Simulation

Statistical Computing, STA3005

Wednesday Mar 20, 2024

Last chapter: Package development

Part I: *Simulation basics*

Why simulate?

R gives us unique access to great simulation tools (unique compared to other languages). Why simulate? Welcome to the 21st century! Two reasons:

- Often, simulations can be easier than hand calculations
- Often, simulations can be made more realistic than hand calculations

Sampling from a given vector

To sample from a given vector, use `sample()`

可以通过 prob argument 来设置概率

```
sample(x=letters, size=10) # Without replacement, the default
```

```
##  [1] "p" "v" "e" "l" "o" "i" "x" "f" "z" "d"
```

```
sample(x=c(0,1), size=10, replace=TRUE) # With replacement
```

(sample size > population size 时必须设置)

```
##  [1] 1 0 1 1 1 0 1 1 1 1
```

```
sample(x=10) # Arguments set as x=1:10, size=10, replace=FALSE
```

```
##  [1]  8  4  9  5 10  3  6  7  1  2
```

Random number generation

To sample from a normal distribution, we have the utility functions:

- `rnorm()` : generate normal random variables
- `pnorm()` : normal distribution function, $\Phi(x) = P(Z \leqslant x)$
- `dnorm()` : normal density function, $\phi(x) = \Phi'(x)$
- `qnorm()` : normal quantile function, $q(y) = \Phi^{-1}(y)$, i.e., $\Phi(q(y)) = y$

Replace "norm" with the name of another distribution, all the same functions apply. E.g., "t", "exp", "gamma", "chisq", "binom", "pois", etc.

Random number examples

Standard normal random variables (mean 0 and variance 1)

```r
n = 100
z = rnorm(n, mean=0, sd=1) # These are the defaults for mean, sd
mean(z)  # Check: sample mean is approximately 0
```

```
## [1] 0.1513339
```

```r
var(z)   # Check: sample variance is approximately 1
```

```
## [1] 0.9852947
```

Estimated distribution function

To compute empirical cumulative distribution function (ECDF)—the standard estimator of the cumulative distribution function (CDF)—use `ecdf()`

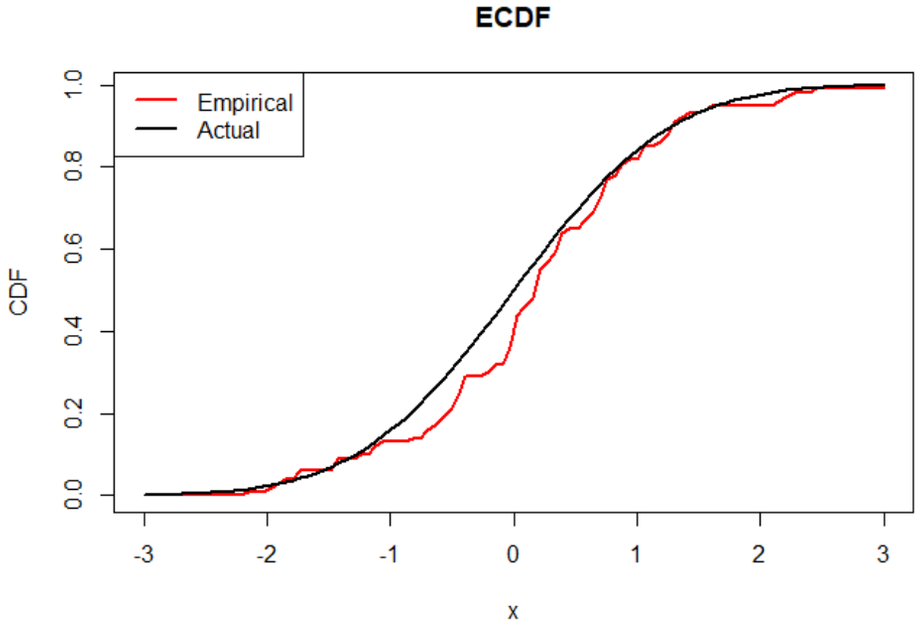
```r
x = seq(-3, 3, length=100)
ecdf.fun = ecdf(z) # Create the ECDF
class(ecdf.fun) # It's a function!
```

```
## [1] "ecdf"     "stepfun"  "function"
```

```r
ecdf.fun(0)
```

```
## [1] 0.38
```

```r
# We can plot it
plot(x, ecdf.fun(x), lwd=2, col="red", type="l", ylab="CDF", main="ECDF")
lines(x, pnorm(x), lwd=2)
legend("topleft", legend=c("Empirical", "Actual"), lwd=2,
       col=c("red","black"))
```



