flo Documentation

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flo is a data workflow utility that is specifically designed to enable rapid iteration and development of complex data pipelines. Its *command line interface* and *task configuration* have many features that make flo ideal for developing data workflows, among them:

- flo hashes the state of each file that it monitors to make it amenible to working with how most distributed version control systems work.
- flo times each step of the analysis, *making it easy to determine how long any particular run will take* before flo does anything.
- flo comes with *command line autocompletion builtin*, making it easy to evaluate your options quickly in the terminal.
- flo's *task configuration is written in YAML*, making it easy to read and write without having to know an *archaic language* (sorry make, its not you, its me).
- flo is written in python, which is a native language to most data-savvy users to make it as easy as possible to maintain by the community.

If you're sold, *get started*. If not, read on:

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op-ed

We built flo because existing tools were not cutting it for us and we kept finding ourselves saying things like:

"It should be easy to swap in development data for production data." - @bo_p

"It should be easy to work on one file at a time." - @mstringer

"It should be easy to avoid making costly mistakes." - @deanmalmgren

There are many ways one could conceivably write a data analysis workflow from scratch, from writing single programs that ingest, analyze and visualize data to simple scripts that each handle one part of the puzzle. Particularly when developing workflows from scratch, we have the strong opinion that writing small scripts with intermediate outputs is a much more effective way to develop a prototype data workflow. In our experience, we find it to be very convenient to edit a script, run it, and repeat several times to make sure it is behaving the way we intend. For one thing, this pattern makes it far easier to spot check results using a litany of available command line tools. For another, this pattern makes it easy to identify weak links (*e.g.* incorrect results, poor performance, etc.) in the analysis and improve them piece by piece after the entire workflow has been written the first time.

1.1 design goals

This package is deliberately designed to help users write small, but compact workflow prototypes using whatever tools they prefer — R, pandas, scipy, hadoop. The goal here is not to provide a substitute for these tools, but rather to be the glue that sticks them together. It takes inspiration from a number of *existing tools* that have similar aims, particularly *GNU make* that has many desirable properties of working with data workflows. Specifically, the design goals for this project are to:

- Provide an easy-to-use framework. This applies for n00bs and pros alike. Use human-readable syntax.
- Prevent, as much as reasonably possible, costly mistakes. Avoid inadvertently rerunning commands that overwrite results or executing commands that take a long time.
- Encourage good development practices, but allow for flexibility. There's a tradeoff here, but we have an opinion on how to do this in a good way.

1.2 prior art

1.2.1 GNU make

GNU make is a very useful tool that was designed mostly for building complicated software packages. It works particularly well when you are compiling a bunch of .c or .h files into .o files because you can use rules to define

how .o files are created from a bunch of dependencies (and usually not too many of them). I've used this to manage data workflows too and, provided you're only working by yourself and you are comfortable with its arcane file format, make is a great tool. A few things make make less desireable, particularly for managing data workflows that tend to take hours or days rather than minutes.

- make uses timestamps, instead of hashes, to determine when a file is out of date with the rest. This isn't so terrible, except when you're working in an asynchronous development environment with hg or git that does not version the timestamp of files.
- Makefiles are extraordinarily picky and not terribly easy for n00bs to use. Even for those that are fluent in Makefile, looking over a Makefile is pretty cumbersome and not easy to read. This is a downer when you're trying to rapidly develop.
- make does not run in parallel or, if it does, it requires a deeper understanding of its arcane format than I am
 comfortable with. Particularly with data workflows that can potentially take days to complete, this is a very
 undesireable behavior.
- make is filesystem based, but doesn't have the ability to test whether databases or cloud storage has been updated. This is pretty important for data workflows.

1.2.2 invoke

Invoke is intended to be a make replacement for python with a nice Fabric-like command line interface. It is function/class based rather than file based and, because its in python, you can basically do anything you need to within an invoke script. Downsides include:

- Because its function/class based, there is a lot of syntactic bloat that does not make invoke scripts considerably longer than they need to be.
- Although invoke does provide a 'pre' keyword argument, it is not possible to run an invoke script without rerunning the *entire* workflow (git issue here). Although its certainly possible to extend invoke to address this use case, its not clear that it'll be enough to address all the use cases that we have in mind.

