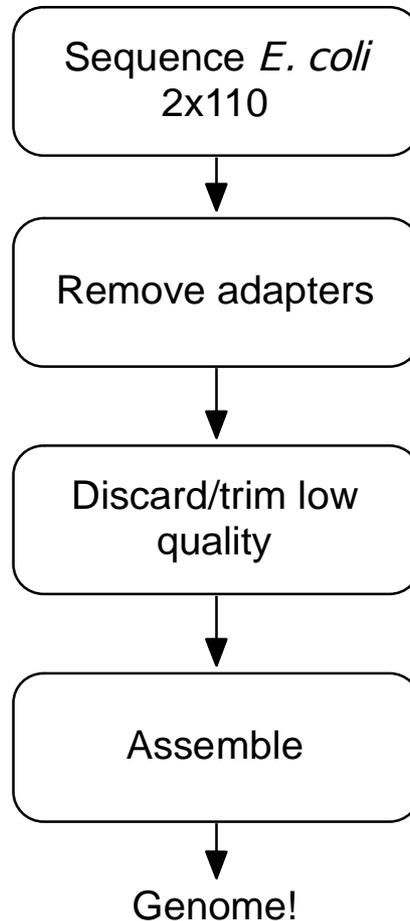


Pipelines!

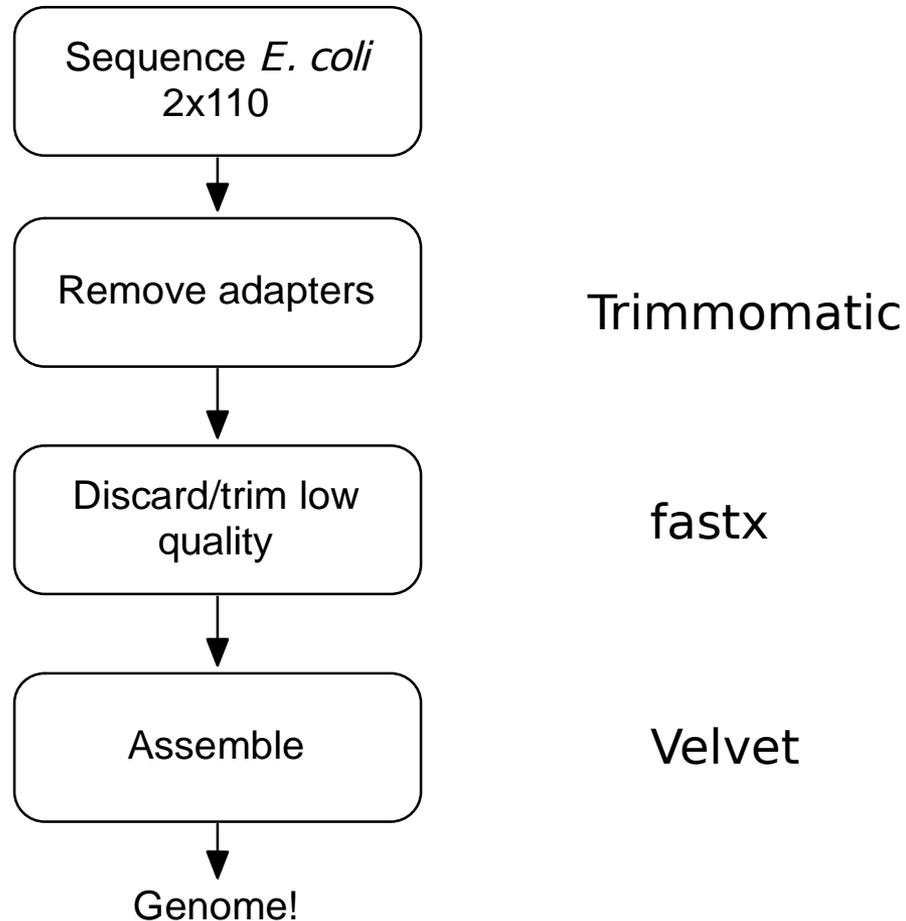