Interlude: Kolmogorov-Smirnov test

One of the most celebrated tests in statistics is due to Kolmogorov in 1933. The *Kolmogorov-Smirnoff (KS) statistic* is:

$$\sqrt{\frac{n}{2}}\sup_x|F_n(x) - G_n(x)|$$

Here F_n is the ECDF of $X_1, \dots, X_n \sim F$, and G_n is the ECDF of $Y_1, \dots, Y_n \sim G$. Under the null hypothesis $F = G$ (two distributions are the same), as $n \to \infty$, the KS statistic approaches the supremum of a Brownian bridge:

$$\sup_{t\in[0,1]}|B(t)|$$

Here, we simulate a Brownian bridge. A Brownian bridge B is a Gaussian process with $B(0) = B(1) = 0$, mean $\mathbb{E}(B(t)) = 0$ for all t, and covariance function

$$\text{Cov}(B(s), B(t)) = s(1-t) \text{ for } s \leqslant t$$

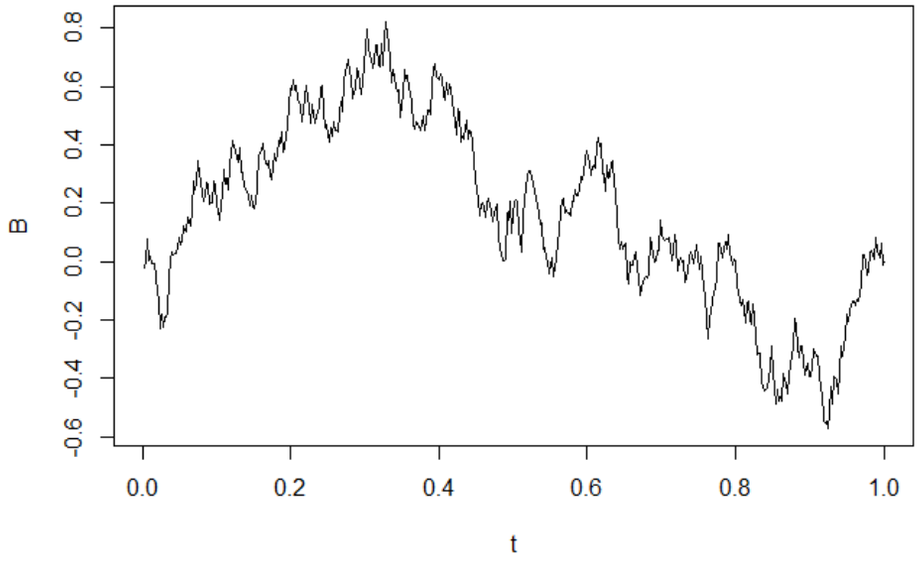
or

$$\text{Cov}(B(s), B(t)) = \min\{s(1-t), t(1-s)\}.$$

```
# Discretize [0,1] interval into 500 grid points
n = 500
t = 1:n/n

# {B(1/500), B(2/500), ..., B(1)} follow a multivariate normal distribution
# Sig represents the covariance matrix
Sig = t %o% (1-t)
Sig = pmin(Sig, t(Sig))
eig = eigen(Sig)

# If AA^T = Sig and Z ~ N(0, I), then AZ ~ N(0, Sig)
Sig.half = eig$vec %*% diag(sqrt(eig$val)) %*% t(eig$vec)
B = Sig.half %*% rnorm(n)
plot(t, B, type="l")
```