1.2.3 Fabric

Fabric is a tool that is intended for application deployment to many different servers simultaneously. It has a great command-line interface for deployment and DevOps, but doesn't provide a lot of out-of-the box functionality for managing data workflows. Downsides include:

- Fabric parallelizes tasks across machines, not tasks. In data analysis situations, you can actually divvy up analysis tasks depending on what data files are or not available.
- fabfiles tend to get big rather quickly, even for relatively mundane jobs. The fact that its in python is nice, but probably not necessary for running a data analysis workflow.
- There is no default way of detecting whether a task needs to be run based on timestamps or hashes. Its certainly possible to extend Fabric to address this issue.

1.2.4 **Drake**

Drake is intended to be the "make for data". Drakefiles have a very similar look and feel of Makefiles. It has some pretty decent advantages over make in that it comes pre-equipped with parallelization and with filesystem, S3 and HDFS integration, but there are a few key disadvantages:

• It is based on timestamps. This makes it tricky to develop when working in an asynchronous development environment like hg or git.

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• Its written in clojure, which makes it difficult for most data people to contribute too (?), or at least difficult for this data person to read.

1.2.5 AWS Data Pipeline

Amazon's Data Pipeline is intended to organize data pipelines that occur entirely in Amazon's cloud. This seems extremely handy if you're playing entirely within Amazon's walls, but not terribly convenient for a wide range or projects where a cloud solution is unnecessarily overkill.

1.2.6 LONI Pipeline

Meh. http://pipeline.bmap.ucla.edu/

1.2.7 Predictive Modeling Markup Language (PMML)

PMML is a language to define workflows in data analysis. There appear to be many tools that will execute PMML workflows, for example Augustus and Zementis for executing on Amazon Web Services. It appears to be geared more toward developing robust, "enterprise" workflows as opposed to rapid development.

1.2.8 Tez

Tez appears to be the Hadoop equivalent of creating data workflows using YARN. If you're nuts about java and everything you do is in hadoop, this is probably great for you.

1.2.9 KNIME

KNIME is a graphical interface for defining data *and* analysis steps in a data workflow. I'm sure its possible to write custom analysis steps in KNIME to make it more practical in real world situations, but the tight coupling between the pipeline definition and actually running an analysis and doing some visualization is highly unappealing for the use cases I have in mind. Nonetheless, its worth mentioning. The GUI is admittedly kinda nice and certainly easier to understand for n00bs.

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quick start

1. Install this package.

pip install flo

- 2. Write a flo.yaml. Create a flo.yaml file in the root of your project. flo.yaml can have many features, but the basic idea is to make it easy to quickly define a sequence of dependent tasks in an easy-to-read way. There are several examples, the simplest of which is the hello-world example. Briefly, every task is a YAML object that has a creates key that represents the resource that is created by this task and a command key that defines the command that are required to create the resource defined in creates. You can optionally define a depends key that lists resources, either filenames on disk or other task creates targets, to quickly set up dependency chains.
- 3. Execute your workflow. From the same directory as the flo.yaml file (or any subdirectory), execute flo run and this will run each task defined in your flo.yaml until everything is complete. If any task definition in the flo.yaml or the contents of its dependencies change, re-running flo run will only redo the parts of the workflow that are out of sync since the last time you ran it. The flo command has several other convenience options to facilitate quickly writing data workflows. Running the hello-world example for the first time yields something like this:
- 4. Repeat steps 2-3 until your data workflow is complete. When developing a data workflow, it is common to write an entire workflow and then go back and revisit particular parts of the analysis. The entire purpose of this package is to make it easy to refine task definitions and quickly re-run workflows with confidence that the user will not ruin previous results or start a simulation that takes a long time.

flo.yaml specification

Individual analysis tasks are defined as YAML objects in a file named flo.yaml (or whatever you prefer) with something like this:

```
creates: "path/to/some/output/file.txt"
depends: "path/to/some/script.py"
command: "python {{depends}} > {{creates}}"
```

Every YAML object that defines a task must have *creates* and *command* keys and can optionally contain a *depends* key. The order of these keys does not matter; the above order is chosen for explanatory purposes only.

