    -p 8888:8888 \
    ploomber-workflow
```

Note: We need to run `docker run` in privileged mode since we'll be running `docker` commands inside the container. More on that here

Upon initialization, JupyterLab will be running at http://127.0.0.1:8888

4.6.3 Refactor notebook

First, we use `soorgeon` to refactor the notebook:

```
soorgeon refactor nb.ipynb -p /mnt/project/output -d parquet
```

We can generate a plot to visualize the dependencies:

```
ploomber plot
```

If you open the generated `pipeline.png`, you'll see that `soorgeon` inferred the dependencies among the sections in the notebook and built a Ploomber pipeline automatically!

Now you can iterate this modular pipeline with Ploomber, but for now, let's go to the next stage and deploy to Kubernetes.

4.6.4 Configure target platform

Soopervisor allows you to configure the target platform using a `soopervisor.yaml` file, let's add it and set the backend to `argo-worflows`:

```
# soopervisor add requires a requirements.lock.txt file
cp requirements.txt requirements.lock.txt

# add the taget environment
soopervisor add training --backend argo-workflows
```

Usually, you'd manually edit `soopervisor.yaml` to configure your environment; for this example, let's use one that we already configured, which tells soopervisor to mount a local directory to every pod so we can review results later:

```
cp /soopervisor-workflow.yaml soopervisor.yaml
```

4.6.5 Submit pipeline

We finished configuring; let's now submit the workflow:

```
# build docker image and generate an argo's yaml spec
soopervisor export training --skip-tests --ignore-git --mode force

# import image to the k8s cluster
k3d image import project:latest --cluster mycluster

# submit workflow
argo submit -n argo --watch training/argo.yaml
```

Congratulations! You just went from a legacy notebook to production-ready pipeline!

Note: `k3d image import` is only required if creating the cluster with `k3d`.

Once the execution finishes, take a look at the generated artifacts:

```
ls /mnt/project
```

Tip: You may also watch the progress from the UI.

```
# port forwarding to enable the UI
kubectl -n argo port-forward --address 0.0.0.0 svc/argo-server 2746:2746
```

Then, open: https://127.0.0.1:2746

4.6.6 Clean up

To delete the cluster:

```
k3d cluster delete mycluster
```

4.7 AWS Lambda

Note: Got questions? Reach out to us on Slack.

AWS Lambda is a serverless compute service. It allows you to deploy functions in the cloud without worrying about servers or scaling. It is a great (and cheap) option to deploy Machine Learning models.

This tutorial shows you how to deploy a Machine Learning model to AWS Lambda. Unlike other frameworks or tutorials, Soopervisor and Ploomber allow you to deploy complete inference DAGs (as opposed to a model file) without changing your training pipeline's code; handling packaging, containerization and deployment.

If you encounter any issues with this tutorial, let us know.

4.7.1 Pre-requisites

- conda
- sam
- docker
- git
- Install Ploomber with `pip install ploomber`

4.7.2 Training vs. serving pipelines

When training an ML model, you may organize the pipeline in several tasks such as "get data", "clean data", "compute feature 1", "compute feature 2" and "train model".

To deploy the model, you have to provide both a model file and all the necessary feature generation steps. Soopervisor and Ploomber allow you to create an online inference pipeline from a training one without code changes.

In our case, your inference pipeline includes "compute feature 1" and "compute feature 2"; and adds two new tasks: one to receive the input raw data and another one to load a model and make a prediction using the feature vector.

This tutorial will walk you through the development and deployment process.

4.7.3 Setting up project

We'll now fetch an example pipeline:

```
git clone https://github.com/ploomber/projects
cd projects/templates/ml-online/
```

Configure the development environment:

```
ploomber install
```

Then, activate the environment:

```
conda activate ml-online
```

4.7.4 Exploring the example code

Before diving into the code, let's plot our pipeline to have a better idea of its structure:

```
# required to generate plots
conda install pygraphviz --channel conda-forge --yes

