# BIOL 343
# Applied Bioinformatics I
## Building pipelines

**Dr. Nic Wheeler**

# Managing computational pipelines

**Problems when using many tools:**

1. Poor file management

   *Input/output files end up in unpredictable locations*

2. Uninformative file names

   *Names tend to get looooong with suffixes like* `_new_reallynew_1.txt`

3. Difficult to checkpoint

   *Re-running one step sometimes requires re-running* ***all*** *the steps*

4. Difficult to take notes

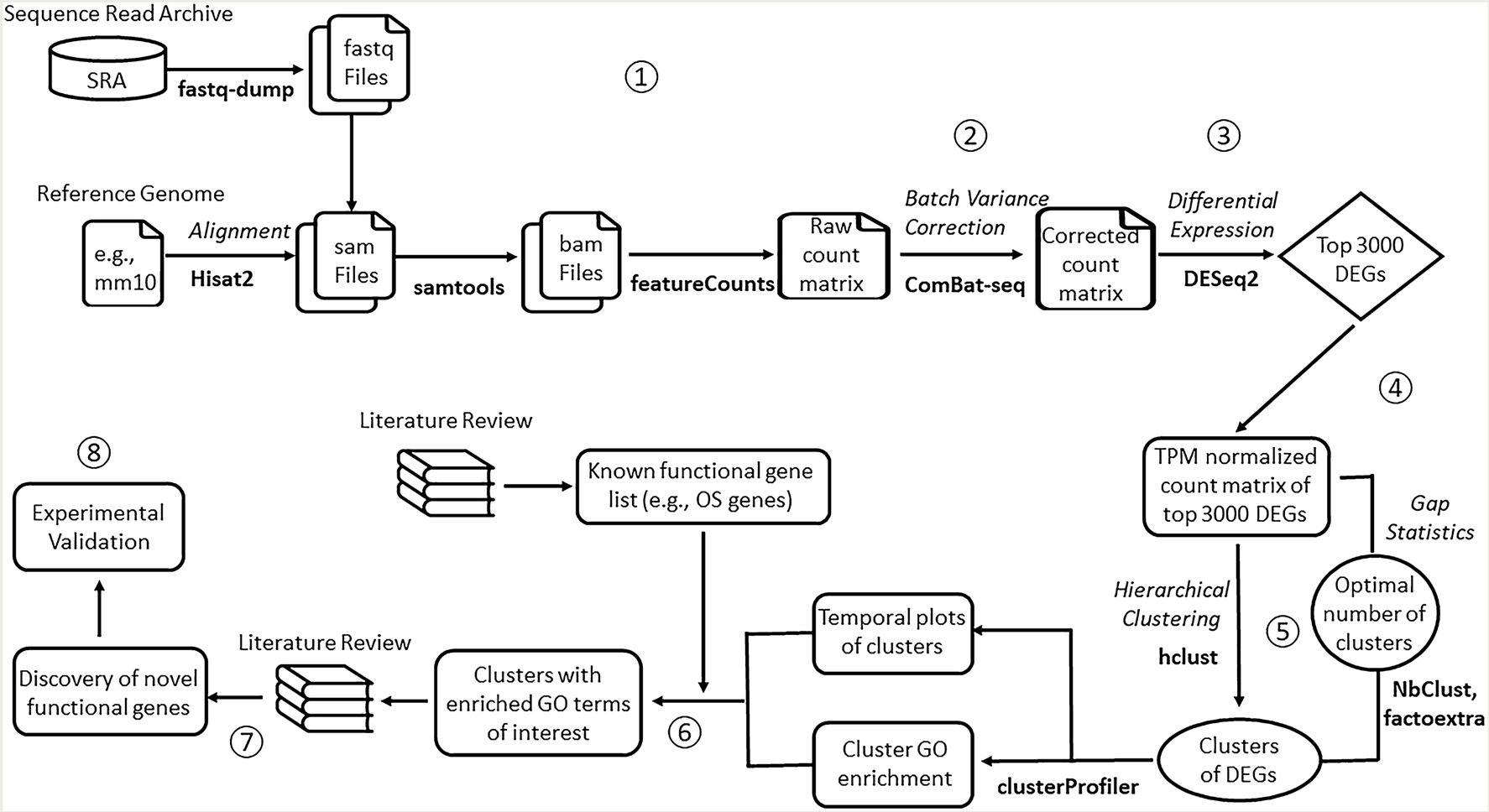
   *When testing new tools, it's difficult to recall what worked and didn't work (and why)*

**Workflow (pipeline) scripts**

# Managing computational pipelines

**Options for managing a pipeline like this:**

- Run one-by-one with CLI
- Run with Jupyter notebook
- Write a script




*Colon 2021, Scientific Reports*

# Managing computational pipelines

**One-by-one**

Good for alpha tests

Difficult to reproduce

Many opportunities for error

**Jupyter notebook**

Good when visualization/ manual inspection is necessary (beta tests)

Single-use

Doesn’t scale

**Scripting**

Good when publishing/ distributing

Generic for multiple uses

Scales well

# Managing computational pipelines

## Scripting options

**Shell script:**

- Ex: https://github.com/zamanianlab/Filarid_IsoSeq/blob/master/main.sh
- Key features:
  - Can manage directories with variables
  - Checkpoint with comments (kind of)
  - Allows use of all command line tools, even Bash commands
  - No special language knowledge required
  - Could be made generic (but this one isn’t)

# Managing computational pipelines

## Scripting options


**Nextflow script:**

- Ex: https://github.com/zamanianlab/Core_RNAseq-nf/blob/master/WB-pe.nf
- Key features:
  - Built-in directory and file management
  - Built-in checkpointing
  - Generic (with some restrictions)
  - Allows use of all command line tools, even Bash commands
  - Requires some Groovy knowledge
  - Large user base, lots of support

# Managing computational pipelines

## Scripting options

snakemake

**Snakelike script:**

- Key features:
  - Built-in directory and file management
  - Built-in checkpointing
  - Generic (with some restrictions)
  - Allows use of all command line tools, even Bash commands
  - Uses Python!
  - Uses conda!
  - Integrates with Slurm!

# Scripting pipelines in BIOL 343

- Each student will script their own pipelines
- Can choose which type you want to use
- Can use all available documentation/support online
- Can use your own conda envs

Live code activity…

1. Complete the snakemake tutorial on BOSE
    a. Start a VS Code session
    b. Install the snakemake extension
    c. Start at Step 2 (above link) to setup the env, then go here and edit your snakefile in a VS Code session