Two remarkable facts about the KS test:

1. It is *distribution-free*, meaning that the null distribution doesn't depend on F, G!

2. We can actually compute the null distribution and use this test, e.g., via `ks.test()`:

```
ks.test(rnorm(n), rt(n, df=1)) # Normal versus t1
```

```
##
##  Asymptotic two-sample Kolmogorov-Smirnov test
##
## data:  rnorm(n) and rt(n, df = 1)
## D = 0.158, p-value = 7.589e-06
## alternative hypothesis: two-sided
```

```
ks.test(rnorm(n), rt(n, df=10)) # Normal versus t10
```

```
##
##  Asymptotic two-sample Kolmogorov-Smirnov test
##
## data:  rnorm(n) and rt(n, df = 10)
## D = 0.046, p-value = 0.6654
## alternative hypothesis: two-sided
```

Note: the larger the degree of freedom of a t distribution is, the more similar it is to a standard normal dsitribution.

Estimated density function

To compute histogram—a basic estimator of the density based on binning—use `hist()`

```
hist.obj = hist(z, breaks=30, plot=FALSE)
class(hist.obj) # It's a list
```

```
## [1] "histogram"
```

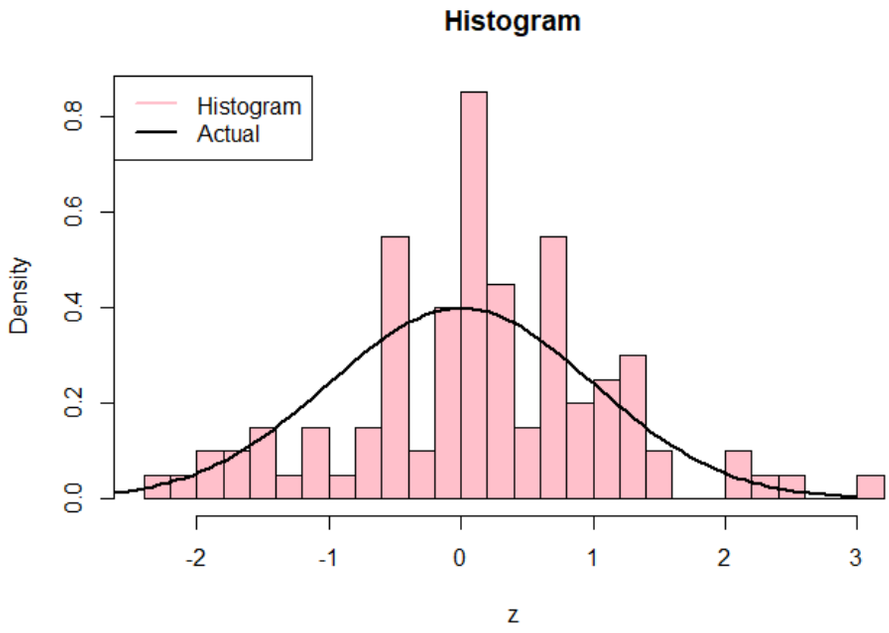
```
hist.obj$breaks # These are the break points that were used
```

```
##  [1] -2.4 -2.2 -2.0 -1.8 -1.6 -1.4 -1.2 -1.0 -0.8 -0.6 -0.4 -0.2  0.0  0.2  0.4
## [16]  0.6  0.8  1.0  1.2  1.4  1.6  1.8  2.0  2.2  2.4  2.6  2.8  3.0  3.2
```

```
hist.obj$density # These are the estimated probabilities
```

```
##  [1] 0.05 0.05 0.10 0.10 0.15 0.05 0.15 0.05 0.15 0.55 0.10 0.40 0.85 0.45 0.15
## [16] 0.55 0.20 0.25 0.30 0.10 0.00 0.00 0.10 0.05 0.05 0.00 0.00 0.05
```

```
# We can plot it 即使在创建 hist object 时设置了 col，在 plot 时仍要额外设置
plot(hist.obj, col="pink", freq=FALSE, main="Histogram")
lines(x, dnorm(x), lwd=2)
legend("topleft", legend=c("Histogram", "Actual"), lwd=2,
       col=c("pink","black"))
```



