Reproducible Programming

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2. don't repeat yourself, use functions
3. avoid magic numbers, expose them
4. cache intermediate results
5. seed random numbers

1. As much as possible, write it in code.

Code written in the console is wiped upon restart, and not particularly reproducible.

Console 1

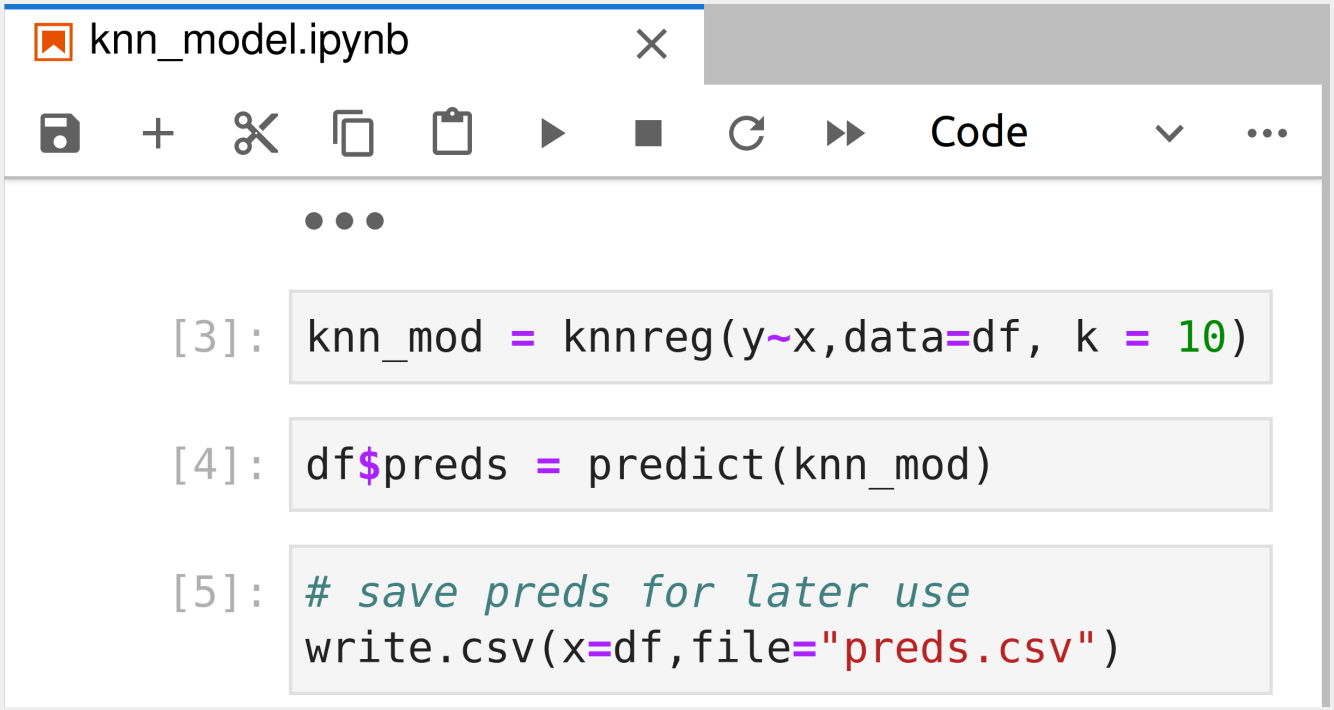
```
[3]: knn_mod = knnreg(y~x,data=df, k = 10)

[4]: df$preds = predict(knn_mod)

[5]: # save preds for later use
     write.csv(x=df,file="preds.csv")

[ ]:
```

For example, I may save model predictions in “preds.csv” but I don’t **exactly** know how they were produced.

1. As much as possible, write it in code.

Following Ellis and Leek (2018), shared analyses should have a "instruction list" documenting how the analysis was performed.

Generally, we think that documenting analysis in a notebook/script helps enhance reproducibility. e.g. the previous code could be put in a notebook:



1. As much as possible, write it in code.

This applies to all stages of analysis, including low-level processing of data before more *traditional* statistical analyses.

