Keeping your Jupyter notebook code quality bar high (and production ready) with Ploomber

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This paper walks through this interactive tutorial. It is highly recommended running this interactively so it's easier to follow and see the results in real-time. There's a binder link in there as well, so you can launch it instantly.

1. Introduction

Notebooks are an excellent environment for data exploration: they allow us to write code interactively and get visual feedback, providing an unbeatable experience for understanding our data.

However, this convenience comes at a cost; if we are not careful about adding and removing code cells, we may have an irreproducible notebook. Arbitrary execution order is a prevalent problem: a recent analysis found that about 36% of notebooks on GitHub did not execute in linear order. To ensure our notebooks run, we must continuously test them to catch these problems.

A second notable problem is the size of notebooks: the more cells we have, the more difficult it is to debug since there are more variables and code involved.

Software engineers typically break down projects into multiple steps and test continuously to prevent broken and unmaintainable code. However, applying these ideas for data analysis requires extra work; multiple notebooks imply we have to ensure the output from one stage becomes the input for the next one. Furthermore, we can no longer press "Run all cells" in Jupyter to test our analysis from start to finish.

Ploomber provides all the necessary tools to build multi-stage, reproducible pipelines in Jupyter that feel like a single notebook. Users can easily break down their analysis into multiple notebooks and execute them all with a single command.

2. Refactoring a legacy notebook

If you already have a python project in a single notebook, you can use our tool Soorgeon to automatically refactor it into a Ploomber pipeline. Soorgeon statically analyzes your code, cleans up unnecessary imports, and makes sure your monolithic notebook is broken down into smaller components. It does that by scanning the markdown in the notebook and analyzing the headers; each H2 header in our example is marking a new self-contained task.

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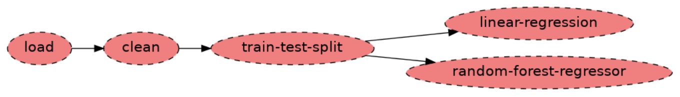


***Fig. 1:** In this pipeline none of the tasks were executed - it's all red.*

In addition, it can transform a notebook to a single-task pipeline and then the user can split it into smaller tasks as they see fit.

To refactor the notebook, we use the `soorgeon refactor` command:

```
soorgeon refactor nb.ipynb
```

After running the refactor command, we can take a look at the local directory and see that we now have multiple python tasks which that are ready for production:

```
ls playground
```

We can see that we have a few new files. `pipeline.yaml` contains the pipeline declaration, and `tasks/` contains the *stages* that Soorgeon identified based on our H2 Markdown headings:

```
ls playground/tasks
```

One of the best ways to onboard new people and explain what each workflow is doing is by plotting the pipeline (note that we're now using `ploomber`, which is the framework for developing pipelines):

```
ploomber plot
```

This command will generate the plot below for us, which will allow us to stay up to date with changes that are happening in our pipeline and get the current status of tasks that were executed or failed to execute.

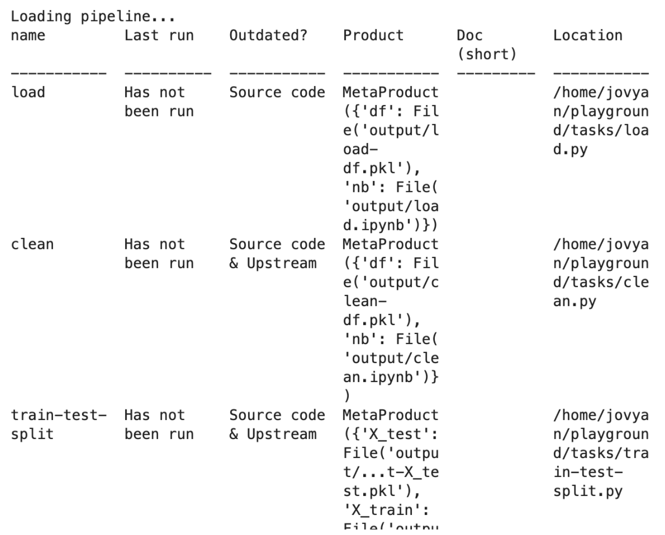
Soorgeon correctly identified the *stages* in our original `nb.ipynb` notebook. It even detected that the last two tasks (`linear-regression`, and `random-forest-regressor`) are independent of each other!