Part II: *Pseudorandomness and seeds*

Same function call, different results

Not surprisingly, we get different draws each time we call `rnorm()`

```
mean(rnorm(n))
```

```
## [1] -0.03837689
```

```
mean(rnorm(n))
```

```
## [1] -0.05118108
```

```
mean(rnorm(n))
```

```
## [1] 0.05634469
```

```
mean(rnorm(n))
```

```
## [1] 0.01551291
```

Is it really random?

Random numbers generated in R (in any language) are not "truly" random; they are what we call **pseudorandom**

- These are numbers generated by computer algorithms that very closely mimick "truly" random numbers
- The study of such algorithms is an interesting research area in its own right!
- The default algorithm in R (and in nearly all software languages) is called the "Mersenne Twister", which a kind of congruetial generators.

Mersenne-Twister

Consider an initial number X_0 and three big integers A, B and m. The next random integer is generated by

$$X_{n+1} \equiv (AX_n + B) \mod m$$

Then, $U_i = \frac{X_i}{m} \in [0, 1), i = 1, 2, \cdots$ can be regarded as a sequence of random number generated from 0-1 uniform distribution.

- For example, $m = 2^{32}, A = 1,664,525, B = 1,013,904,223$ for a huge period
- Always repeat after sufficient large number of iterations
- Type `?Random` in your R console to read more about this (and to read how to change the algorithm used for pseudorandom number generation, which you should never really have to do, by the way)

Setting the random seed

All pseudorandom number generators depend on what is called a **seed** value

- This puts the random number generator in a well-defined "state", so that the numbers it generates, from then on, will be reproducible
- The seed is just an integer, and can be set with `set.seed()`
- The reason we set it: so that when someone else runs our simulation code, they can see the same—albeit, still random—results that we do

Seed examples

```
# Getting the same 5 random normals over and over
set.seed(0); rnorm(5)
```

```
## [1]  1.2629543 -0.3262334  1.3297993  1.2724293  0.4146414
```

```
set.seed(0); rnorm(5)
```

```
## [1]  1.2629543 -0.3262334  1.3297993  1.2724293  0.4146414
```

```
set.seed(0); rnorm(5)
```

```
## [1]  1.2629543 -0.3262334  1.3297993  1.2724293  0.4146414
```

```
# Different seeds, different numbers
set.seed(1); rnorm(5)
```

```
## [1] -0.6264538  0.1836433 -0.8356286  1.5952808  0.3295078
```

```
set.seed(2); rnorm(5)
```

```
## [1] -0.89691455  0.18484918  1.58784533 -1.13037567 -0.08025176
```

```
set.seed(3); rnorm(5)
```

```
## [1] -0.9619334 -0.2925257  0.2587882 -1.1521319  0.1957828
```

```r
# Each time the seed is set, the same sequence follows (indefinitely)
set.seed(0); rnorm(3); rnorm(2); rnorm(1)
```

```
## [1]  1.2629543 -0.3262334  1.3297993
```

```
## [1] 1.2724293 0.4146414
```

```
## [1] -1.53995
```

```r
set.seed(0); rnorm(1); rnorm(2); rnorm(3)
```

(normal r.v. generator 需要2个 unif r.v. generator)

↓

Box-Muller method

```
## [1] 1.262954
```

```
## [1] -0.3262334  1.3297993
```

```
## [1]  1.2724293  0.4146414 -1.5399500
```

```r
set.seed(0); rnorm(6)
```

```
## [1]  1.2629543 -0.3262334  1.3297993  1.2724293  0.4146414 -1.5399500
```

Generate discrete random variables by inverse method

Suppose we have a sequence of 0-1 uniform random number $U_i, i = 1, 2, \cdots, N$. We want to generate X_i i.i.d. from a discrete distribution with a known probability distribution

$$Pr(X_i \leqslant x) = p_x, x = 0, 1, 2, \cdots$$

Let $X_i = x$, if $U_i \leqslant p_x$ and $U > p_{x-1}$. Then, $X_i \sim p_x$.

