Reproducible Programming

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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")

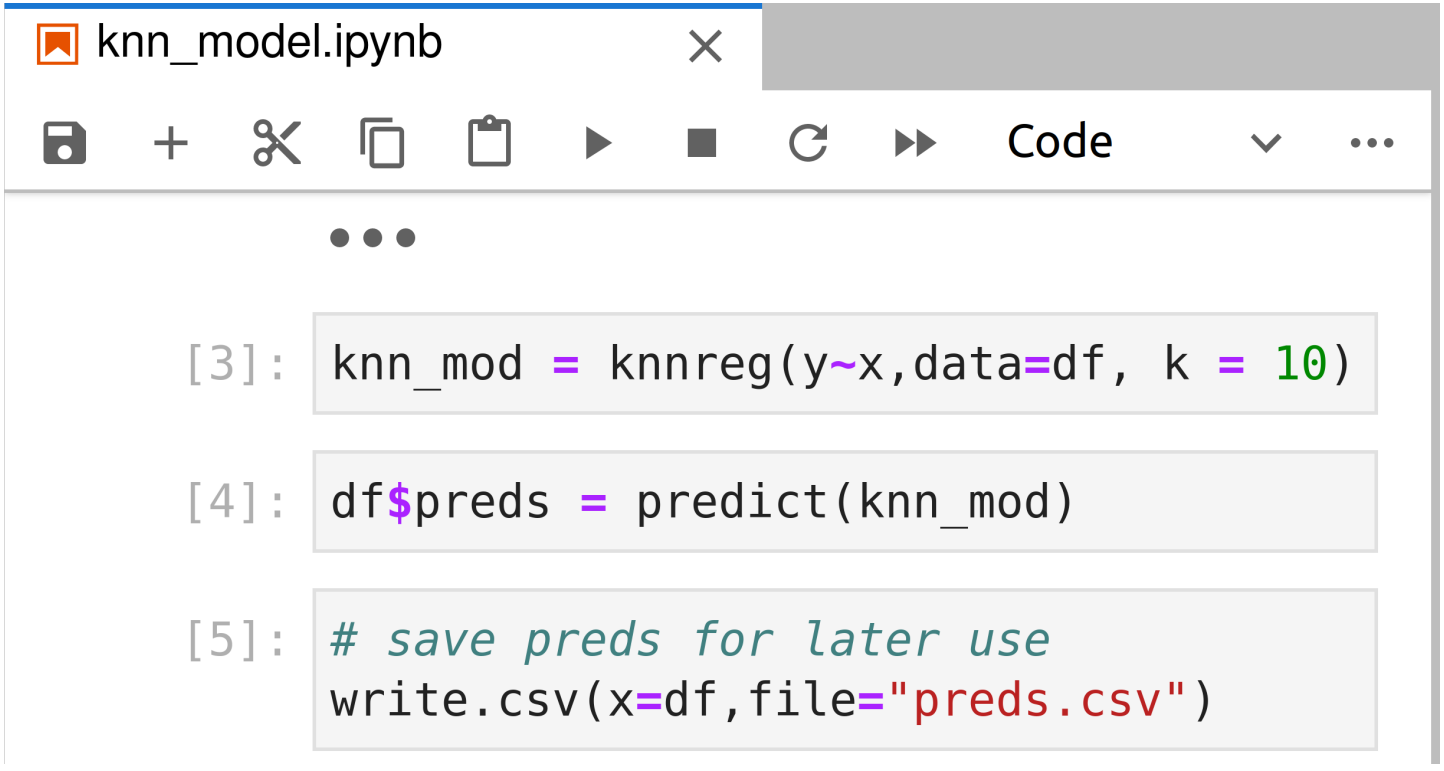
[ ]:
```

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.

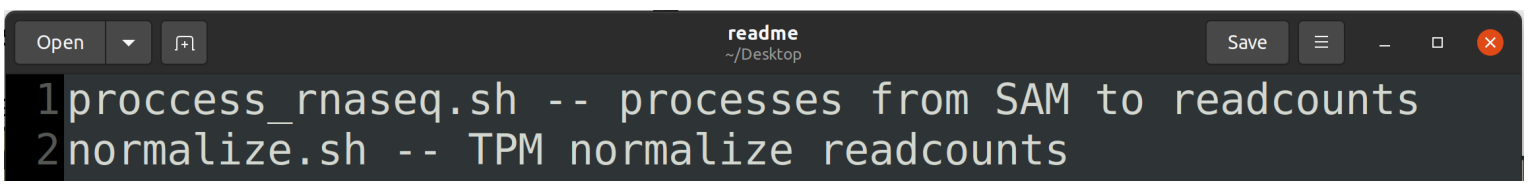
Example, aligning RNA-seq data:

```
$> 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.

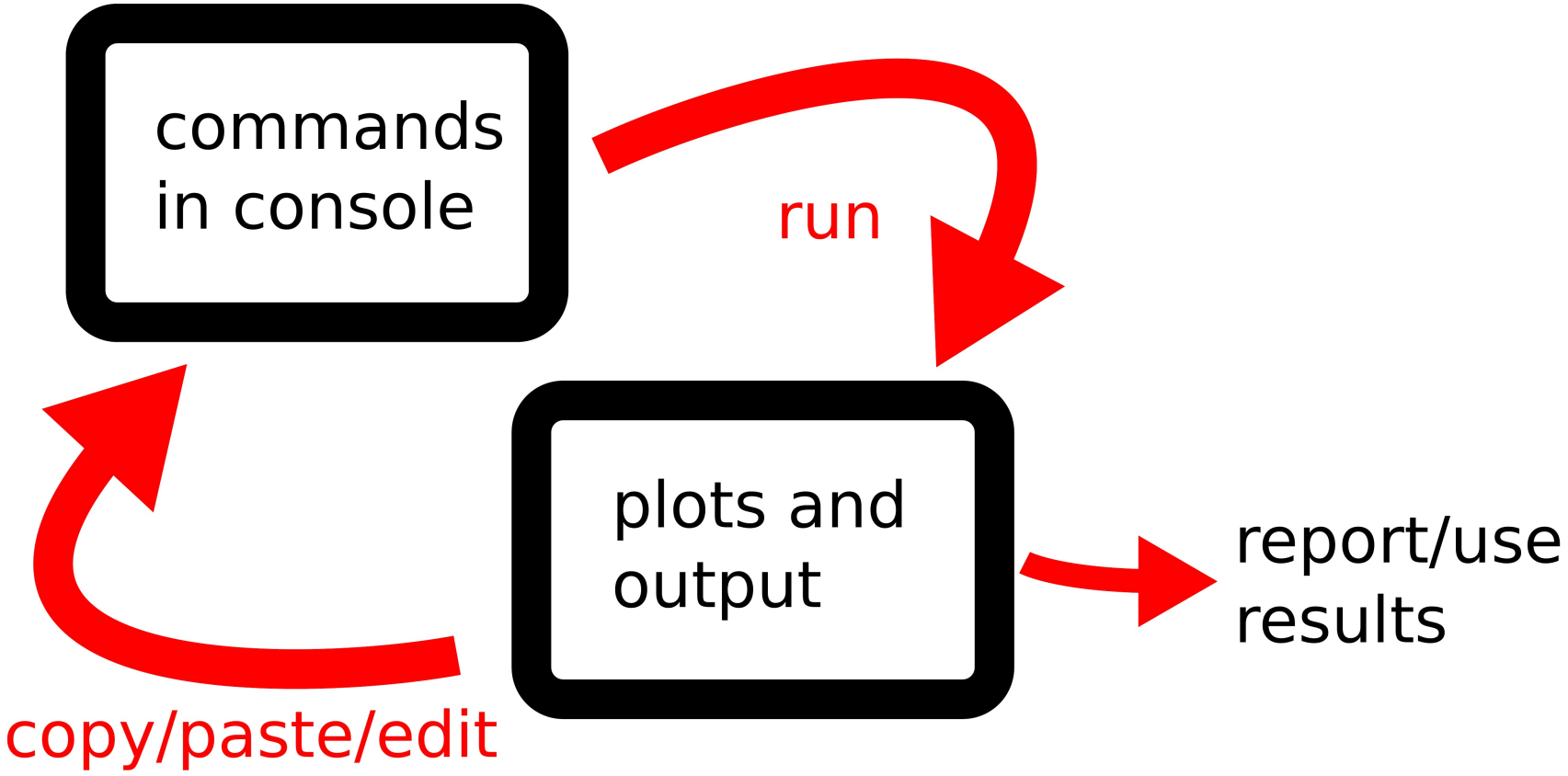
Run with the command `make` and pass in a named argument

```
#>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.