CTB

6/15/13

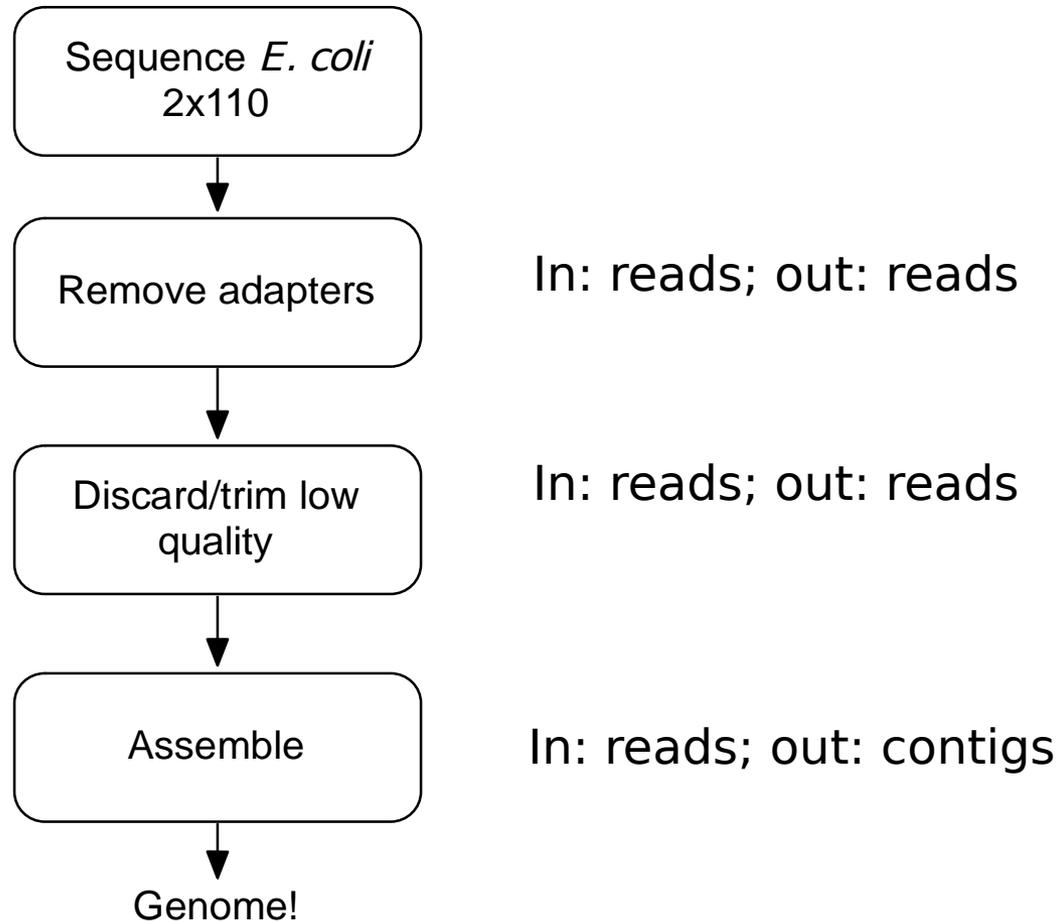
A pipeline view of the world



