Scatter/gather-operations in Snakemake

What does scatter/gather mean?

- Scatter: turn input into several pieces of output
- Gather: bring together (aggregate) results from the different pieces

Snakemake now has built-in support for scatter/gather processes via the `scattergather` directive. Described further in the documentation: Defining scatter-gather processes. Currently not very flexible though.

When are scatter-gather processes handy?

- demultiplexing sequencing runs
    - multiple samples per plate
    - split plates into separate files per sample
- extract reads from bam files
    - reads mapped to several genomes
    - split sequences per genome
- parallelize analyses
    - e.g. multiple sequences per sample
    - split input into smaller chunks and run analyses in parallell

etc...

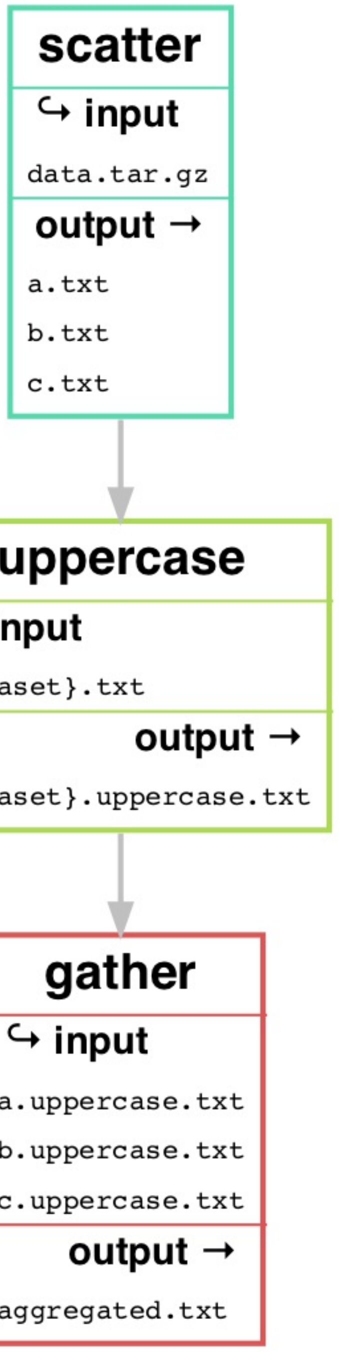
Between scattering and gathering there's some type of analyses performed.

The basics

```
DATASETS = ["a", "b", "c"]

rule scatter:
    output:
        expand('{dataset}.txt', dataset=DATASETS)
    input:
        data = 'data.tar.gz'
    shell:
        """
        tar xvf {input}
        """

rule uppercase:
    input:
        "{dataset}.txt"
    output:
        "{dataset}.uppercase.txt"
    shell:
        """
        tr [a-z] [A-Z] < {input} > {output}
        """

rule gather:
    output:
        "aggregated.txt"
    input:
        expand("{dataset}.uppercase.txt", dataset=DATASETS)
    shell:
        """
        cat {input} > {output}
        """
```

```
snakemake -c 1

Job stats:
job          count    min threads    max threads
---------  -------  -------------  -------------
gather           1              1              1
scatter          1              1              1
uppercase        3              1              1
total            5              1              1
```

The basics


scatter
↪ input
data.tar.gz
output →
a.txt
b.txt
c.txt
uppercase
↪ input
{dataset}.txt
output →
{dataset}.uppercase.txt
gather
↪ input
a.uppercase.txt
b.uppercase.txt
c.uppercase.txt
output →
aggregated.txt

Example: split files for parallelization

- one fastq file per sample

```
data
├── sample1.fastq
└── sample2.fastq
```

- split into several files (scatter)

```
splits
├── sample1
│   ├── sample1.1.fastq
│   ├── sample1.2.fastq
│   ├── sample1.3.fastq
|   ├── sample1.4.fastq
│   └── sample1.5.fastq
├── sample2
|   ├── sample2.1.fastq
|   ├── sample2.2.fastq
|   ├── sample2.3.fastq
|   ├── sample2.4.fastq
└   └── sample2.5.fastq
```

Example: split files for parallelization

- process individual files (parallelization)

```
rc
├─── sample1
│     ├─── sample1.1.rc.fastq
│     ├─── sample1.2.rc.fastq
│     ├─── sample1.3.rc.fastq
|    ├─── sample1.4.rc.fastq
│     └─── sample1.5.rc.fastq
├─── sample2
|    ├─── sample2.1.rc.fastq
|    ├─── sample2.2.rc.fastq
|    ├─── sample2.3.rc.fastq
|    ├─── sample2.4.rc.fastq
└─    └─── sample2.5.rc.fastq
```

- aggregate results (gather)

```
sample1.rc.fastq
sample2.rc.fastq
```

Example: split files for parallelization

We start with defining the number of splits

```
splits = 5
scatteritems = range(1, splits+1]
```

Then define a rule to scatter each sample fastq

```
rule scatter:
    output:
        expand("splits/{{sample}}/{{sample}}.{scatteritem}.fastq", scatteritem = scatteritems)
    input:
        "data/{sample}.fastq"
    log:
        "logs/{sample}.scatter.log"
    conda:
        "envs/seqkit.yml"
    params:
        parts = splits,
        outdir = lambda wildcards, output: os.path.dirname(output[0])
    shell:
        """
        seqkit split -p {params.parts} -O {params.outdir} {input} > {log} 2>&1
        rename 's/part_0*//' {params.outdir}/{wildcards.sample}.*.fastq
        """
```

Here `scatteritem` is not a wildcard because it is expanded using the `scatteritems` list.