3.1 creates

The creates key uniquely identifies the resource that is created. By default, it is interpreted as a path to a file (relative paths are interpreted as relative to the flo.yaml file) or a directory. Importantly, every task is intended to create a single file or directory. If you have a task that creates multiple files, you can either (i) split that into separate tasks or (ii) have all of those files embedded in a directory and use the directory name as the creates value like this:

In this case, the directory path/to/output/directory is passed as the first argument to path/to/some/script.py, which can then add as many files as necessary to that directory. When this task is complete, flo checks the hash of all files in path/to/output/directory and all of its child directories to determine if it is in sync or not.

3.2 depends

The depends key defines the resource(s) on which this task depends. It is common for depends to specify many things, including data analysis scripts or other tasks from within the flo.yaml. Multiple dependencies can be defined in a YAML list like this:

```
depends:
```

```
- "path/to/some/script.py"
```

^{- &}quot;another/task/creates/target.txt"

These dependencies are what flo uses to determine if a task is out of sync and needs to be re-executed. Importantly, flo obeys the dependencies when it constructs the task graph but always runs in a *deterministic order*. If a specified depends does not exist immediately prior to flo running the task, flo throws an informative error.

3.3 command

The command key is mandatory and it defines the command(s) that should be executed to produce the resource specified by the creates key. Like the depends key, multiple steps can be defined in a YAML list like this:

```
command:
   - "mkdir -p $(dirname {{creates}})"
   - "python {{depends}} > {{creates}}"
```

3.4 templating variables

Importantly, the command is rendered as a jinja template to avoid duplication of information that is already defined in that task. Its quite common to use { depends } and { creates } in the command specification, but you can also use other variables like this:

```
creates: "path/to/some/output/file.txt"
sigma: "2.137"
depends: "path/to/some/script.py"
command: "python {{depends}} {{sigma} > {{creates}}}"
```

In the aforementioned example, sigma is only available when rendering the jinja template for that task. If you'd like to use sigma in several other tasks, you can alternatively put it in a global namespace in a flo.yaml like this (similar example here):

```
sigma: "2.137"
tasks:

creates: "path/to/some/output/file.txt"
  depends: "path/to/some/script.py"
  command: "python {{depends}} {{sigma} > {{creates}}"

creates: "path/to/another/output/file.txt"
  depends:
    - "path/to/another/script.py"
    - "path/to/some/output/file.txt"
  command: "python {{depends[0]}} {{sigma}} < {{depends[1]}} > {{creates}}"
```

Another common use case for global variables is when you have several tasks that all depend on the same file. You can also use jinja templating in the creates and depends attributes of your flo.yaml like this:

```
creates: "data/names.dat"
depends:
    - "src/extract_names.py"
    - "{{input}}"
command: "python {{depends|join(' ')}} > {{creates}}"

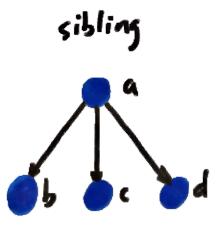
creates: "data/symbols.dat"
depends:
    - "src/extract_symbols.py"
    - "{{input}}"
command: "python {{depends|join(' ')}} > {{creates}}"
```

There are several examples for more inspiration on how you could use the flo.yaml specification. If you have suggestions for other ideas, please add them!

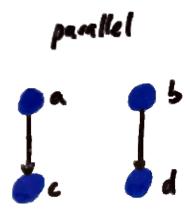
3.5 deterministic execution order

flo is guaranteed to run in the exact same order every single time and its important that users understand how it works. When flo is executed, it makes sure to obey the dependencies specified in the YAML configuration. In the event of ties flo is executed in the same order as the tasks appear in the YAML configuration. Technically, this is very similar to a breadth first search originating from the set of tasks that have no dependencies except that we order things based on the maximum distance that each task is from any given source node and we break ties based on the order in the YAML configuration file.