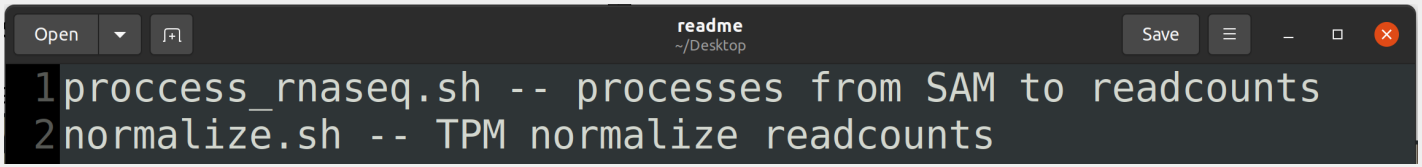
Example, aligning RNA-seq data:

```
$> samtools sort -@ 8 -o UHR_Rep1.bam UHR_Rep1.sam
$> samtools sort -@ 8 -o UHR_Rep2.bam UHR_Rep2.sam
$> cd $RNA_HOME/alignments/hisat2
$> java -Xmx2g -jar $PICARD MergeSamFiles -OUTPUT
UHR.bam -INPUT UHR_Rep1.bam -INPUT UHR_Rep2.bam -INPUT
UHR_Rep3.bam
$> ls -l *.bam | wc -l
$> hisat2 --very-sensitive --no-spliced-alignment -x
grch38 -U SRR1806626.fastq.gz > SRR1806626.fastq.sam
```

Write scripts:

```
$> bash process_rnaseq.sh
```

and readmes:



1. As much as possible, write it in code.

In a **linux** environment `makefiles` can be helpful for unifying and self-documenting this process.

This is a file called `makefile` that is run with the command `make`

Open

makefile
~/Desktop

```
1 .PHONY: preproc analysis plots
2
3 preproc:
4         bash ./pre_proc.sh
5
6 analyze:
7         Rscript analyze.R
8
9 plot:
10        Rscript plot.R
```

1. As much as possible, write it in code.

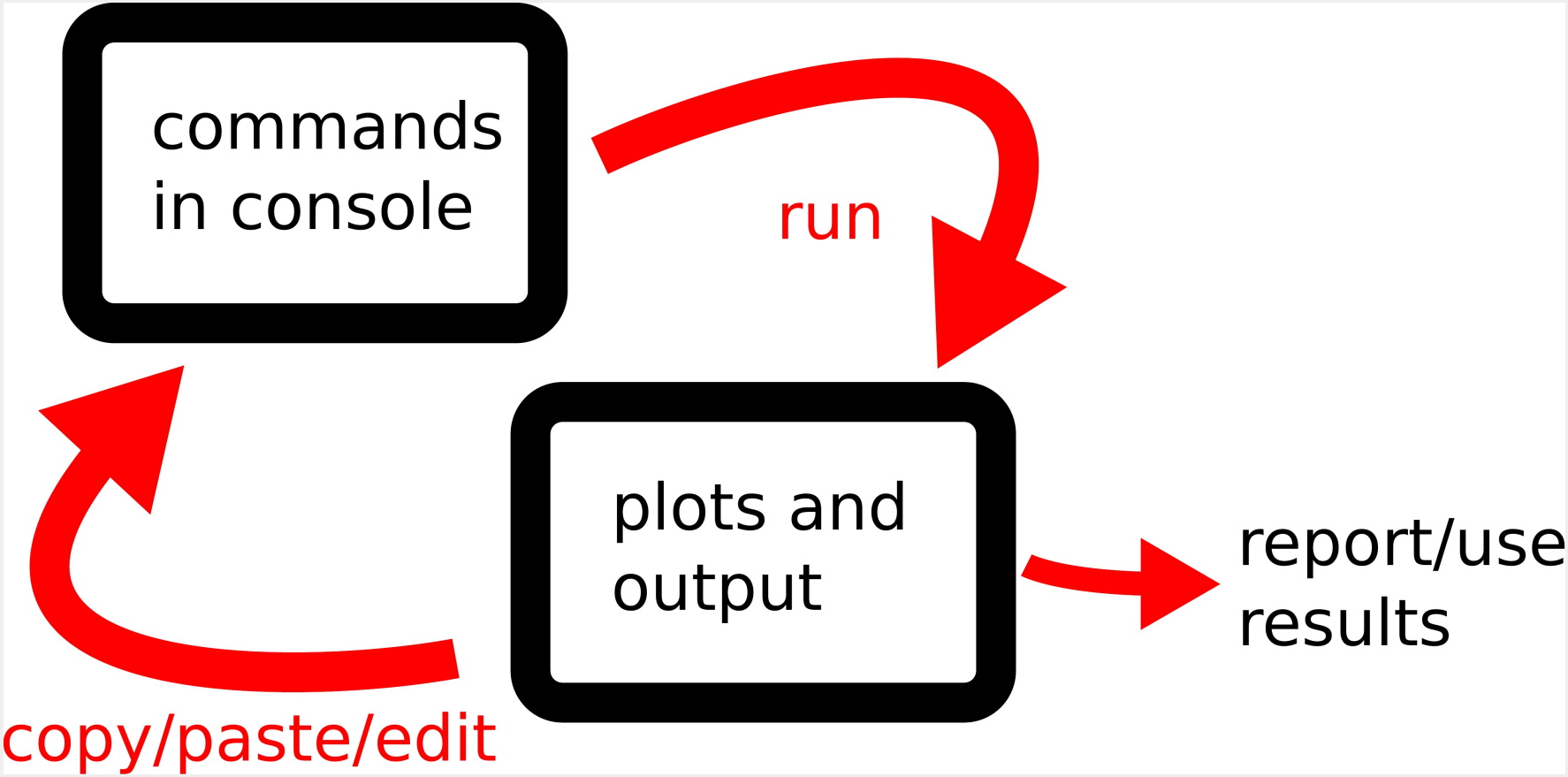
Run with the command `make` and pass in a named argument

```
#>make preproc
bash ./pre_proc.sh
Pre-processing raw data...
Pre-processing done: output in data.csv
#>
#>make analyze
Rscript analyze.R
Analyzing data...
Analysis done: results for plotting in plot_data.csv
#>
#>make plot
Rscript plot.R
Saving plots in plot.pdf
null device
          1
```

