BIOL 343
Applied Bioinformatics I

Building pipelines

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Learning Objectives

You will be able to:

1.

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)

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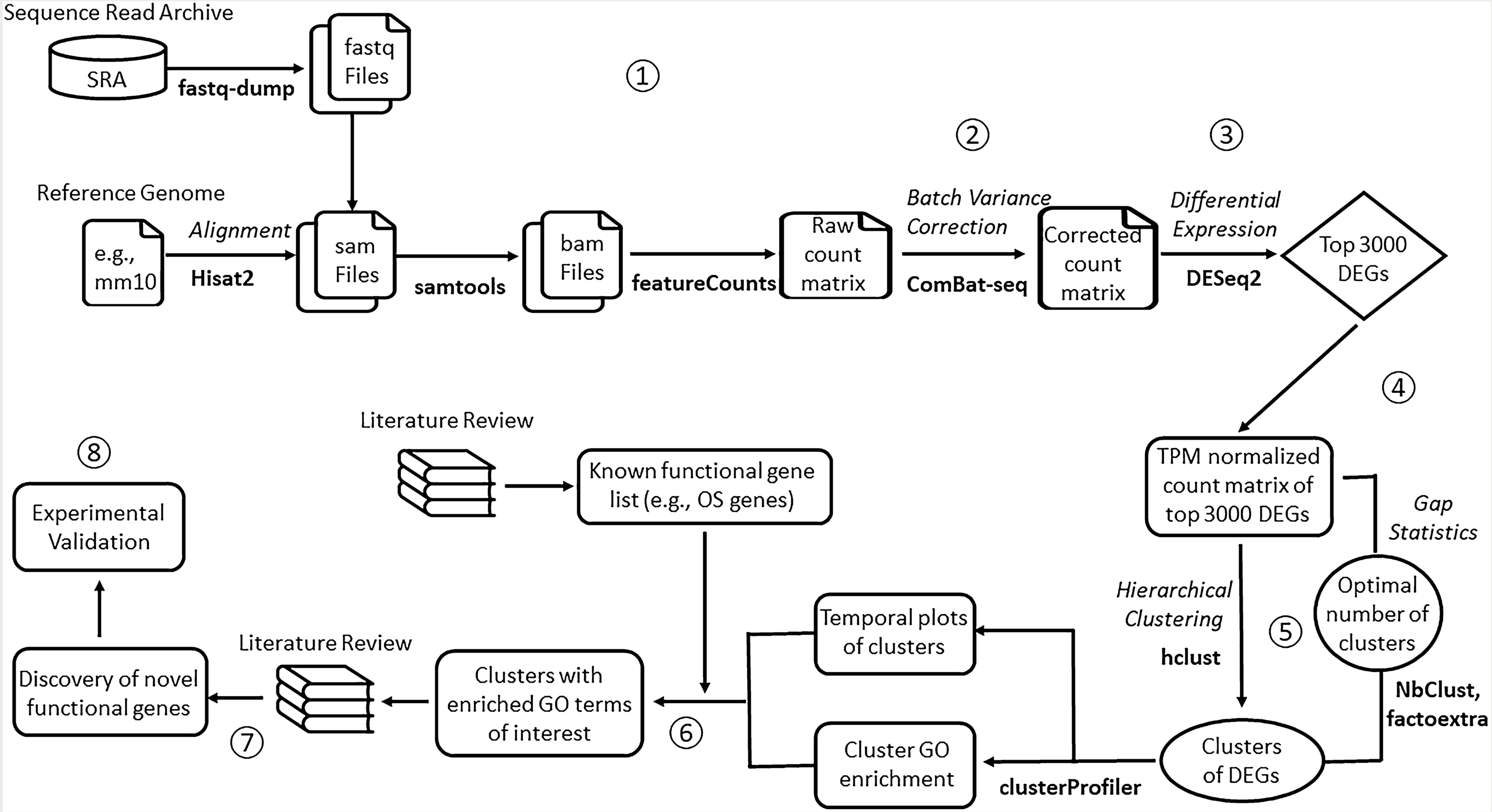
Workflow (pipeline) scripts

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

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. Convert your Jupyter notebook from last week to a Shell script
   - Strict file and directory management
2. Complete the snakemake tutorial on BOSE
   - Start at Step 2, then go here and edit your snakefile in a VS Code session
   - Install the snakemake extension
3. Convert your Shell script to a snakemake script