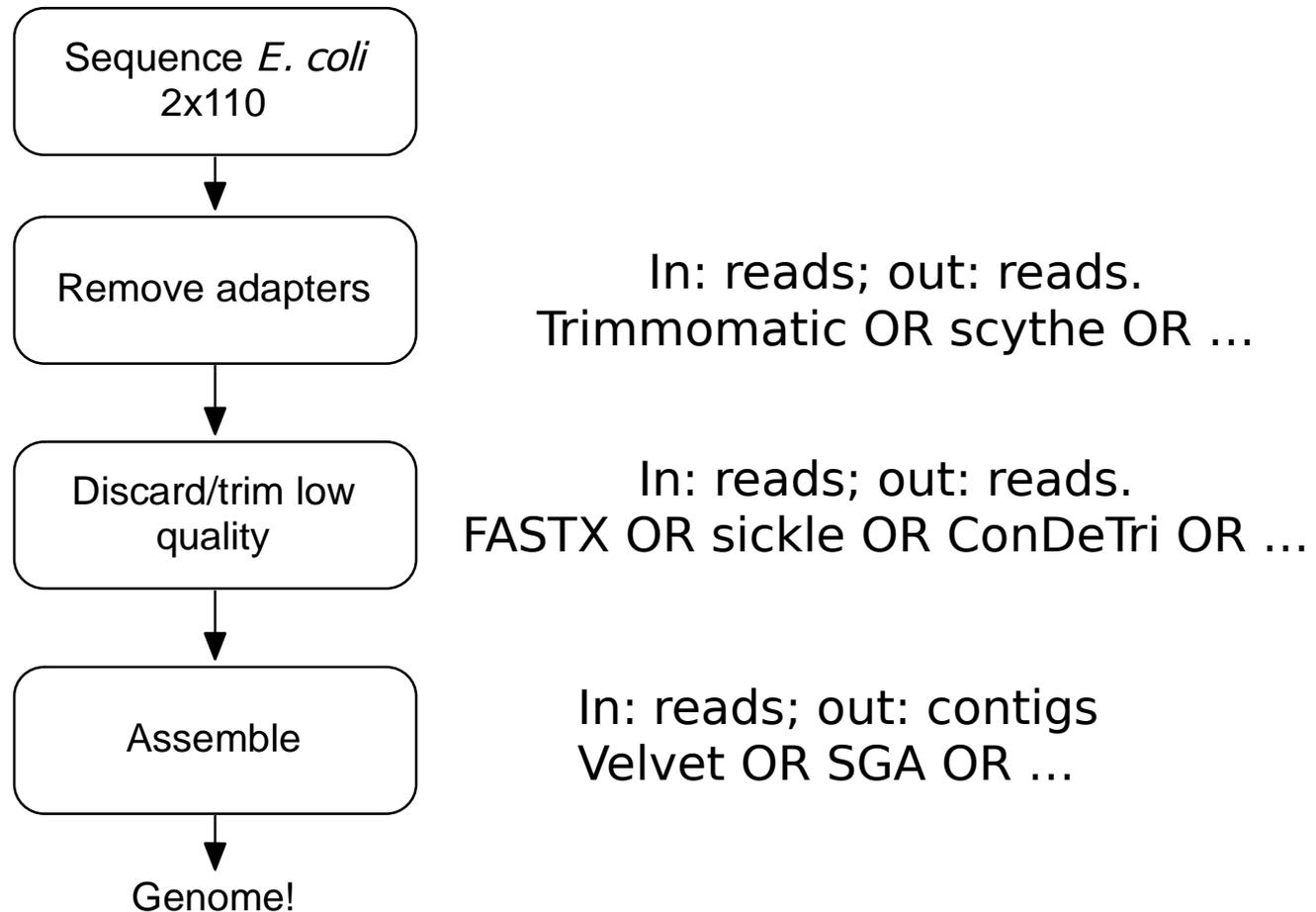
Each computational step is one or more commands