Example: split files for parallelization

Next, a rule to do something with the split files per sample

```
rule reversecomplement:
    output:
        "rc/{sample}/{sample}.{scatteritem}.rc.fastq"
    input:
        "splits/{sample}/{sample}.{scatteritem}.fastq"
    conda:
        "envs/seqkit.yml"
    shell:
        """
        seqkit seq --reverse --complement {input} > {output}
        """
```

Here both `scatteritem` and `sample` are wildcards. The rule is generalized to work on any value for these wildcards.

Example: split files for parallelization

Then a rule to gather the results per sample

```
rule gather:
    output:
        "{sample}.rc.fastq"
    input:
        expand("rc/{{sample}}/{{sample}}.{scatteritem}.rc.fastq", scatteritem = scatteritems)
    shell:
        "cat {input} > {output}"
```

Here `scatteritem` is not a wildcard, but `sample` is. The rule can gather split files for any sample.

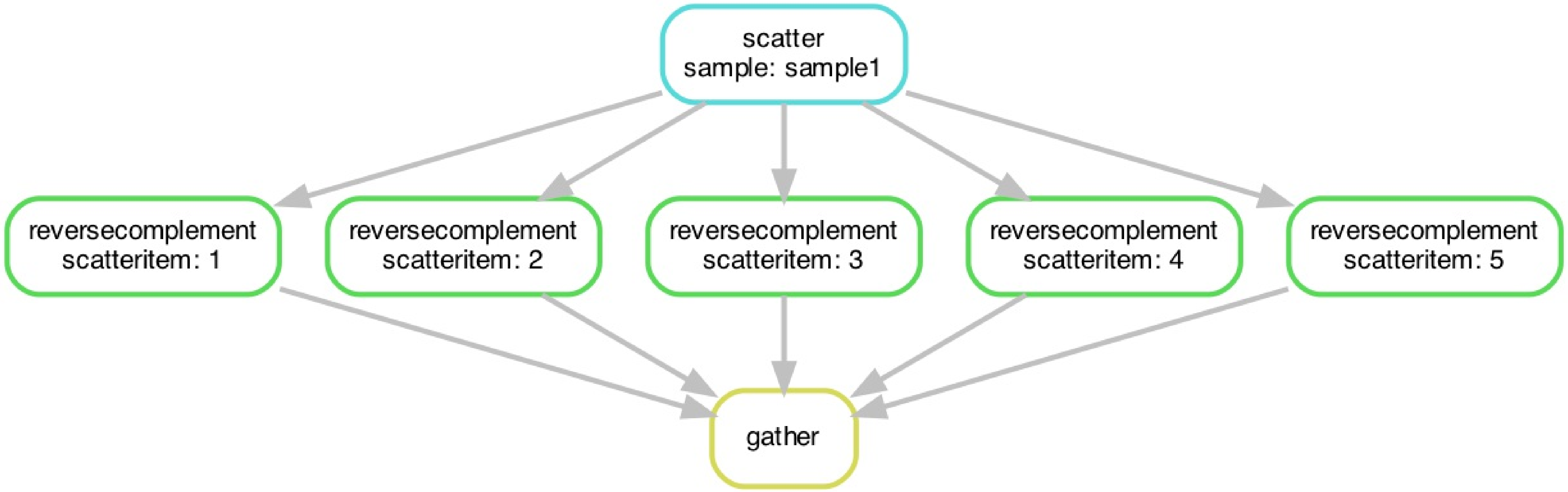
Example: split files for parallelization

Finally we put everything together, and define a pseudo rule 'all' that takes as input the gathered results for all samples.

```
samples = ["sample1", "sample2"]

splits = 5
scatteritems = range(1, splits+1)

rule all:
    input:
        expand("{sample}.rc.fastq", sample = samples)

rule scatter:
    output:
        expand("splits/{{sample}}/{{sample}}.{scatteritem}.fastq", scatteritem = scatteritems)
    input:
        "data/{sample}.fastq"

rule reversecomplement:
    output:
        "rc/{sample}/{sample}.{scatteritem}.rc.fastq"
    input:
        "splits/{sample}/{sample}.{scatteritem}.fastq"

rule gather:
    output:
        "{sample}.rc.fastq"
    input:
        expand("rc/{{sample}}/{{sample}}.{scatteritem}.rc.fastq", scatteritem = scatteritems)
```

Example: split files for parallelization

```
snakemake -c 1 --use-conda

Building DAG of jobs...
Job stats:
job                 count    min threads    max threads
-----------------   -------  -------------  -------------
all                     1            1             1
gather                  2            1             1
reversecomplement      10            1             1
scatter                 2            1             1
total                  15            1             1
```



This example workflow is available at the course GitHub repository: workshop-snakemake-byoc/tree/main/lectures/scatter-gather/

Questions?