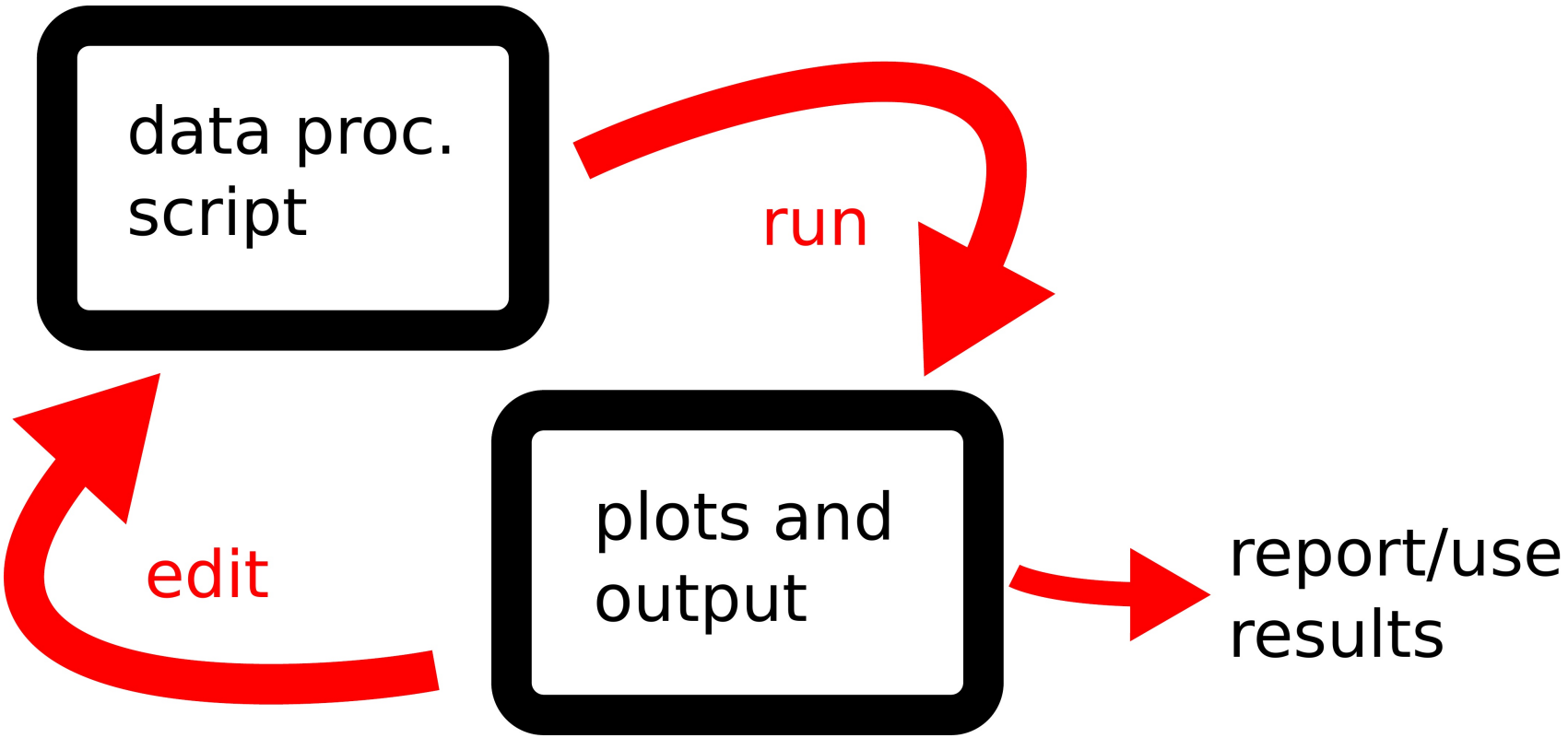
A **less** reproducible process:



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.

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)
```