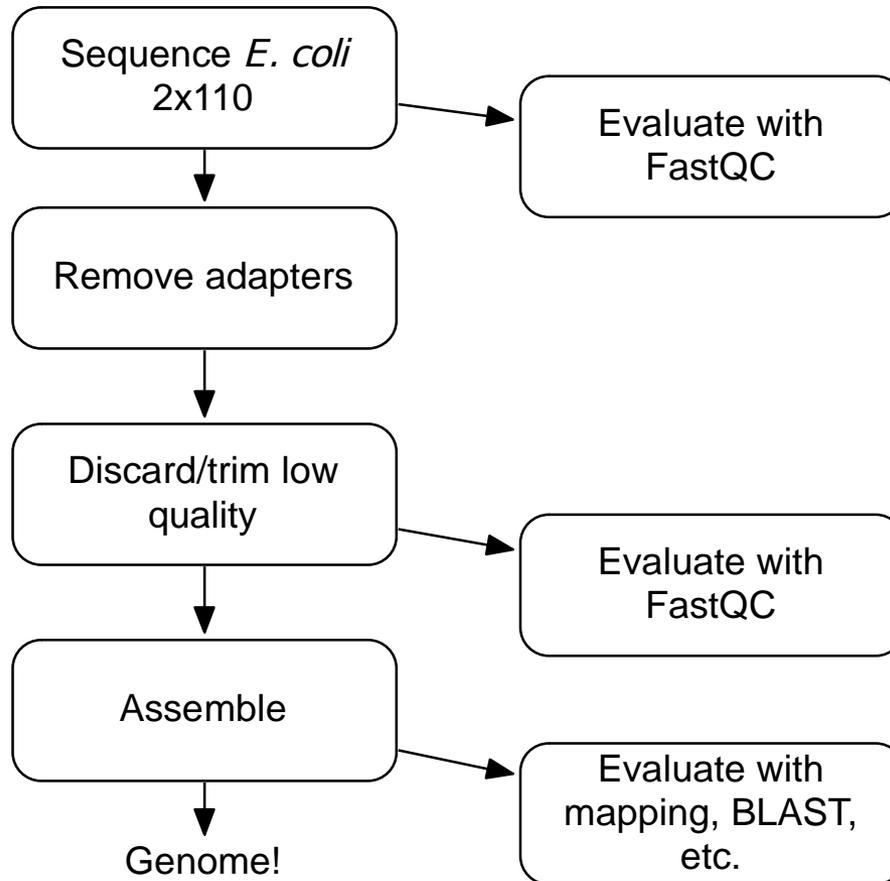
The breakdown into steps is dictated by input/output...



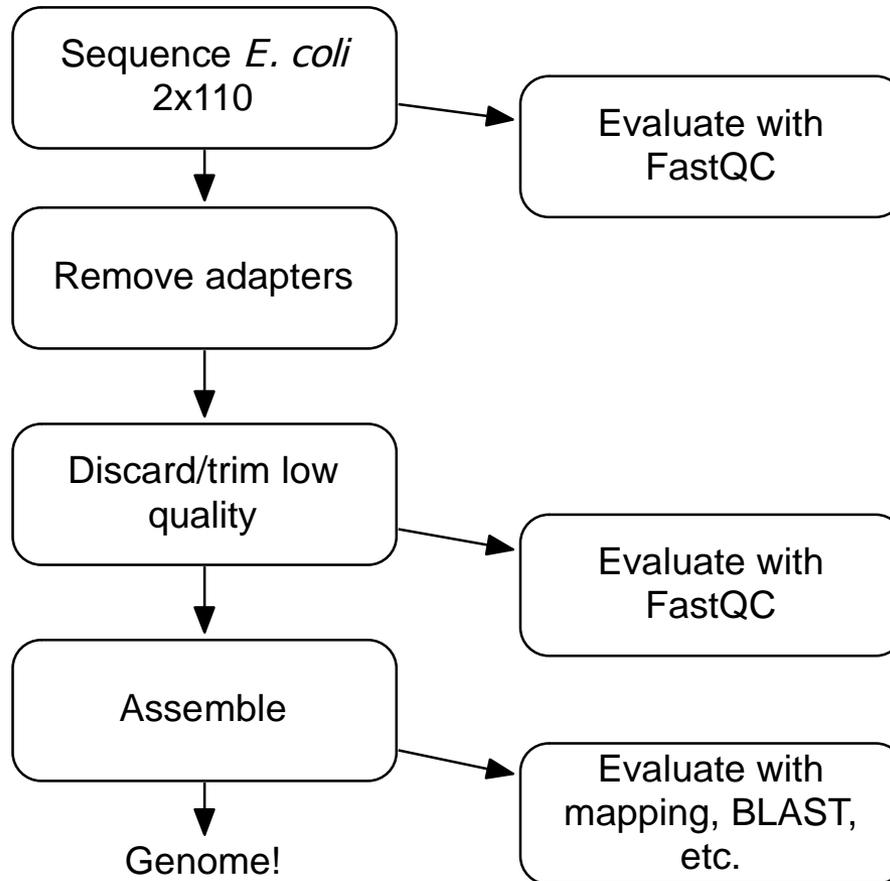
The breakdown into steps is driven by input/output and “concept”