# generate plot
ploomber plot
```

Open the generated `pipeline.png` file. The left-most task in the pipeline obtains data for training, then we have a of couple tasks that generate some extra feature, a task that joins all features into a single data frame and one that fits a model.

Those tasks are declared in the `src/ml_online/pipeline.yaml` file. Open the file to review the content, you will see that there are two tasks in the `tasks` section (to get data and to fit the model), the remaining tasks are coming from the `src/ml_online/pipeline-features.yaml`; this separation allows us to convert the feature engineering portion of the pipeline into an inference pipeline without code changes.

Note that for this to work, all feature engineering tasks must be Python functions with a configured `serializer` and `unserializer`. The other tasks can be of any type.

4.7.5 Training a model

Let's now train a model:

```
ploomber build
```

Once the pipeline finishes, copy the trained model from `products/model.pickle` to the standard model location: `src/ml_online/model.pickle`.

```
# on linux/mac
cp products/model.pickle src/ml_online/model.pickle
```

That's it. We're ready to export to AWS Lambda.

4.7.6 Generating files

Let's now create the necessary files to export to AWS Lambda:

```
soopervisor add serve --backend aws-lambda
```

Note: You don't have to install `soopervisor` manually; it should've been installed when running `ploomber install`. If missing, install it with `pip install soopervisor`.

You have to provide a few details before you can run the model in AWS Lambda. First, edit the `serve/test_aws_lambda.py` file. This file contains a unit test to ensure your model works as expected.

The test case is already configured, you only have to replace the line that contains, `body = None` for a sample input value. In our case, it looks like this:

```
body = {
    'sepal length (cm)': 5.1,
    'sepal width (cm)': 3.5,
    'petal length (cm)': 1.4,
    'petal width (cm)': 0.2,
}
```

Important: You should also remove the line that raises the `NotImplementedError`.

Next, we have to tell Lambda, how to handle an incoming API request, this happens in the `serve/app.py` file. The request body is received as a string but our model receives a data frame as input. The sample code already implements a "string to data frame" implementation, hence, you only have to delete the line that raises the `NotImplementedError`. When you use this for your own model, write the applicable parsing logic.

To deploy to AWS Lambda, `soopervisor` packages your code and creates a Docker image. We can build such Docker image (without actually deploying to AWS Lambda) to test our API with the following command:

```
soopervisor export serve --until-build
```

The command will take a few minutes since it has to create a Docker image, subsequent runs will be much faster.

Once finished, you may start the API locally with:

```
cd serve
sam local start-api
```

Open a new terminal and call the API:

```
curl http://127.0.0.1:3000/predict -X POST -d '{"sepal length (cm)": 5.1, "sepal width␣
↪(cm)": 3.5, "petal length (cm)": 1.4, "petal width (cm)": 0.2}'
```

Try calling with other values to get a different prediction

Note: Due to the way the local API is built this will take a few seconds

Congratulations! You just ran Ploomber on AWS Lambda!

Deployment

```
soopervisor export serve
```

explain the –guided thing and add some link

you must be authenticated to use lambda, s3, and CloudFormation

4.7.7 About `template.yaml`

To deploy to Lambda, AWS requires a `template.yaml` file to specify your serverless application. A sample file that configures an API Gateway is provided, but you may need to edit it for your application. Click here to learn more.

4.8 Airflow

Note: This is a quick reference. For a full tutorial, *click here.*

4.8.1 Step 1: Add target environment

Tip: To get a sample pipeline to try this out, see this.

KubernetesPodOperator

```
# add a target environment named 'airflow' (uses KubernetesPodOperator)
soopervisor add airflow --backend airflow
```

Note: Using the `--preset` option requires `soopervisor>=0.7`

```
# add a target environment named 'airflow-k8s' (uses KubernetesPodOperator)
soopervisor add airflow-k8s --backend airflow --preset kubernetes
```

BashOperator

Important: If using `--preset bash`, the `BashOperator` tasks will use `ploomber` CLI to execute your pipeline. Edit the `cwd` argument in `BashOperator` so your DAG runs in a directory where it can import your project's `pipeline.yaml` and source code.