This helps self-document and collect all processing steps across languages/programs etc.

1. As much as possible, write it in code.

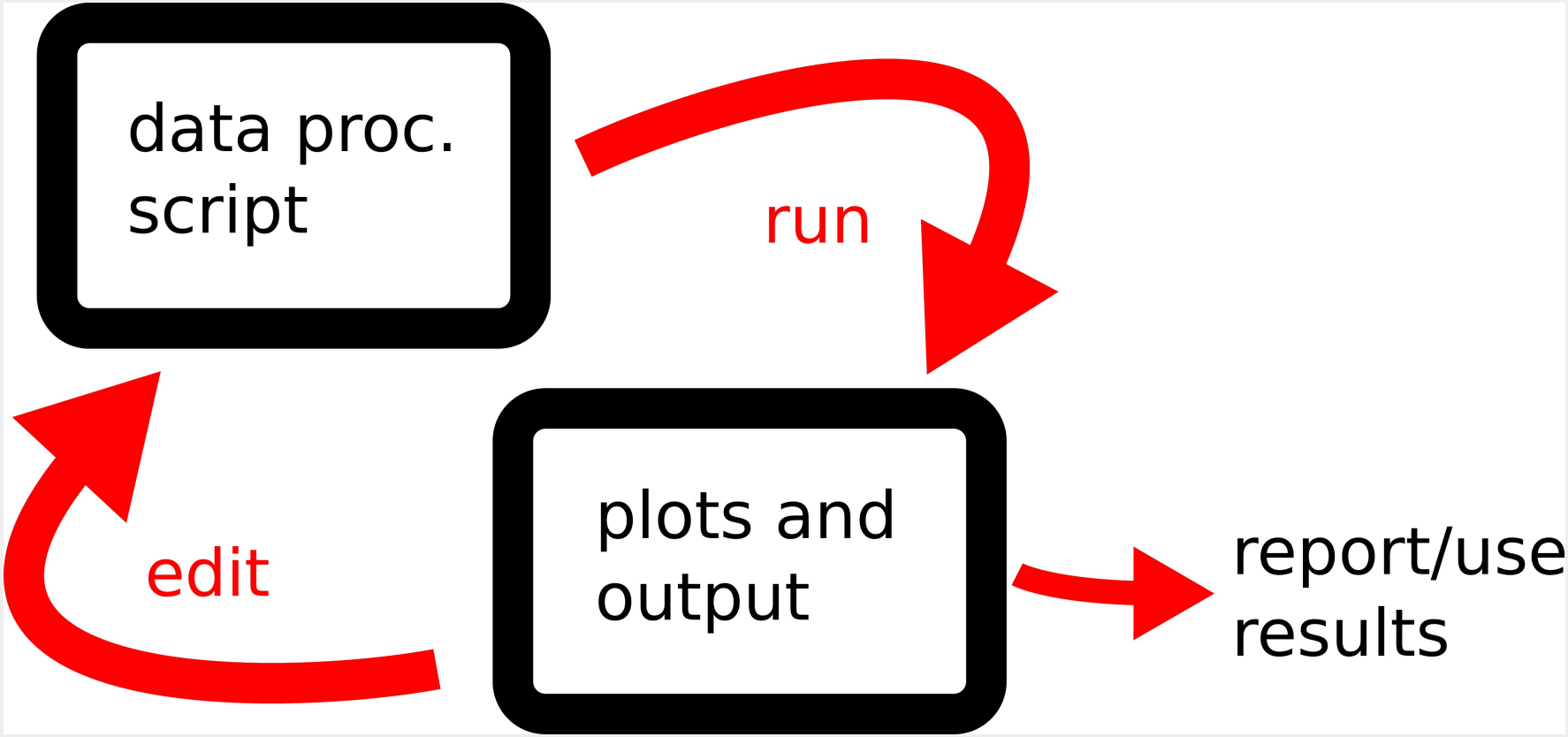
A **less** reproducible process:



After closing down the console, I **don't** have a reproducible record of what I did to get results.

1. As much as possible, write it in code.

A **more** reproducible process:



Afterwards, I have a **more reproducible script** that shows exactly what was run to get results.

Exercise 1: Makefiles

Create some scripts and a makefile to run them

- Write two notebooks: `analysis.ipynb` and `plotting.ipynb`
- Mirror the outputs to `.R` scripts using `jupytext`
- `analysis.ipynb` should load up `palmerpenguins` and save it as a `.csv`
- `plotting.ipynb` should read in the `.csv`, make a plot, save it as a `.pdf`
- Create a `makefile` with three options: `analyze`, `plot`, and `all` to run the scripts, respectively.

2. Don't repeat yourself (DRY), use functions.

Copying / pasting can create code that is difficult to maintain / understand.

For example, often see code like this:

```
knn_mod10 = knnreg(y~x,data=df, k = 10)
```

```
knn_mod5 = knnreg(y~x,data=df, k = 5)
```

```
knn_mod1 = knnreg(y~x,data=df, k = 1)
```

2. Don't repeat yourself, use functions.

Refactoring as a function is a much more scalable solution:

```
fit_knn = function(K){
    knn_mod = knnreg(y~x,data=df, k = K)
    return(knn_mod)
}
```

```
K_seq = c(10,5,1)
```

```
knn_mods = lapply(K_seq,fit_knn)
```

2. Don't repeat yourself, use functions.

DRY advantages:

1. makes your code easier to change / maintain (avoiding errors)

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- **be careful**, one can over-do it:

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- General rule:

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2. Second time, copy it.
3. Third* time, refactor it.

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- **be careful**, one can over-do it:
- General rule:

1. First time, write it.
2. Second time, copy it.
3. Third* time, refactor it.

- * May not actually be the *third* time.

2. Don't repeat yourself, use functions.

"Premature optimization is the root of all evil." – Don Knuth

```
fit_model = function(df, fit_fn, ...){
    mdl = fit_fn(y~x,data=df,...)
    return(mdl)
}
```

```
mod_lm = fit_model(df,lm)
mod_knn = fit_model(df,knnreg,K=5)
```

In this particular case, factoring out the call to `lm` and `knnreg` increased the number of lines of code and made it harder to read.

Exercise 2: Refactoring as Functions

Write a script to fit a KNN regression to predict one variable from another using `palmerpenguins`.

- You can use `knnreg` from the `caret` package
- Refactor this routine as a function with a single argument `K`, the number of neighbors, and return the KNN model from the function
- Apply this function over the sequence `K=1,5,10,15` and put the output in a `list`

3. Magic numbers should be variables, variables should often be arguments.

An R example:

```
run_sim=function(){
    x = sort(runif(200,-4*pi,4*pi)) # simulated data
    eps = rnorm(200,0,.25)
    y = sin(x)+eps

    smoothed = locPolSmootherC(x=x,y=y,xeval=x,deg=0,
                               kernel=gaussK,bw=.5)
    preds = smoothed$beta0
    return(preds)
}
```

```
run_sim()
```