We can also get a summary of the pipeline with `ploomber status`:

```
cd playground
ploomber status
```

3. The `pipeline.yaml` file

To develop a pipeline, users create a `pipeline.yaml` file and declare the tasks and their outputs as follows:



```
Loading pipeline...
name         Last run    Outdated?    Product      Doc          Location
                                                   (short)
-----------  ----------  -----------  -----------  ---------  -----------
load         Has not     Source code  MetaProduct               /home/jovya
             been run                 ({'df': Fil               n/playgroun
                                      e('output/l               d/tasks/loa
                                      oad-                      d.py
                                      df.pkl'),
                                      'nb': File(
                                      'output/loa
                                      d.ipynb')})
clean        Has not     Source code  MetaProduct               /home/jovya
             been run    & Upstream   ({'df': Fil               n/playgroun
                                      e('output/c               d/tasks/cle
                                      lean-                     an.py
                                      df.pkl'),
                                      'nb': File(
                                      'output/cle
                                      an.ipynb')}
                                      )
train-test-  Has not     Source code  MetaProduct               /home/jovya
split        been run    & Upstream   ({'X_test':               n/playgroun
                                      File('outpu               d/tasks/tra
                                      t/...t-X_te               in-test-
                                      st.pkl'),                 split.py
                                      'X_train':
                                      File('outpu
```

Fig. 2: In here we can see the status of each of our pipeline's tasks, runtime and location.

```yaml
tasks:
  - source: script.py
    product:
      nb: output/executed.ipynb
      data: output/data.csv

  # more tasks here...
```

The previous pipeline has a single task (`script.py`) and generates two outputs: `output/executed.ipynb` and `output/data.csv`. You may be wondering why we have a notebook as an output: Ploomber converts scripts to notebooks before execution; hence, our script is considered the source and the notebook a byproduct of the execution. Using scripts as sources (instead of notebooks) makes it simpler to use git. However, this does not mean you have to give up interactive development since Ploomber integrates with Jupyter, allowing you to edit scripts as notebooks.

In this case, since we used `soorgeon` to refactor an existing notebook, we did not have to write the `pipeline.yaml` file.

4. Building the pipeline

Let's build the pipeline (this will take ~30 seconds):

```
cd playground
ploomber build
```

We can see which are the tasks that ran during this command, how long they took to execute, and the contributions of each task to the overall pipeline execution runtime.

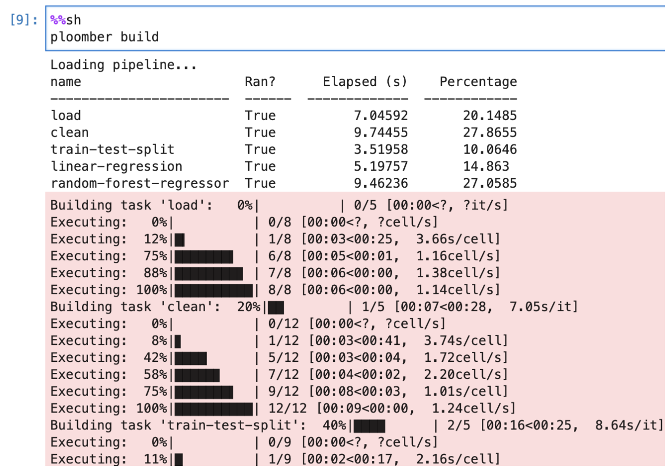
Navigate to `playground/output/` and you'll see all the outputs: the executed notebooks, data files and trained model.

```
ls playground/output
```

In this figure, we can see all of the data that was collected during the pipeline, any artifacts that might be useful to the user, and some of the execution history that is saved on the notebook's context.