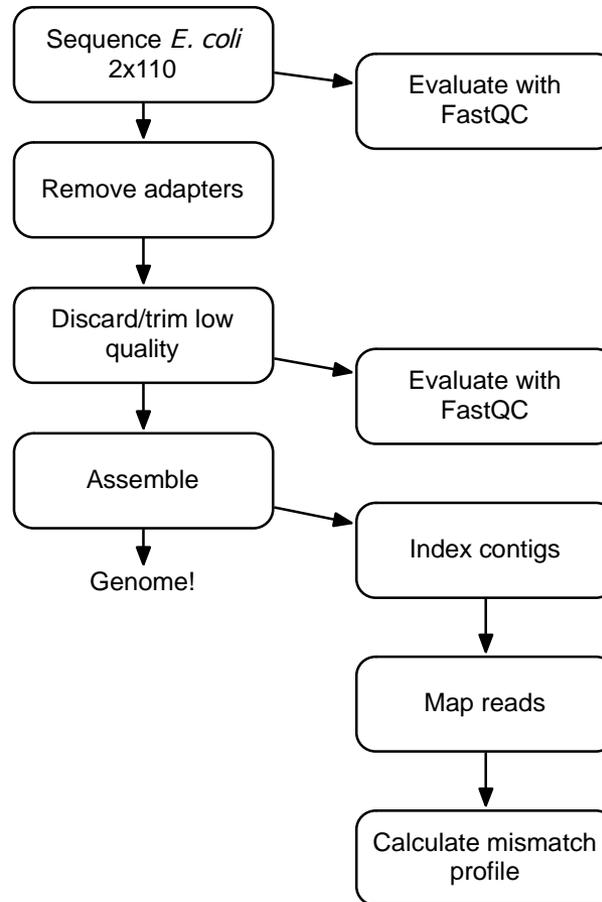
Generally, I don't include diagnostic steps as part of the main "flow".



Generally, I don't include diagnostic steps as part of the main "flow".



...but there isn't exactly a standard :)



What *is* a pipeline, anyway?

- Conceptually: series of data in/data out steps.
- Practically: series of commands that load data, process it, and save it back to disk.
 - This is generally true in bioinformatics
 - You can also have programs that do multiple steps, which involves less disk “traffic”
- Actually: a bunch of UNIX commands.

“Shell scripting”

- The shell (bash, csh, etc) is specialized for exactly this: running commands.
- Shell “scripting” is putting together a series of commands – “scripting actions” to be run.
- Scripting vs programming – fuzzy line.
 - Scripting generally involves less complex organization.
 - Scripting typically done w/in single file

Writing a shell script:

It's just a series of shell commands, in a file.

```
# trim adapters
```

```
... Trimmomatic ...
```

```
# shuffle reads together
```

```
Interleave.py ...
```

```
trim-and-assemble.sh
```

```
# Trim bad reads
```

```
fastx_trimmer
```

```
# Run velvet
```

```
velveth...
```

```
velvetg...
```

Back to pipelines

- *Automated* pipelines are good things.
 - Encode each and every step in a script;
 - Provide all the details, incl parameters;
- Explicit: each command is present.
- Reusable: can easily tweak a parameter, re-run & re-evaluate.
- Communicable: you can give to lab mate, PI, etc.
- Minimizes confusion as to what you actually did :)
- Automated: start & walk away from long-running pipelines.

Why pipelines?

- Automation:
 - Convenience
 - Reuse
 - **Reproducibility**

Pipelines encode *knowledge* in an explicit & executable computational representation.

Reproducibility

- *Most groups can't reproduce their own results, 6 months later.*
- *Other groups don't even have a chance.*
- Limits:
 - Reusability
 - Bug finding/tracking/fixing
 - Both convenience and correctness.*

Some nonobvious corollaries

- Each processing step from the raw data onwards is interesting; so you need to provide close-to-raw data.
- Making the figures is part of the pipeline; but Excel cannot be automated.
- Keeping track of what exact *version* of the pipeline script you used to generate the results now becomes a problem...

Click to edit Master text styles
Second level

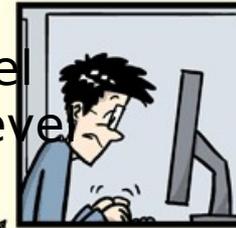
Third level

Fourth level

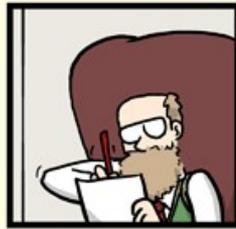
Fifth level



FINAL.doc!