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DRY advantages:

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

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3. Third* time, refactor it.

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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.

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, . . .

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    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()
```

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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

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2. enhances reproducibility by
   - flagging these analysis choices,
   - exposing them via an interface for easy (third party) experimentation

4. Cache Intermediate Results

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

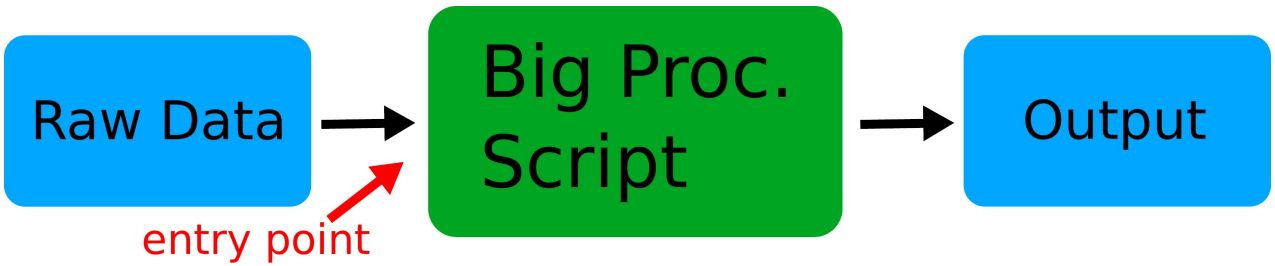
- raw sources, to
- cleaned-up processed data, to
- final results/plots/output

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.

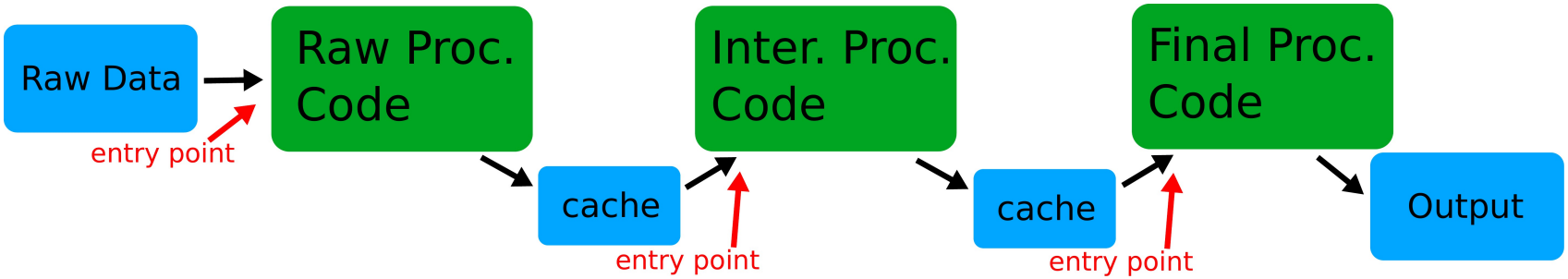
4. Cache Intermediate Results

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...
```

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

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

```
0.261476556288769
```

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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())
```

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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...
0.280758108258287
```

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
```

Testing/Cleaning: good every-so-often practices:

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

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   - re-run your whole analysis (ideally via a `makefile`)
3. code review
   - have someone else look at your code
4. avoid proprietary software

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?

Example: Making code more reproducible.

1. Download the following https://go.wm.edu/qDS1gz
2. Take **five** minutes to refactor this code so that it is more *proactively reproducible*.

We'll reconviene and discuss thoughts.