Creating simulated data sets in R

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Contents

The ability to simulate data is a useful tool for better understanding statistical analyses and planning experimental designs. These notes illustrate how to simulate data using a variety of different functions in the R programming language, then discuss how data simulation can be used in research. These notes borrow heavily from a Stirling Coding Club session on randomisation, and to a lesser extent from a session on linear models. After working through these notes, the reader should be able to simulate their own data sets and use them to explore data visualisations and statistical analysis. These notes are also available as a PDF.

Introduction: Simulating data

The ability generate simulated data is very useful in a lot of research contexts. Simulated data can be used to better understand statistical methods, or in some cases to actually run statistical analyses (e.g., simulating a null distribution against which to compare a sample). Here I want to demonstrate how to simulate data in R. This can be accomplished with base R functions including `rnorm`, `runif`, `rbinom`, `rpois`, or `rgamma`;

all of these functions sample univariate data (i.e., one variable) from a specified distribution. The function `sample` can be used to sample elements from an R object with or without replacement. Using the MASS library, the `mvtnorm` function will sample multiple variables with a known correlation structure (i.e., we can tell R how variables should be correlated with one another) and normally distributed errors.

Below, I will first demonstrate how to use some common functions in R for simulating data. Then, I will illustrate how these simulated data might be used to better understand common statistical analyses and data visualisation.

Univariate random numbers

Below, I introduce some base R functions that simulate (pseudo)random numbers from a given distribution. Note that most of what follows in this section is a recreation of a similar section in the notes for randomisation analysis in R.

Sampling from a uniform distribution

The `runif` function returns some number (`n`) of random numbers from a uniform distribution with a range from a (`min`) to b (`max`) such that $X \sim \mathcal{U}(a, b)$ (verbally, X is sampled from a uniform distribution with the parameters a and b), where $-\infty < a < b < \infty$ (verbally, a is greater than negative infinity but less than b, and b is finite). The default is to draw from a standard uniform distribution (i.e., $a = 0$ and $b = 1$) as done below.

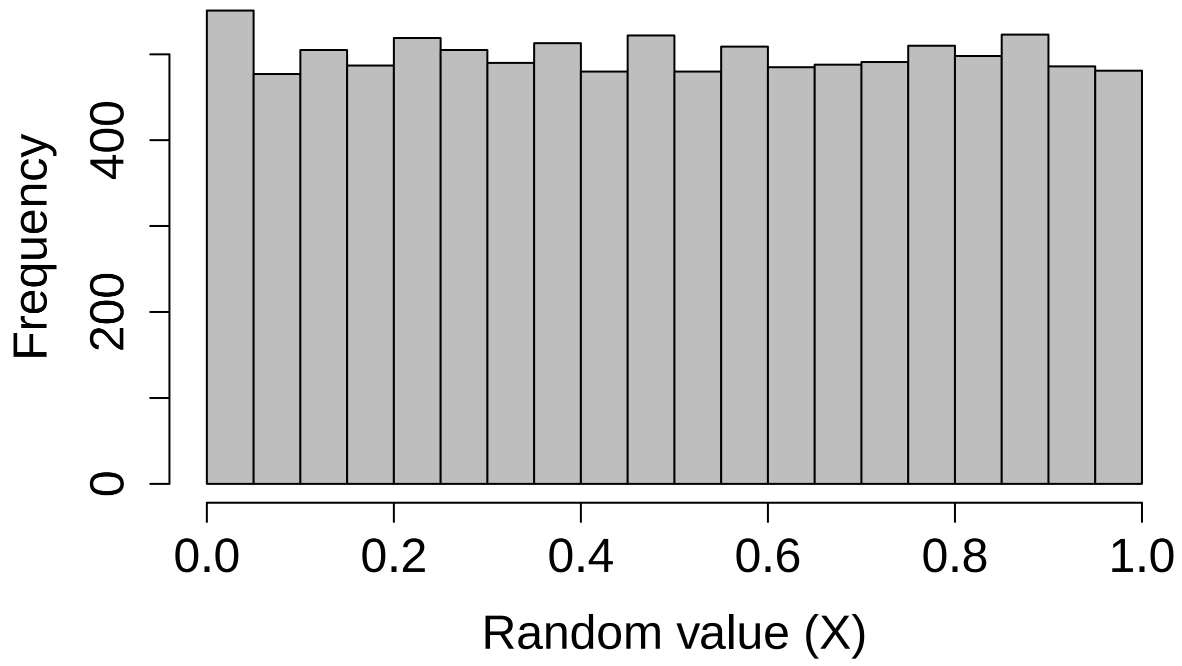
```r
rand_unifs_10 <- runif(n = 10, min = 0, max = 1);
```

The above code stores a vector of ten numbers `rand_unifs_10`, shown below. Note that the numbers will be different each time we re-run the `runif` function above.

```
##  [1] 0.7509029 0.7572325 0.6623544 0.7408719 0.9491530 0.7507392 0.3800938
##  [8] 0.9743183 0.1405556 0.8090658
```

We can visualise the standard uniform distribution that is generated by plotting a histogram of a very large number of values created using `runif`.

```r
rand_unifs_10000 <- runif(n = 10000, min = 0, max = 1);
hist(rand_unifs_10000, xlab = "Random value (X)", col = "grey",
     main = "", cex.lab = 1.5, cex.axis = 1.5);
```



The random uniform distribution is special in some ways. The algorithm for generating random uniform numbers is the starting point for generating random numbers from other distributions using methods such as rejection sampling, inverse transform sampling, or the Box Muller method (Box and Muller 1958).