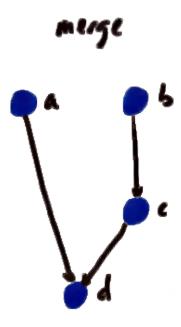
The deterministic order example contains a few different YAML configuration files to demonstrate how this works in practice, the highlights of which are summarized here.



For sibling tasks, sibling tasks are executed in the order in which they appear in the YAML configuration file, but always after the their dependencies have been satisfied. In this example, the task graph looks like this and the tasks are guaranteed to run in alphabetical order.



For parallel threads, task threads are executed based on their distance from the source tasks and secondarily based on their ordering in the YAML configuration file. In this example, the task graph looks something like this and the tasks are guaranteed to run in alphabetical order.



For merging task graphs, tasks are executed based on their maximal distance from any source task. In this example, the task graph looks something like this and the tasks are guaranteed to run in alphabetical order.

command line interface

This package ships with the flo command, which embodies the entire command line interface for this package. This command can be run from the directory that contains flo.yaml or any of its child directories. Output has been formatted to be as useful as possible, including the task names that are run, the commands that are run, and how long each task takes. For convenience, this information is also stored in .flo/flo.log.

To make the command line interface as usable as possible, autocompletion of available options with workflow is enabled by @kislyuk's amazing argcomplete package. Follow instructions to enable global autocomplete and you should be all set. As an example, this is also configured in the virtual machine provisioning for this project. Here, we elaborate on a few key features of flo; see flo --help for details about all available functionality.

4.1 running workflows

By default, the flo run command will execute the entire workflow, or at least the portion of it that is "out of sync" since the last time it ran. Executing flo run twice in a row without editing any files in the interim will not rerun any steps. If you edit a particular file in the workflow and re-execute flo run, this will only re-execute the parts that have been affected by the change. This makes it very easy to iterate quickly on data analysis problems without having to worry about re-running an arsenal commands — you only have to remember one, flo run.

Importantly, if you edit a particular task in the flo.yaml itself, this will cause that particular task to be re-run as well:

```
flo run
edit flo.yaml  # change a particular task's command
flo run  # rerun's that command and any dependent task
```

The flo command is able to do this by tracking the status of all creates, depends, and task definitions by hashing the contents of these resources. If the contents in any depends or the task itself has changed since the last time that task was run, flo will run that task. For reference, the hashes of all of the creates, depends, and workflow task definitions are in .flo/state.csv.

4.2 same project, different workflows

Naturally, there will be times when you'll want to have separate sets of steps to accomplish different things. One simple way to separate your workflow configuration is by putting them in two separate files, say figures.yaml and analysis.yaml. You can then specify running these separate workflows on the command line with the ——config option like this:

```
flo run --config figures.yaml
flo run --config analysis.yaml
```

All other behaviors of the YAML configuration and use of the flo command remain exactly the same.

4.3 limiting flo run execution

Oftentimes we do not want to run the entire workflow, but only a particular component of it. Like GNU make, you can specify a particular task by its creates value on the command line like this:

```
flo run path/to/some/output/file.txt
```

This limits flo to only executing the task defined in path/to/some/output/file.txt and all of its recursive upstream dependencies. Other times we do not want to run the entire workflow, but run everything after a specific task. We can do that like this:

```
flo run --start-at path/to/some/file.txt
```

This limits flo to only executing the task defined in path/to/some/file.txt and all of its recursive **down-stream** dependencies. This can be combined with flo run task_id to only all tasks between two specified tasks like this:

```
flo run --start-at path/to/some/file.txt path/to/some/output/file.txt
```

If you ever want to only run one task, say a task that creates path/to/some/file.txt, you can specify that task as both the starting and ending point of the workflow run with --only:

```
# these two things are the same
flo run --only path/to/some/file.txt
flo run --start-at path/to/some/file.txt path/to/some/file.txt
```

In some situations — especially with very long-running tasks that you know haven't been affected by changes — it is convenient to be able to skip particular tasks like this:

```
flo run --skip path/to/some/file.txt
```

This eliminates the task associated with path/to/some/file.txt from the workflow but preserves the dependency chain so that other tasks are still executed in the proper order.