• • •

3. Magic numbers should be variables, variables should often be arguments.

Magic numbers: sample size, kernel type, bandwidth, ...

```
run_sim=function(){
    x = sort(runif(200,-4*pi,4*pi)) # simulated data
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    smoothed = locPolSmootherC(x=x,y=y,xeval=x,deg=0,
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    preds = smoothed$beta0
    return(preds)
}
```

```
run_sim()
```

• • •

3. Magic numbers should be variables, variables should often be arguments.

Better: expose those magic numbers as parameters

```
run_sim=function(N=200,sig=.25,bandw=.5,kern=gaussK){
    x = sort(runif(N,-4*pi,4*pi)) # simulated data
    eps = rnorm(N,0,sig)
    y = sin(x)+eps

    smoothed = locPolSmootherC(x=x,y=y,xeval=x,deg=0,
                               kernel=kern,bw=bandw)
    preds = smoothed$beta0
    return(preds)
}
```

```
run_sim()
```

•••

```
run_sim(bandw=1,sig=2)
```

3. Magic numbers should be variables, variables should often be arguments.

Naming **magic numbers** and other parameter choices

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Naming **magic numbers** and other parameter choices

1. makes the code easier to read and more self-documenting
2. enhances reproducibility by
   - flagging these analysis choices,
   - exposing them via an interface for easy (third party) experimentation

Exercise 3: Magic Numbers

Write a function to generate data from the model

$$y = \beta_0 + \beta x + e$$

where $x \sim U(0, 1)$ and $e \sim N(0, \sigma^2)$. After generating the data, fit a KNN regression with some number of neighbors K. Return the KNN model.

- The arguments of this function should allow me to change: β_0,β, and K.
- Run this simulation over the cases of $\beta_0 = 0, \beta = 1, \sigma^2 = 1$ and $K = 1, 5, 10$, and,
- $\beta_0 = 3, \beta = 5, \sigma^2 = 3$ and $K = 1, 5, 10$.
- Keep the respective outputs as lists.

4. Cache Intermediate Results

Ideally, reproducible analysis takes data from (e.g.)

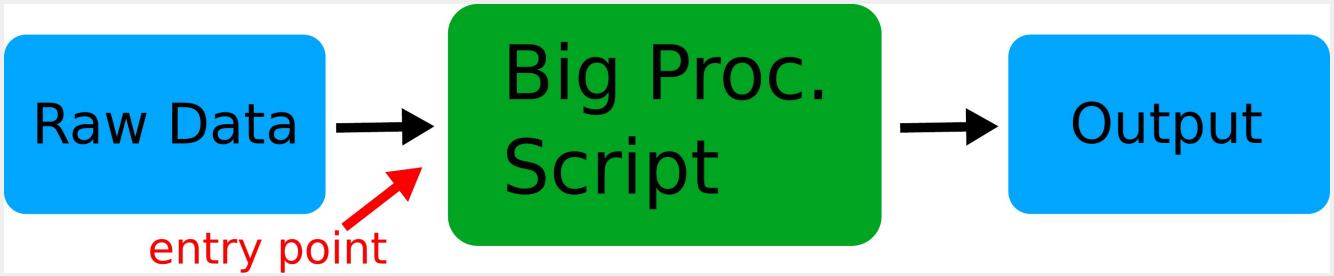
- raw sources, to
- cleaned-up processed data, to
- final results/plots/output

If this is all one long script that processes data without saving any intermediate results along the way, it can be difficult to reproduce the analysis.

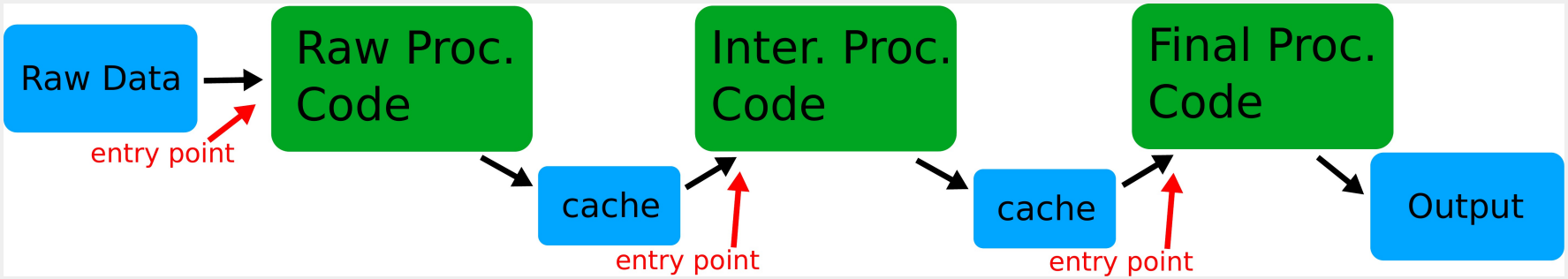
4. Cache Intermediate Results

It is good practice to **cache** intermediate results to enhance reproducibility by creating multiple entry-points into the analysis.