5. Testing and quality checks

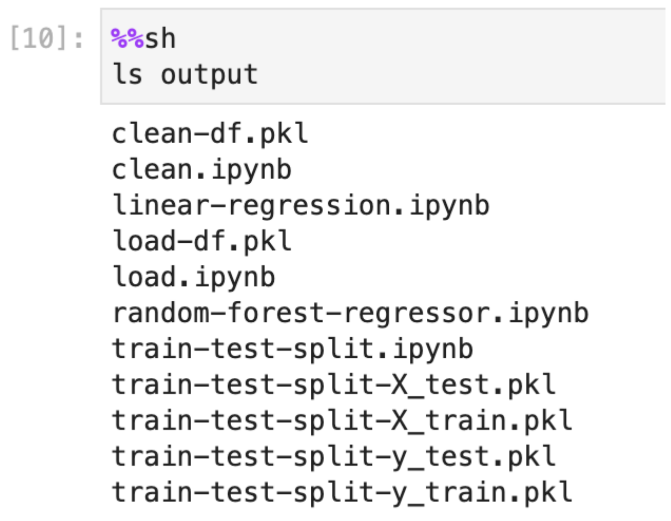
** Open *tasks/train-test-split.py* as a notebook by right-clicking on it and then *Open With -> Notebook* and add the following code after the cell with *# noqa*:



```
[9]: %%sh
     ploomber build
```

```
Loading pipeline...
name                     Ran?      Elapsed (s)    Percentage
-----------------------  ------  -------------  ------------
load                     True          7.04592       20.1485
clean                    True          9.74455       27.8655
train-test-split         True          3.51958       10.0646
linear-regression        True          5.19757       14.863
random-forest-regressor  True          9.46236       27.0585
Building task 'load':   0%|          | 0/5 [00:00<?, ?it/s]
Executing:   0%|          | 0/8 [00:00<?, ?cell/s]
Executing:  12%|█         | 1/8 [00:03<00:25,  3.66s/cell]
Executing:  75%|███████▌  | 6/8 [00:05<00:01,  1.16cell/s]
Executing:  88%|████████▊ | 7/8 [00:06<00:00,  1.38cell/s]
Executing: 100%|██████████| 8/8 [00:06<00:00,  1.14cell/s]
Building task 'clean':  20%|██        | 1/5 [00:07<00:28,  7.05s/it]
Executing:   0%|          | 0/12 [00:00<?, ?cell/s]
Executing:   8%|▊         | 1/12 [00:03<00:41,  3.74s/cell]
Executing:  42%|████▏     | 5/12 [00:03<00:04,  1.72cell/s]
Executing:  58%|█████▊    | 7/12 [00:04<00:02,  2.20cell/s]
Executing:  75%|███████▌  | 9/12 [00:08<00:03,  1.01s/cell]
Executing: 100%|██████████| 12/12 [00:09<00:00,  1.24cell/s]
Building task 'train-test-split':  40%|████      | 2/5 [00:16<00:25,  8.64s/it]
Executing:   0%|          | 0/9 [00:00<?, ?cell/s]
Executing:  11%|█         | 1/9 [00:02<00:17,  2.16s/cell]
```

Fig. 3: Here we can see the build outputs



```
[10]: %%sh
      ls output
```

```
clean-df.pkl
clean.ipynb
linear-regression.ipynb
load-df.pkl
load.ipynb
random-forest-regressor.ipynb
train-test-split.ipynb
train-test-split-X_test.pkl
train-test-split-X_train.pkl
train-test-split-y_test.pkl
train-test-split-y_train.pkl
```

Fig. 4: These are the post build artifacts

```python
# Sample data quality checks after loading the raw data
# Check nulls
assert not df['HouseAge'].isnull().values.any()

# Check a specific range - no outliers
assert df['HouseAge'].between(0,100).any()

# Exact expected row count
assert len(df) == 11085
```

** We'll do the same for *tasks/linear-regression.py*, open the file and add the tests:

```python
# Sample tests after the notebook ran
# Check task test input exists
assert Path(upstream['train-test-split']['X_test']).exists()

# Check task train input exists
assert Path(upstream['train-test-split']['y_train']).exists()

# Validating output type
assert 'pkl' in upstream['train-test-split']['X_test']
```

Adding these snippets will allow us to validate that the data we're looking for exists and has the quality we expect. For instance, in the first test we're checking there are no missing rows, and that the data sample we have are for houses up to 100 years old.