Sometimes it is convenient to rerun an entire workflow, regardless of the current status of the files that were generated.

```
flo run
# don't do anything for several months
echo "Rip Van Winkle awakens and wonders, where did I leave off again?"
echo "Screw it, lets just redo the entire analysis"
flo run --force
```

For long-running workflows, it is convenient to be alerted when the entire workflow completes. The --notify command line option makes it possible to have the last 100 lines of the .flo/flo.log sent to an email address specified on the command line.

```
flo run --notify j.doe@example.com
```

4.4 I'm nervous, what's going to happen?

While we don't recommend it, its not uncommon to get "in the zone" and make several edits to analysis scripts before re-running your workflow. Because we're human, its easy to incorrectly remember the files you edited and how they may affect re-running the workflow. To help, the flo status command lets you see which commands will be run and approximately how much time it should take (!!!).

```
flo run
edit path/to/some/script.py
edit path/to/another/script.py
echo "a long time passes"
flo status  # don't run anything, just report what would be done
```

For reference, flo stores the duration of each task in .flo/duration.csv. Another way you can comfort yourself is by looking at the status visualization.

```
flo status --serve
```

which displays something like this:

4.5 Starting over

Sometimes you want to start with a clean slate. Perhaps the data you originally started with is dated or you want to be confident a workflow properly runs from start to finish before inviting collaborators. Whatever the case, the flo clean command can be useful for removing all creates targets that are defined in flo.yaml. With the --force command line option, you can remove all files without having to confirm that you want to remove them. If you just want to remove a particular target, you can use flo clean task_id to only remove that creates target.

```
flo clean  # asks user if they want to remove 'creates' results
flo clean --force  # removes all 'creates' targets without confirmation
flo clean a/task  # only remove the a/task target
```

4.6 Saving results

Before removing or totally redoing an analysis, I've often found it useful to backup my results and compare the differences later. The flo archive command makes it easy to quickly backup an entire flo (including generated creates targets, source code specified in depends, and the underlying flo.yaml) and compare it to previous versions.

developing

1. Fork and clone the project:

```
qit clone https://github.com/YOUR-USERNAME/flo.git
```

2. Install Vagrant and Virtualbox and launch the development virtual machine:

```
vagrant up && vagrant provision
```

On vagrant sshing to the virtual machine, note that the PYTHONPATH and PATH environment variables have been altered in this virtual machine so that any changes you make to your local data workflow scripts are automatically reloaded.

3. On the virtual machine, make sure everything is working by executing workflows in examples/*/flo.yaml

```
cd examples/reuters-tfidf
flo run
```

4. To be more thorough, there is an automated suite of functional tests to make sure any patches you have made haven't disturbed the behavior of this package in any substantiative way.

```
./tests/run_functional_tests.sh
```

These functional tests are designed to be run on an Ubuntu 12.04 LTS server, just like the virtual machine and the server that runs the travis-ci test suite. There are some other tests that have been added along the way in the Travis configuration. For your convenience, you can run all of these tests with:

```
./tests/run.py
```

Current build status:

5. Contribute! There are several open issues that provide good places to dig in. Check out the contribution guidelines and send pull requests; your help is greatly appreciated!

changelog

This project uses semantic versioning to track version numbers, where backwards incompatible changes (highlighted in **bold**) bump the major version of the package.

6.1 latest

- enforce that depends must exist prior to running any commands (#59)
- more informative error messages (#56, #57, #58)
- several bug fixes, including:
 - properly handling backspacing output of subprocessed commands (#53)

6.2 1.0.0

- removed pseudotask creation (every task must have a command key)
- specifying alternative yaml configuration (#62)
- incorporated deterministic ordering in a predictable and explainable manner (#65, #70)
- introduced flo status command; removed "flo run -dry-run" in favor of "flo status" (#55)
- incorporated the --only option (#37)
- several bug fixes, including:
 - making sure that the TaskGraph is a directed acyclic graph (#61)
 - ensuring that creates exists after a task has been run (#60)
 - clarifying output on flo status and flo run (#64)

6.3 0.2.0

· Initial release