Example: Draw from Binomial(3,0.5)

```r
# Inverse method
pmf <- dbinom(0:3, 3, 0.5)
x_inv <- sample(0:3, size = 1000, replace = TRUE, prob = pmf)

table(x_inv)/1000
```

```
## x_inv
##     0     1     2     3
## 0.129 0.372 0.379 0.120
```

```r
pmf
```

```
## [1] 0.125 0.375 0.375 0.125
```

Generate continuous random variables by inverse method

Instead, we want to generate X_i i.i.d. from a continuous distribution with a known probability distribution

$$Pr(X_i \leqslant x) = F(x)$$

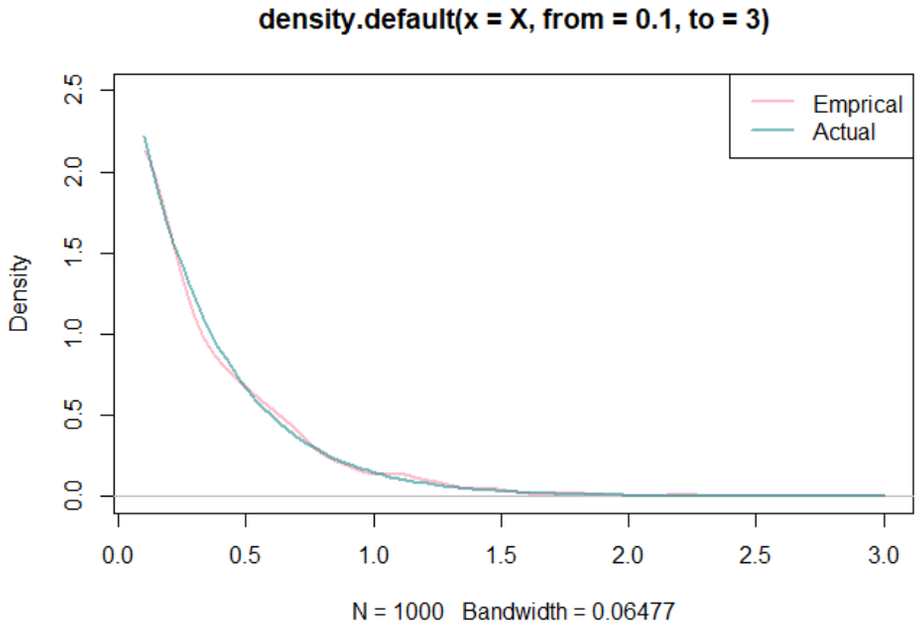
Let $X_i = F^{-1}(U_i)$, where F^{-1} is the inverse function of F. Then, $X_i \sim F(x)$.

Example: Draw from Exp(3)

$$F(x) = 1 - \exp(-3x) \Rightarrow x = F^{-1}(u) = -\frac{\log(1-u)}{3}$$

```
# Inverse method
n <- 1000
U <- runif(n)
X <- - log(1-U)/3
plot(density(X, from  = 0.1, to = 3),  col = "pink", ylim = c(0,2.5), lwd = 2)

x_seq = seq(0.1, 3, length=100)
lines(x_seq, dexp(x_seq,3), lwd=2, col = rgb(0,0.5,0.5,0.5))
legend("topright", legend=c("Emprical", "Actual"), lwd=2,
       col=c("pink",rgb(0,0.5,0.5,0.5)))
```



Part III: *Iteration and simulation*

Drug effect model

- Let's start with a motivating example: suppose we had a model for the way a drug affected certain patients.
- We guess those who aren't given the drug experience a reduction in tumor size of percentage

$$X_{\text{no drug}} \sim 10 \cdot \text{Exp}(\text{mean} = R), \quad R \sim \text{Unif}(0, 1)$$

- And those who were given the drug experience a reduction in tumor size of percentage

$$X_{\text{drug}} \sim 10 \cdot \text{Exp}(\text{mean} = 2)$$

(Here Exp denotes the exponential distribution, and Unif does the uniform distribution)

What would you do?