```
# add a target environment named 'airflow-bash' (uses BashOperator)
soopervisor add airflow-bash --backend airflow --preset bash
```

DockerOperator

Important: Due to a bug in the DockerOperator, we must set `enable_xcom_pickling = True` in `airflow.cfg` file. By default, this file is located at `~/airflow/airflow.cfg`.

```
# add a target environment named 'airflow-docker' (uses DockerOperator)
soopervisor add airflow-docker --backend airflow --preset docker
```

4.8.2 Step 2: Generate Airflow DAG

```
# export target environment named 'airflow'
soopervisor export airflow
```

Important: For your pipeline to run successfully, tasks must write their outputs to a common location. You can do this either by creating a shared disk or by adding a storage client. *Click here to learn more.*

4.9 Kubernetes (Argo)

Note: This is a quick reference. For a full tutorial, *click here.*

4.9.1 Step 1: Add target environment

Tip: To get a sample pipeline to try this out, see this.

```
# add a target environment named 'argo'
soopervisor add argo --backend argo-workflows
```

The command above will generate a pre-configured `argo/Dockerfile` and a new entry named `argo` in the `soopervisor.yaml` file. For information on the configuration schema, *click here.*

At the very least, you'll have to modify `repository` to point it to the container repository.

4.9.2 Step 2: Generate Argo Spec (`YAML`)

```
# generate argo yaml spec
soopervisor export argo --skip-tests  --ignore-git
```

The command will build the docker image, push it to the repository and generate an Argo spec at `argo/argo.yaml`.

Note that the command above will only export outdated tasks (the ones whose source code has changed since the last execution), to force exporting all tasks:

```
# force exporting all tasks regardless of status
soopervisor export argo --skip-tests  --ignore-git --mode force
```

Important: For your pipeline to run successfully, tasks must write their outputs to a common location. You can do this either by creating a shared disk or by adding a storage client. *Click here to learn more.*

To submit the workflow:

```
# submit workflow
argo submit -n argo argo/argo.yaml
```

For more information, refer to Argo's CLI documentation.

4.10 SLURM

Note: This is a quick reference. For a full tutorial, *click here.*

4.10.1 Step 1: Add target environment

Tip: To get a sample pipeline to try this out, see this.

```
# add a target environment named 'slurm'
soopervisor add slurm --backend slurm
```

The command above will generate an entry named `slurm` in the `soopervisor.yaml` file, and a `slurm/template.sh` file, you can use the latter to customize how Soopervisor executes the tasks in your pipeline. Under the hood, Soopervisor executes a `sbatch job.sh` command for each task in your pipeline, where `job.sh` is generated by using `template.sh` as a template. For more information and customization options, *click here.*

4.10.2 Step 2: Submit jobs

To submit the jobs to SLURM:

```
# submit pipeline to the cluster
soopervisor export slurm --skip-tests --ignore-git
```

Note that the command above will only export outdated tasks (the ones whose source code has changed since the last execution), to force exporting all tasks:

```
# force exporting all tasks regardless of status
soopervisor export slurm --skip-tests --ignore-git --mode force
```

Important: For your pipeline to run successfully, tasks must write their outputs to a common location. You can do this either by creating a shared disk or by adding a storage client. *Click here to learn more.*

4.11 Task communication

Since `soopervisor` executes tasks in isolated environments, you must provide a way to pass the output files of each task to upcoming tasks that use them as inputs.

There are two ways of doing so: either mount a shared disk on all containers, or configure a `File` client to use remote storage; we describe both options in the next sections.

4.11.1 Shared disk

If using K8s/Argo, you can mount a volume on each pod by adding some configuration to your `soopervisor.yaml` file. Refer to the *Kubernetes* configuration schema documentation for details.

Note that the configuration flexibility is limited; if you need a more flexible approach, you can generate the Argo YAML Spec (by running the `soopervisor export` command), and then edit the generated spec to suit your needs (the spec is generated in `{name}/argo.yaml`, where `{name}` is the name of your target environment).

When using Airflow, the `soopervisor add` generates an output `.py` file with the Airflow DAG, you can edit this file to configure a shared disk and execute `soopervisor export` afterwards. The *Airflow* tutorial shows how to do this, you can see the `.py` file that the tutorial uses here.

To execute pipelines in AWS Batch, you must create a compute environment, map it to a job queue, and include the job queue name in your `soopervisor.yaml` file. You can configure a shared disk using Amazon EFS, click here to learn how to configure EFS in your compute environment.

If running on SLURM, sharing a disk depends on your cluster configuration, so ensure you can mount a disk in all nodes and that your pipeline writes their outputs in the shared disk.

Important: If using a shared disk, execute `soopervisor export` with the `--skip-tests` flag, otherwise Soopervisor will raise an error if your pipeline does not have a `File` client configured.

4.11.2 Using remote storage

As an alternative, you can configure a `File` client to ensure each task has their input files before execution. We currently support Amazon S3 and Google Cloud Storage.

To configure a client, add the following to your `pipeline.yaml` file:

Listing 1: pipeline.yaml