Don’t structure analysis like this:



Structure it like this:



4. Cache Intermediate Results

A very simplified version in R uses the idioms `saveRDS(object,file)` and `object = readRDS(file)`:

```
raw_data = read.csv('raw_data.csv')
# ... do some analysis to produce `basic_data`
```

```
saveRDS(object=basic_data,file='basic_data_cache.rds')
```

```
basic_data = readRDS(file='basic_data_cache.rds')
# .. do some analysis to produce `intermed_data`
```

```
saveRDS(object=intermed_data,file='intermed_data_cache.rds')
```

```
intermed_data = readRDS(file='intermed_data_cache.rds')
#...
```

4. Cache Intermediate Results

A useful idiom if I have a single function's results I want to cache:

```
read_or_run = function(cache_file,func){
    if(!file.exists(cache_file)){
        cat("Running func...");flush.console()
        obj = func()
        saveRDS(object=obj,file=cache_file)
    } else {
        cat("Reading from cache...");flush.console()
        obj = readRDS(file=cache_file)
    }
    return(obj)
}
```

4. Cache Intermediate Results

An example of this idiom:

```
proc_df = read_or_run('proc_cache.rds',proc_data)
```

```
Running func...
```

```
proc_df = read_or_run('proc_cache.rds',proc_data)
```

```
Reading from cache...
```

Exercise 4: Caching

Cache and read-in analysis.

- Using previous analysis, save the output to a `.RDS` file using `saveRDS`.
- Start a new notebook/session, read in the cached output using `readRDS`
- Do this over, but now use our `read_or_run` function in both places.

5. Seed Random Numbers

For statistical analyses, our results often depend on **randomness**. To make randomness **reproducible** we need to identically set the pseudo-random number generators (PRNG) state each time.

In R we can do this with `set.seed(number)` or `set.seed(NULL)`

Example: a simple MC estimate of the mean of a U(0,1)

```
x = runif(10)
mean(x^2)
```

```
0.504305202849137
```

```
x = runif(10)
mean(x^2)
```

```
0.432056724361968
```

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In R we can do this with `set.seed(number)` or `set.seed(NULL)`

Example: a simple MC estimate of the mean of a U(0,1)

```
set.seed(887561)
x = runif(10)
mean(x^2)
```

```
0.261476556288769
```

```
set.seed(887561)
x = runif(10)
mean(x^2)
```

```
0.261476556288769
```

5. Seed Random Numbers

In R the PRNG state is saved in `.Random.seed`

```
head(.Random.seed)
```

10403 · 30 · -1808316273 · -469104443 · 837650556 · 1438237906

A useful idiom:

```
get_rseed = function(){
    if(!exists(".Random.seed"))
        set.seed(NULL)
    return(.Random.seed)
}
```

```
head(get_rseed())
```

10403 · 624 · -1849901807 · 114181022 · 809053063 · -1333479908

5. Seed Random Numbers

We can use this state to cache the PRNG state reproducibly without explicitly setting it

```
rseed = read_or_run("random_seed", get_rseed)
.Random.seed = rseed

x = runif(10)
mean(x^2)
```

```
 Running func...
0.280758108258287
```

```
rseed = read_or_run("random_seed", get_rseed)
.Random.seed = rseed

x = runif(10)
mean(x^2)
```

```
 Reading from cache...
```

5. Seed Random Numbers

If we want to generate a new seed we just remove the cache

```
system('rm random_seed')
```

```
rseed = read_or_run("random_seed", get_rseed)
.Random.seed = rseed

x = runif(10)
mean(x^2)
```

```
 Running func...
0.376071728383279
```

5. Beware: Functions

Careful with functions:

```
mc_est = function(){
    set.seed(887561)
    x = runif(10)
    mean(x^2)
}
```

```
N_rep = 5
var(replicate(N_rep,mc_est()))
```