What would you do if you had such a model, and your scientist collaborators asked you: *how many patients would we need to have in each group (drug, no drug), in order to reliably see that the average reduction in tumor size is significantly different between two groups?*

- Answer used to be: get out your pen and paper, make some approximations
- Answer is now: simulate from the model, no approximations required!

So, let's simulate!

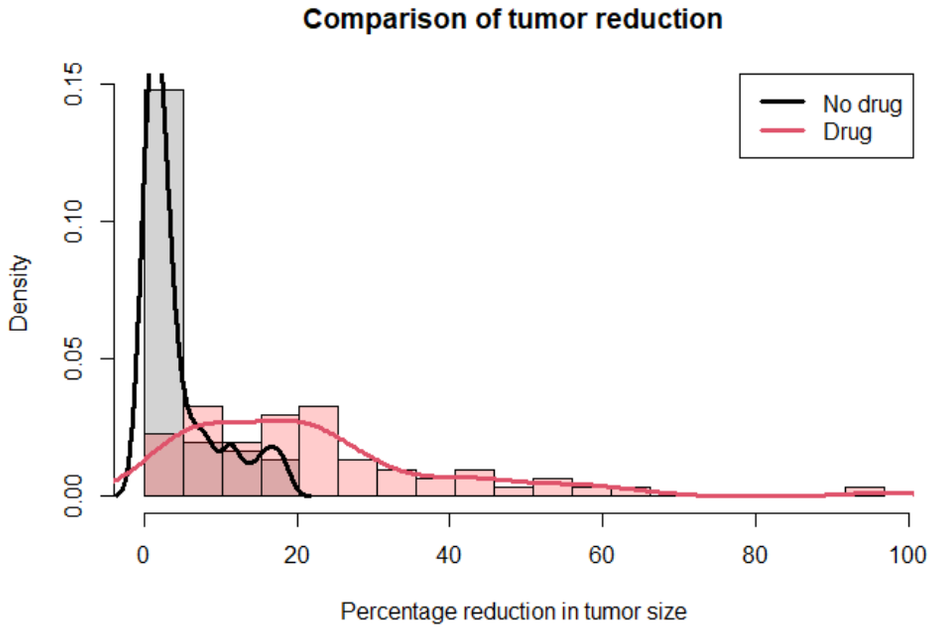
```
# Simulate, supposing 60 subjects in each group
set.seed(0)
n = 60
mu.drug = 2
mu.nodrug = runif(n, min=0, max=1)
x.drug = 10*rexp(n, rate=1/mu.drug)
x.nodrug = 10*rexp(n, rate=1/mu.nodrug)
```

```
# Find the range of all the measurements together, and define breaks
x.range = range(c(x.nodrug,x.drug))
breaks = seq(min(x.range),max(x.range),length=20)

# Produce hist of the non drug measurements, then drug measurements on top
hist(x.nodrug, breaks=breaks, probability=TRUE, xlim=x.range,
     col="lightgray", xlab="Percentage reduction in tumor size",
     main="Comparison of tumor reduction")

# Plot a histogram of the drug measurements, on top
hist(x.drug, breaks=breaks, probability=TRUE, col=rgb(1,0,0,0.2), add=TRUE)

# Draw estimated densities on top, for each dist
lines(density(x.nodrug), lwd=3, col=1)
lines(density(x.drug), lwd=3, col=2)
legend("topright", legend=c("No drug","Drug"), lty=1, lwd=3, col=1:2)
```




```
# Two sample t-test
test <- t.test(x.nodrug, x.drug)
test
```

```
##
##  Welch Two Sample t-test
##
## data:  x.nodrug and x.drug
## t = -7.401, df = 67.675, p-value = 2.743e-10
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  -22.69881 -13.05739
```

```
## sample estimates:
## mean of x mean of y
##  4.255374 22.133476
```