```yaml
# configure a client
clients:
    # note the capital F
    File: clients.get
tasks:
    # content continues...
```

Then, create a `clients.py` file (in the same directory as your `pipeline.yaml`) and declare a `get` function that returns a `File` client instance:

Listing 2: clients.py

```python
from ploomber.clients import S3Client

def get():
    return S3Client(bucket_name='YOUR-BUCKET-NAME',
                    parent='PARENT-FOLDER-IN-BUCKET',
                    json_credentials_path='credentials.json')
```

Click here to see the S3Client documentation.

Listing 3: clients.py

```
from ploomber.clients import GCloudStorageClient

def get():
    return GCloudStorageClient(bucket_name='YOUR-BUCKET-NAME',
                               parent='PARENT-FOLDER-IN-BUCKET',
                               json_credentials_path='credentials.json')
```

Click here to see the GCloudStorageClient documentation.

Next, create a `credentials.json` (in the same directory as your `pipeline.yaml`) with your authentication information. The file should look like this:

```
{
    "aws_access_key_id": "YOUR-ACCESS-KEY-ID",
    "aws_secret_access_key": "YOU-SECRET-ACCESS-KEY"
}
```

```
{
    "type": "service_account",
    "project_id": "project-id",
    "private_key_id": "private-key-id",
    "private_key": "private-key",
    "client_email": "client-email",
    "client_id": "client-id",
    "auth_uri": "https://accounts.google.com/o/oauth2/auth",
    "token_uri": "https://oauth2.googleapis.com/token",
    "auth_provider_x509_cert_url": "https://www.googleapis.com/oauth2/v1/certs",
    "client_x509_cert_url": "https://www.googleapis.com/robot/v1/metadata/x509/service-
↪account.iam.gserviceaccount.com"
}
```

Note: If you're using a Docker-based exporter (K8s/Argo, Airflow, or AWS Batch),you must ensure that your `credentials.json` file is included in your Docker image. You can ensure this by adding the following to your `soopervisor.yaml`

Listing 4: soopervisor.yaml

```yaml
some-name:
    # tell soopervisor to include the credentials.json file
    include: [credentials.json]
    # continues
```

You can check your local configuration by loading your pipeline using `ploomber status`. If you see a table listing your tasks, it means the client has been configured successfully.

Furthermore, when executing the `soopervisor export` command and using a Docker-based exporter (K8s/Argo, Airflow, and AWS Batch), Soopervisor will check that the `File` client in the Docker image is correctly configured by trying to establish a connection with your credentials to the remote storage.

4.12 Docker building process

Note: This guide does not apply if using SLURM.

4.12.1 Installing dependencies

To install dependencies in the Docker image, Soopervisor looks for a `requirements.lock.txt` (if using pip) or an `environment.lock.yml` (if using conda). Although not strictly enforced, such files should contain specific versions of each dependency so that breaking changes from any dependency do not break the pipeline. For example, if your project uses `ploomber`, `pandas`, and `scikit-learn`; your dependencies may look like this:

```
ploomber
pandas
scikit-learn
```

```yaml
dependencies:
  - ploomber
  - pandas
  - scikit-learn
```

The `lock` files generated from such files look like this:

```
ploomber==0.11
pandas==1.2.4
scikit-learn==0.24.2
# many other lines...
```

```yaml
dependencies:
  - ploomber==0.11
  - pandas==1.2.4
  - scikit-learn==0.24.2
  # many other lines...
```

You can generate such files with the following commands:

```
pip freeze > requirements.lock.txt
```

```
conda env export --no-build --file environment.lock.yml
```

Tip: If you use `ploomber install`, `lock` files are automatically generated.

4.12.2 Included files

To export to any of the supported platforms, Soopervisor creates a Docker image from your project. In most cases, there are files in your project that you want to exclude from the Docker image to reduce its size. Common examples are: virtual environments, data files, or exploratory notebooks.

The process to determine which files to include changes if your project isn't a package (i.e., there isn't a `setup.py` file) file or it is a package.

Non-packaged projects

If your project isn't a package and you're using git, Soopervisor copies every file tracked by your repository. To see the list of currently tracked files, run the following command:

```
git ls-tree -r HEAD --name-only
```

This means that you can control what file goes into the Docker image by changing your `.gitignore` file. If there are git tracked that you want to exclude, use the `exclude` key in `soopervisor.yaml`

```
some-target:
    exclude:
        - file-to-exclude.txt
```

Note: If you're not using git, all files are copied into the Docker image by default. You can control what to exclude using the `exclude` key.

If there are files that git ignores but you want to include, use the `include` key:

```
some-target:
    include:
        - file-to-include.txt
```

Tip: It's recommended that you use `.gitignore` to control which files to exclude. The `include` and `exclude` keys in `soopervisor.yaml` should only be used to list a few particular files.

Packaged projects

If your project is a package (i.e., it has a `setup.py` file), a source distribution is generated and copied into the Docker image. This implies that the process to control which files are included is the same used to control which files to include in a source distribution. Unfortunately, there is more than one way to do this. The most reliable way is to use a `MANIFEST.in` file, click here to learn more.

Tip: You can use `ploomber scaffold --package` to quickly generate a pre-configured base packaged project. You can then modify the `MANIFEST.in` file to customize your build.

4.13 Non-packaged vs Packaged

Soopervisor supports two types of projects: non-packaged and packaged.

4.13.1 Non-packaged

Non-packaged are simpler projects that require fewer configuration files. They only need a `pipeline.yaml` file to be valid. Non-packaged projects are a good option for small projects. To create one:

```
# create a base non-packaged project
ploomber scaffold
```

4.13.2 Packaged

Packaged projects have more structure and require more configuration files. The main advantage is they allow you to organize your work better.

For example, if you have some Python modules that you reuse in several files, you must to modify your `PYTHONPATH` or `sys.path` to ensure that such modules are importable. If your project is packaged, this isn't necessary, since you can install your project with pip:

```
pip install --editable path/to/myproject
```

After installation, you can import modules from your project anywhere in a Python session, notebook, or other modules inside your project, making it simpler to create modular code.

To create a base package project:

```
# create a base packaged project
ploomber scaffold --package
```

4.14 Command line interface

Soopervisor has two commands, `add` and `export`.

4.14.1 `soopervisor add`

Adds a new target environment:

```
soopervisor add {name} --backend {backend}
```

- `{name}` is any identifier you want to identify this configuration
- `{backend}` is one of `aws-batch`, `aws-lambda`, `argo-workflows`, `airflow`, or `slurm`

The command adds a new section in a `soopervisor.yaml` file (creates one if needed) with the `{name}`, and adds a few necessary files in a `{name}` directory.

Example:

```
soopervisor add train-cluster --backend argo-workflows
```

4.14.2 `soopervisor export`

Exports a target environment:

```
soopervisor export {name}
```

Where `{name}` is the name of a target environment.

`soopervisor export` has a few options.

Execution mode: `--mode {mode}/ -m`

- `incremental` (default) only export tasks whose source has changed.
- `regular` all tasks are exported, status (execute/skip) determined at runtime.
- `force` all tasks are exported and executed regardless of status.

Example:

```
soopervisor export train-cluster --mode force
```

`--ignore-git / -i`

Note: `--ignore-git` has no effect when using SLURM

If you are using `soopervisor` inside a git repository, `soopervisor` will only copy the files tracked by your repository into the Docker image. For example, if you have a `secrets.json` file, but your `.gitignore` file has a `secrets.json` entry, `soopervisor` wil not copy it to the Docker image. If you pass `--ignore-git`, **the status of your git repository is ignored and all files are copied.**

Example:

```
soopervisor export train-cluster --ignore-git
```

`--skip-tests / -s`

Note: `--skip-tests` has no effect when using SLURM

Soopervisor tests the pipeline before submitting, for example, it checks that a `File.client` is configured, use this flag to **skip docker image tests**:

Example:

```
soopervisor export train-cluster --skip-tests
```

4.15 Kubernetes

Configuration schema for Kubernetes.

4.15.1 Example

Listing 5: soopervisor.yaml

```
k8s-config:
  exclude: [my-venv/]
  repository: my-docker.repository.io/some-name
  mounted_volumes:
    - name: shared-folder
      spec:
        hostPath:
          path: /host
```

The above `soopervisor.yaml`, translates into the following Argo spec:

Listing 6: argo.yaml

```
  apiVersion: argoproj.io/v1alpha1
  kind: Workflow
  spec:
    templates:
      script:
        volumeMounts:
        - mountPath: /mnt/shared-folder
          name: shared-folder
          subPath: ''
        # continues ...
    - dag:
        tasks:
          # continues...
    volumes:
```

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```
    - hostPath:
        path: /host
      name: shared-folder
```

4.15.2 Schema

class soopervisor.abc.**AbstractConfig**
Abstract class for configuration objects

Parameters **preset** (*str*) – The preset to use, this determines certain settings and is backend-specific

class soopervisor.argo.config.**ArgoConfig**
Configuration for exporting to Argo

Parameters

- **repository** (*str*) – Repository for uploading the Docker image.

  Important: If `repository` is `null`, it sets the `imagePullPolicy` in the generated spec to `Never`.

- **mounted_volumes** (*list, optional*) – List of volumes to mount on each Pod, described with the `ArgoMountedVolumes` schema.

class soopervisor.argo.config.**ArgoMountedVolume**
Volume to mount in the Pod at `/mnt/{name}`

Parameters

- **name** (*str*) – Volume's name
- **sub_path** (*str, default=''*) – Sub path from the volume to mount in the Pod (set in `volumeMounts[*].subPath`). Defaults to the volume's root
- **spec** (*dict*) – The volume spec, passed directly to the output spec. e.g: `{'persistentVolumeClaim': {'claimName': 'someName'}}`

4.16 SLURM

4.16.1 The `template.sh` file

When using SLURM as backend, the `soopervisor add {env-name}` command wil create an `{env-name}/template.sh` file.

Under the hood, Soopervisor uses the `template.sh` for all tasks in your pipeline and executes a `sbatch job.sh` command for each one.

`template.sh` contains two placeholders `{{name}}` and `{{command}}`, these placeholders are mandatory and should not be removed, at runtime Soopervisor will replace them with the name of the task and the command execute, one per task in your pipeline. However, you may add other commands to `template.sh` to customize execution. Typically, you'll have to add any preparation steps, like activating a virtual environment:

```
#!/bin/bash
#SBATCH --job-name={{name}}
#SBATCH --output=result.out
#

# activate conda environment
conda activate myenv
# execute task
srun {{command}}
```

4.16.2 Customizing task execution

You may want to use different settings for each task in your pipeline in some scenarios. To achieve that, you can add more files next to the `template.sh` file, and Soopervisor will choose which one to use depending on the task's name.

The resolution logic is as follows. Say you have a task named `fit-gpu`:

1. Look for an exact match (i.e., `fit-gpu.sh`)
2. Look for a file with a double underscore placeholder (e.g., `fit-__.sh`, or `__-gpu.sh`)
3. If no matches, use `template.sh`

You can use this templating feature to customize the submitted jobs, for example to pass custom parameters to the `srun` command.

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