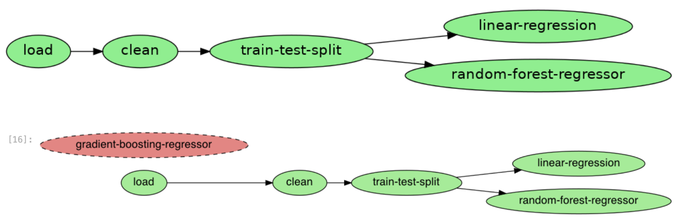


***Fig. 5:** Now we see an independent new task*

In the second snippet, we're checking that there are train and test inputs which are crucial for training the model.

6. Maintaining the pipeline

Let's look again at our pipeline plot:

```
Image('playground/pipeline.png')
```

The arrows in the diagram represent input/output dependencies and depict the execution order. For example, the first task (`load`) loads some data, then `clean` uses such data as input and processes it, then `train-test-split` splits our dataset into training and test sets. Finally, we use those datasets to train a linear regression and a random forest regressor.

Soorgeon extracted and declared this dependencies for us, but if we want to modify the existing pipeline, we need to declare such dependencies. Let's see how.

We can also see that the pipeline is green, meaning all of the tasks in it have been executed recently.

7. Adding a new task

Let's say we want to train another model and decide to try Gradient Boosting Regressor. First, we modify the `pipeline.yaml` file and add a new task:

Open `playground/pipeline.yaml` and add the following lines at the end

```
- source: tasks/gradient-boosting-regressor.py
  product:
    nb: output/gradient-boosting-regressor.ipynb
```

Now, let's create a base file by executing `ploomber scaffold`:

```
cd playground
ploomber scaffold
```

This is the output of the command: ` `Found spec at 'pipeline.yaml' Adding /Users/ido/ploomber-workshop/playground/ tasks/ gradient-boosting-regressor.py... Created 1 new task sources.` `

We can see it created the task sources for our new task, we just have to fill those in right now.

Let's see how the plot looks now:

```
cd playground
ploomber plot
```

You can see that Ploomber recognizes the new file, but it does not have any dependency, so let's tell Ploomber that it should execute after `train-test-split`:

Open

```
playground/tasks/gradient-boosting-regressor.py
```

as a notebook by right-clicking on it and then `Open With -> Notebook`:

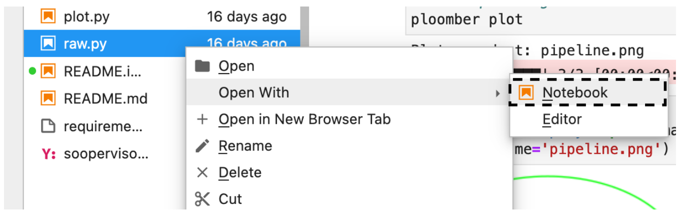


***Fig. 6:** lab-open-with-notebook*

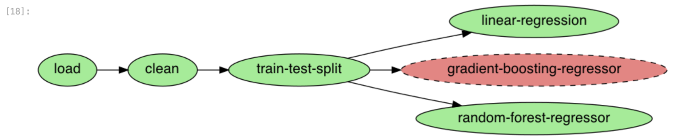


***Fig. 7:** The new task is attached to the pipeline*

At the top of the notebook, you'll see the following:

```
upstream = None
```

This special variable indicates which tasks should execute before the notebook we're currently working on. In this case, we want to get training data so we can train our new model so we change the `upstream` variable:

```
upstream = ['train-test-split']
```

Let's generate the plot again:

```
cd playground
ploomber plot
```

Ploomber now recognizes our dependency declaration!