Sampling from a normal distribution

The `rnorm` function returns some number (`n`) of randomly generated values given a set mean (μ; `mean`) and standard deviation (σ; `sd`), such that $X \sim \mathcal{N}(\mu, \sigma^2)$. The default is to draw from a standard normal (a.k.a., "Gaussian") distribution (i.e., $\mu = 0$ and $\sigma = 1$).

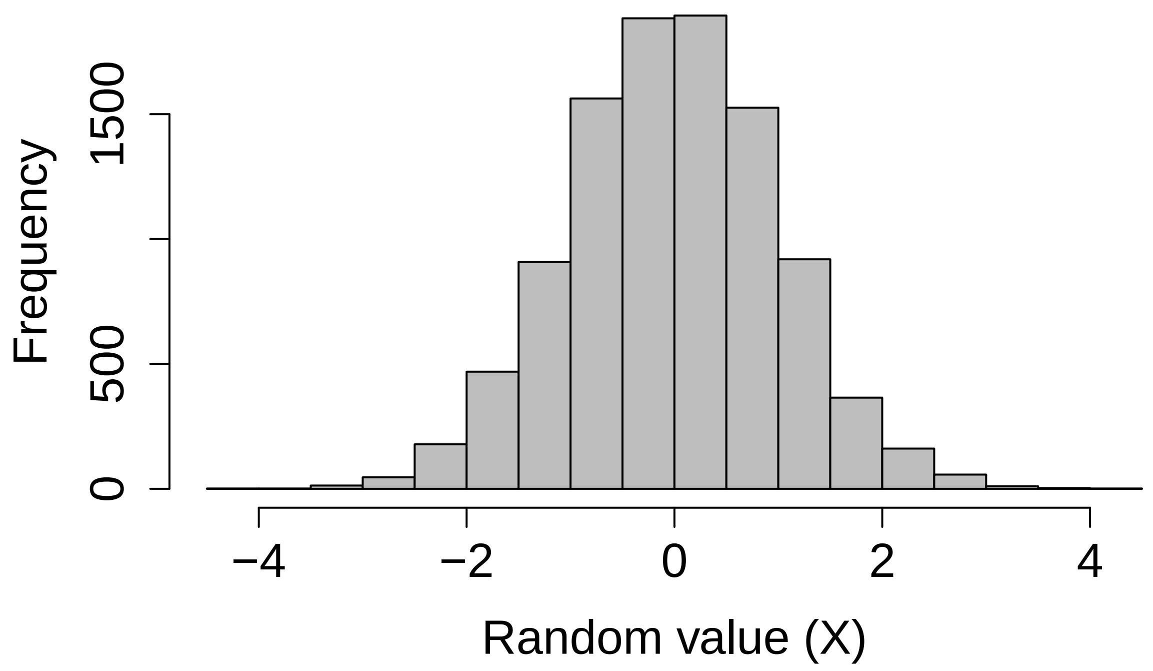
```
rand_norms_10 <- rnorm(n = 10, mean = 0, sd = 1);
```

The above code stores a vector of 10 numbers, shown below.

```
##  [1] -0.8756363  2.3899310 -0.5227091  1.2904072 -1.5955765 -1.2644592
##  [7]  0.7433444 -1.3839452 -2.1338794 -0.1006011
```

We can verify that a standard normal distribution is generated by plotting a histogram of a very large number of values created using `rnorm`.

```
rand_norms_10000 <- rnorm(n = 10000, mean = 0, sd = 1);
hist(rand_norms_10000, xlab = "Random value (X)", col = "grey",
     main = "", cex.lab = 1.5, cex.axis = 1.5);
```



Generating a histogram using data from a simulated distribution like this is often a useful way to visualise distributions, or to see how samples from the same distribution might vary. For example, if we wanted to compare the above distribution with a normal distribution that had a standard deviation of 2 instead of 1, then we could simply sample 10000 new values in `rnorm` with `sd = 2` instead of `sd = 1` and create a new histogram with `hist`. If we wanted to see what the distribution of sampled data might look like given a low sample size (e.g., 10), then we could repeat the process of sampling from `rnorm(n = 10, mean = 0, sd = 1)` multiple times and looking at the shape of the resulting histogram.