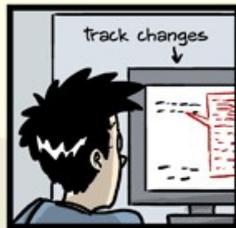
FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc



FINAL_rev.8.comments5.
CORRECTIONS.doc



FINAL_rev.18.comments7.
corrections9.MORE.30.doc



FINAL_rev.22.comments49.
corrections.10.#@\$%WHYDID
ICOMETOGRADSCHOOL?????.doc

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This is what *version control* is about.

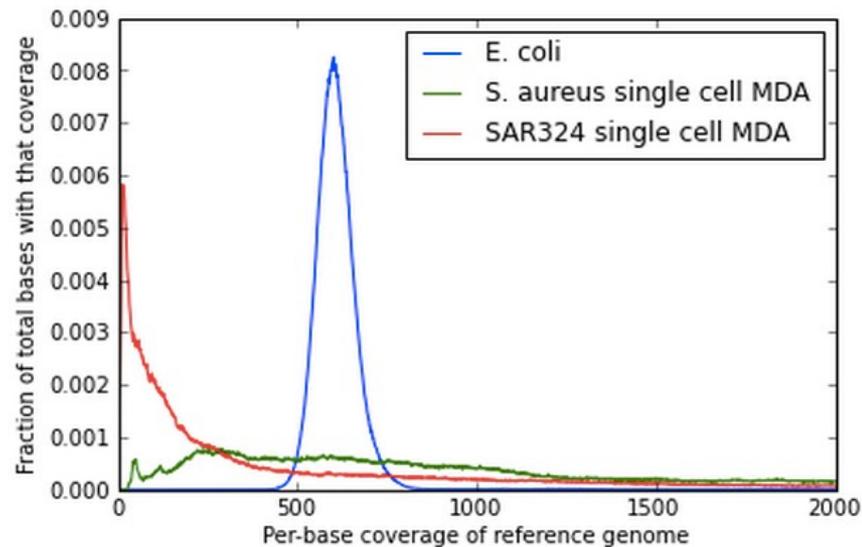
- Version control gives you an explicit way to track, mark, and annotate changes to collections of files.
- (Git is one such system.)
- In combination with Web sites like github.com, you can:
 - View changes and files online
 - Download specific marked versions of files

An actual pipeline

- The results in our digital normalization paper are about 80% automated.
 - Raw data
 - Single command to go from raw data to fully processed data.
 - Single IPython Notebook to go from raw data to figures.
 - (Super special) single command to go from figures + paper source to submission PDF.
 - Figures & text are tied to a specific *version* of our pipeline => 100% reproducible.

IPython Notebook

```
In [16]: plot(ecoli_cov[:,0], ecoli_cov[:,1])
plot(staph_cov[:,0], staph_cov[:,1])
plot(sar_cov[:,0], sar_cov[:,1])
xlabel("Per-base coverage of reference genome")
ylabel("Fraction of total bases with that coverage")
legend(["E. coli", "S. aureus single cell MDA", "SAR324 single cell MDA"])
axis(xmax=2000)
savefig('/tmp/diginorm-coverage2-raw.pdf')
```



```
In [17]: ecoli_kcov = numpy.loadtxt(datadir + 'ecoli.keep.rawreads.map.gz.cov')
ecoli_kcov = 1 / (sum(ecoli_kcov) + 1)
```

This morning

- Let's automate read trimming, mapping, & mismatch calculation!
 - Write script; run on subset of reads
 - Write notebook => figures
 - Put in version control, post to github.
- A quick tour of github
 - Forking, cloning, editing, pushing back
- Encoding assembly

Tips & tricks

- Develop a systematic naming scheme for files => easier to investigate results.
- Work with a small data set first & develop the pipeline; then, once it's working, apply to full data set.
- Put in friendly “echo” commands.
- Advanced: use *loops* and *wildcards* to write generic processing steps.