Repetition and reproducibility

- One single simulation is not always trustworthy (depends on the situation, of course)
- In general, simulations should be repeated and aggregate results reported—requires iteration!
- To make random number draws reproducible, we must set the seed with `set.seed()`
- More than this, to make simulation results reproducible, we need to follow **good programming practices**
- Gold standard: any time you show a simulation result (a figure, a table, etc.), you have code that can be run (by anyone) to produce exactly the same result

```
drug.sim = function(n.sample, mu.drug=2, mu.nodrug.range=c(0,1)) {
  mu.nodrug <- runif(n.sample, mu.nodrug.range[1], mu.nodrug.range[2])
  x.drug = 10*rexp(n.sample, rate=1/mu.drug)
  x.nodrug = 10*rexp(n.sample, rate=1/mu.nodrug)
  drug.test <- t.test(x.drug, x.nodrug)
  return(drug.test$p.value)
}
```

Iteration and simulation (and functions): good friends

- Writing a **function** to complete a single run of your simulation is often very helpful
- This allows the simulation itself to be intricate (e.g., intricate steps, several simulation parameters), but makes running the simulation simple
- Then you can use **iteration** to run your simulation over and over again
- Good design practice: write another function for this last part (running your simulation many times)

Code sketch

Consider the code below for a generic simulation. Think about how you would frame this for the drug effect example, which you'll revisit in the assignment

```
# Function to do one simulation run
one.sim = function(param1, param2=value2, param3=value3) {
  # Possibly intricate simulation code goes here
}

# Function to do repeated simulation runs
rep.sim = function(nreps, param1, param2=value2, param3=value3, seed=NULL) {
  # Set the seed, if we need to
  if(!is.null(seed)) set.seed(seed)

  # Run the simulation over and over
  sim.objs = vector(length=nreps, mode="list")
  for (r in 1:nreps) {
    sim.objs[r] = one.sim(param1, param2, param3)
  }

  # Aggregate the results somehow, and then return something
}
```

Saving results

Sometimes simulations take a long time to run, and we want to save intermediate or final output, for quick reference later

There two different ways of saving things from R (there are more than two, but here are two useful ones):

- `saveRDS()` : allows us to save single R objects (like a vector, matrix, list, etc.), in (say) .rds format. E.g.,

```
saveRDS(my.mat, file="my.matrix.rds")
```

- `save()` : allows us to save any number of R objects in (say) .rdata format. E.g.,

```
save(mat.x, mat.y, list.z, file="my.objects.rdata")
```

- `save.image()` : allows use to save the entire global enviroment (workspace) in .rdata format. E.g.,

```
save.image(file="my.wk.space.rdata")
```

Note: there is a big difference between how these two treat variable names

Loading results

Corresponding to the two different ways of saving, we have two ways of loading things into R:

- `readRDS()` : allows us to load an object that has been saved by `savedRDS()` , and **assign a new variable name**. E.g.,

```
my.new.mat = readRDS("my.matrix.rds")
```

- `load()` : allows us to load all objects that have been saved through `save()` , **according to their original variables names**. E.g.,

```
load("my.objects.rdata")
```

Note: you can also load the entire workspace by `load()`

Summary

- Running simulations is an integral part of being a statistician in the 21st century
- R provides us with a utility functions for simulations from a wide variety of distributions
- To make your simulation results reproducible, you must set the seed, using `set.seed()`
- Inverse method generates random numbers based on a sequence of uniform random numbers
- There is a natural connection between iteration, functions, and simulations
- Saving and loading results can be done in two formats: rds and rdata formats