0

```
replicate(N_rep,mc_est())
```

1. 0.261476556288769
2. 0.261476556288769
3. 0.261476556288769
4. 0.261476556288769

5. Beware: Functions

Set the seed *outside* the function

```
set.seed(887561)

mc_est = function(){
    x = runif(10)
    mean(x^2)
}

N_rep = 5
var(replicate(N_rep,mc_est()))
```

```
0.0177441652674178
```

5. Beware: Parallelization

As instructed, we set the seed outside the function call:

```
library(parallel)
cl <- makeCluster(5)
```

```
mc_est = function(i){
    x = runif(10)
    mean(x^2)
}
```

```
set.seed(887561)
out = clusterApply(cl, 1:5, mc_est)
out
```

1. 0.437248451074948
2. 0.394221360173399
3. 0.177918863126196
4. 0.311512514403605
5. 0.246496561791708

5. Beware: Parallelization

Re-running it, it's not the same.

```
set.seed(887561)
clusterApply(cl, 1:5, mc_est)
```

1. 0.394305944271141
2. 0.454497342889293
3. 0.398544956729978
4. 0.582426639255505
5. 0.41182331119249

Each parallel instance starts its own session, and thus resets the PRNG.

5. Beware: Parallelization

An ok solution:

```
set.seed(887561)
seeds = sample.int(100000000,5)
seeds
```

1. 33786065
2. 90525536
3. 40106588
4. 15296196
5. 84095680

```
mc_est = function(i){
    set.seed(seeds[i])
    x = runif(10)
    mean(x^2)
}

cl <- makeCluster(5)
clusterExport(cl=cl, varlist="seeds", envir=environment())

clusterApply(cl, 1:5, mc_est)
```

5. Beware: Parallelization

The built-in solution:

```
cl <- makeCluster(5)
clusterSetRNGStream(cl, iseed = 887561)
mc_est = function(i){
    x = runif(10)
    mean(x^2)
}

clusterApply(cl, 1:5, mc_est)
```

1. 0.390381338040286
2. 0.353646776895175
3. 0.338523872182183
4. 0.261878172684988

5. Beware: Parallelization

This will fail if I change parallelization parameters e.g. the number of workers.

```
cl <- makeCluster(2)
clusterSetRNGStream(cl, iseed = 887561)
mc_est = function(i){
    x = runif(10)
    mean(x^2)
}

clusterApply(cl, 1:5, mc_est)
```

1. 0.390381338040286
2. 0.353646776895175
3. 0.327037352615337
4. 0.30747298222943

5. Beware: Parallelization

A very reproducible way is to use the `future.apply` package:

```
mc_est = function(i){
    x = runif(10)
    mean(x^2)
}
```

```
library('future.apply')
plan(multisession,workers=5)
future_lapply(1:5,FUN=mc_est,future.seed=887561)
```

```
Loading required package: future
```

1. 0.392439730744121
2. 0.288707857966789
3. 0.442395305412029
4. 0.568664612085185
5. 0.408235991591878

This will still work even if we change parallelization parameters.

Exercise 5: Random Numbers

Write a function to estimate $E[\log(X)]$ for $X \sim U(0, 1)$.

- Set the seed for this simulation and check that it reproduces the same result.
- Use the `future.apply` function/package to run this simulation 10 times in parallel. Check that it is reproducible.

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1. cleaning up your pipeline. Go back periodically, and do things like:

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   - break apart code into better logically structured chunks/scripts
2. testing your pipeline (from soup to nuts)
   - delete all your cached intermediate results

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1. cleaning up your pipeline. Go back periodically, and do things like:
   - delete those commented out lines
   - refactor copy-and-pasted code chunks,
   - rename your poorly named variables,
   - break apart code into better logically structured chunks/scripts
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   - have someone else look at your code
4. avoid proprietary software

Exercise 6: Putting it all together.

1. Open up the messy code messy.ipynb
2. Refactor this code so that it is more *proactively reproducible*. Remember the five idioms and try to incorporate them into your solution:

- write it in code, not the console
- don't repeat yourself, use functions
- avoid magic numbers, expose them
- cache intermediate results
- seed random numbers

Discussion

- How often do you go back and clean-up code?
- What practices do you find most helpful for creating good, reproducible code?
- What do you find gets in the way of applying good practices?