Open

```
playground/tasks/gradient-boosting-regressor.py
```

as a notebook by right-clicking on it and then `Open With -> Notebook` and add the following code:

```
from pathlib import Path
import pickle

import seaborn as sns
from sklearn.ensemble import GradientBoostingRegressor

y_train = pickle.loads(Path(
   upstream['train-test-split']['y_train']).read_bytes())
y_test = pickle.loads(Path(
   upstream['train-test-split']['y_test']).read_bytes())
X_test = pickle.loads(Path(
   upstream['train-test-split']['X_test']).read_bytes())
X_train = pickle.loads(Path(
   upstream['train-test-split']['X_train']).read_bytes())

gbr = GradientBoostingRegressor()
gbr.fit(X_train, y_train)

y_pred = gbr.predict(X_test)
sns.scatterplot(x=y_test, y=y_pred)
```

8. Incremental builds

Data workflows require a lot of iteration. For example, you may want to generate a new feature or model. However, it's wasteful to re-execute every task with every minor change. Therefore, one of Ploomber's core features is incremental builds, which automatically skip tasks whose source code hasn't changed.

Run the pipeline again:

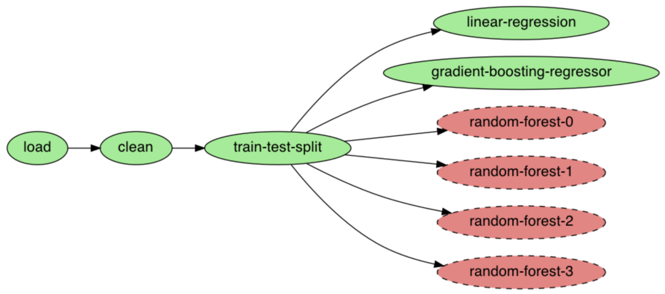


Fig. 8: *We can see this pipeline has multiple new tasks.*

```
cd playground
ploomber build
```

You can see that only the `gradient-boosting-regressor` task ran!

Incremental builds allow us to iterate faster without keeping track of task changes.

Check out `playground/output/gradient-boosting-regressor.ipynb`,

which contains the output notebooks with the model evaluation plot.

9. Parallel execution and Ploomber cloud execution

This section can run locally or on the cloud. To setup the cloud we'll need to register for an api key

Ploomber cloud allows you to scale your experiments into the cloud without provisioning machines and without dealing with infrastrucutres.

Open *playground/pipeline.yaml* and add the following code instead of the source task:

```
- source: tasks/random-forest-regressor.py
```

This is how your task should look like in the end

```
- source: tasks/random-forest-regressor.py
  name: random-forest-
  product:
    nb: output/random-forest-regressor.ipynb
  grid:
        # creates 4 tasks (2 * 2)
        n_estimators: [5, 10]
        criterion: [gini, entropy]
```

In addition, we'll need to add a flag to tell the pipeline to execute in parallel. Open *playground/pipeline.yaml* and add the following code above the *-tasks* section (line 1):

yaml

# Execute independent tasks in parallel executor: parallel

```
ploomber plot
```

```
ploomber build
```

10. Execution in the cloud

When working with datasets that fit in memory, running your pipeline is simple enough, but sometimes you may need more computing power for your analysis. Ploomber makes it simple to execute your code in a distributed environment without code changes.

Check out Soopervisor, the package that implements exporting Ploomber projects in the cloud with support for:

- Kubernetes (Argo Workflows)
- AWS Batch
- Airflow

11. Resources

Thanks for taking the time to go through this tutorial! We hope you consider using Ploomber for your next project. If you have any questions or need help, please reach out to us! (contact info below).

Here are a few resources to dig deeper:

- GitHub
- Documentation
- Code examples
- JupyterCon 2020 talk
- Argo Community Meeting talk
- Pangeo Showcase talk (AWS Batch demo)
- Jupyter project

10. Contact

- Twitter
- Join us on Slack
- E-mail us