Sampling from a poisson distribution

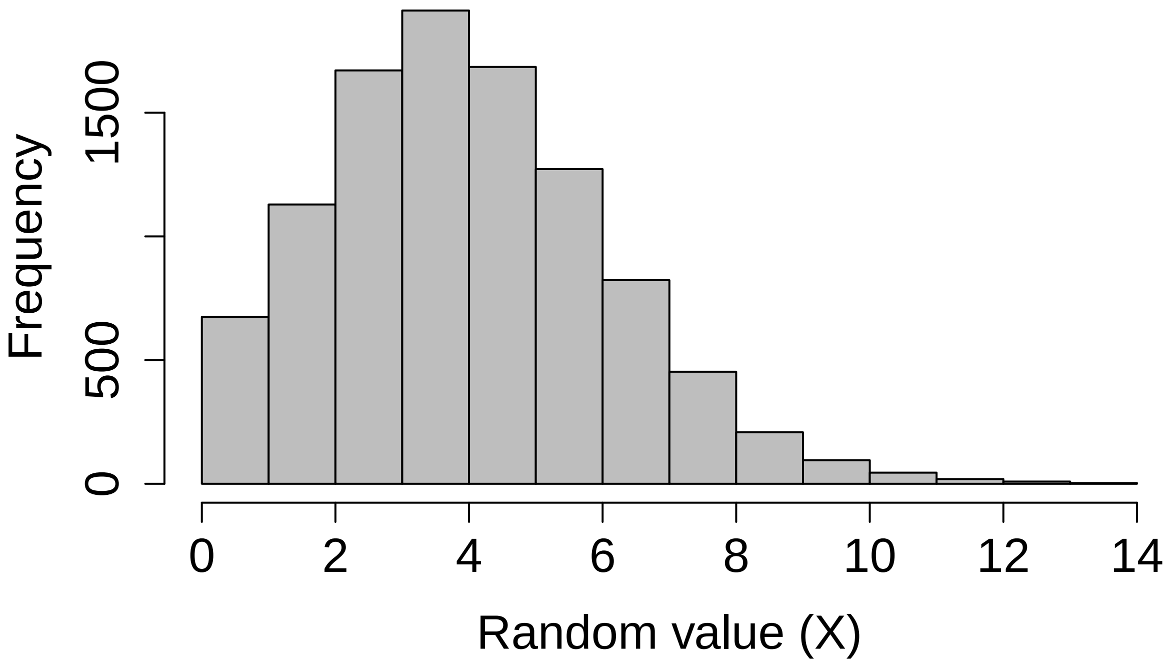
Many processes in biology can be described by a Poisson distribution. A Poisson process describes events happening with some given probability over an area of time or space such that $X \sim Poisson(\lambda)$, where the rate parameter λ is both the mean and variance of the Poisson distribution (note that by definition, $\lambda > 0$, and although λ can be any positive real number, data are always integers, as with count data). Sampling from a Poisson distribution can be done in R with `rpois`, which takes only two arguments specifying the number of values to be returned (`n`) and the rate parameter (`lambda`).

```
rand_poissons <- rpois(n = 10, lambda = 1.5);
print(rand_poissons);
```

```
##  [1] 1 1 4 4 2 1 1 3 1 3
```

There are no default values for `rpois`. We can plot a histogram of a large number of values to see the distribution when $\lambda = 4.5$ below.

```
rand_poissons_10000 <- rpois(n = 10000, lambda = 4.5);
hist(rand_poissons_10000, xlab = "Random value (X)", col = "grey",
     main = "", cex.lab = 1.5, cex.axis = 1.5);
```



Sampling from a binomial distribution

Sampling from a binomial distribution in R with `rbinom` is a bit more complex than using `runif`, `rnorm`, or `rpois`. Like those previous functions, the `rbinom` function returns some number (`n`) of random numbers, but the arguments and output can be slightly confusing at first. Recall that a binomial distribution describes the number of 'successes' for some number of independent trials ($\Pr(success) = p$). The `rbinom` function returns the number of successes after `size` trials, in which the probability of success in each trial is `prob`. For a concrete example, suppose we want to simulate the flipping of a fair coin 1000 times, and we want to know how many times that coin comes up heads ('success'). We can do this with the following code.

```
coin_flips <- rbinom(n = 1, size = 1000, prob = 0.5);
print(coin_flips);
```

```
## [1] 497
```

The above result shows that the coin came up heads 497 times. Note, however, the (required) argument `n` above. This allows the user to set the number of sequences to run. In other words, if we set `n = 2`, then this could simulate the flipping of a fair coin 1000 times once to see how many times heads comes up, then repeating the whole process a second time to see how many times heads comes up again (or, if it is more intuitive, the flipping of two separate fair coins 1000 times).

```
coin_flips_2 <- rbinom(n = 2, size = 1000, prob = 0.5);
print(coin_flips_2);
```

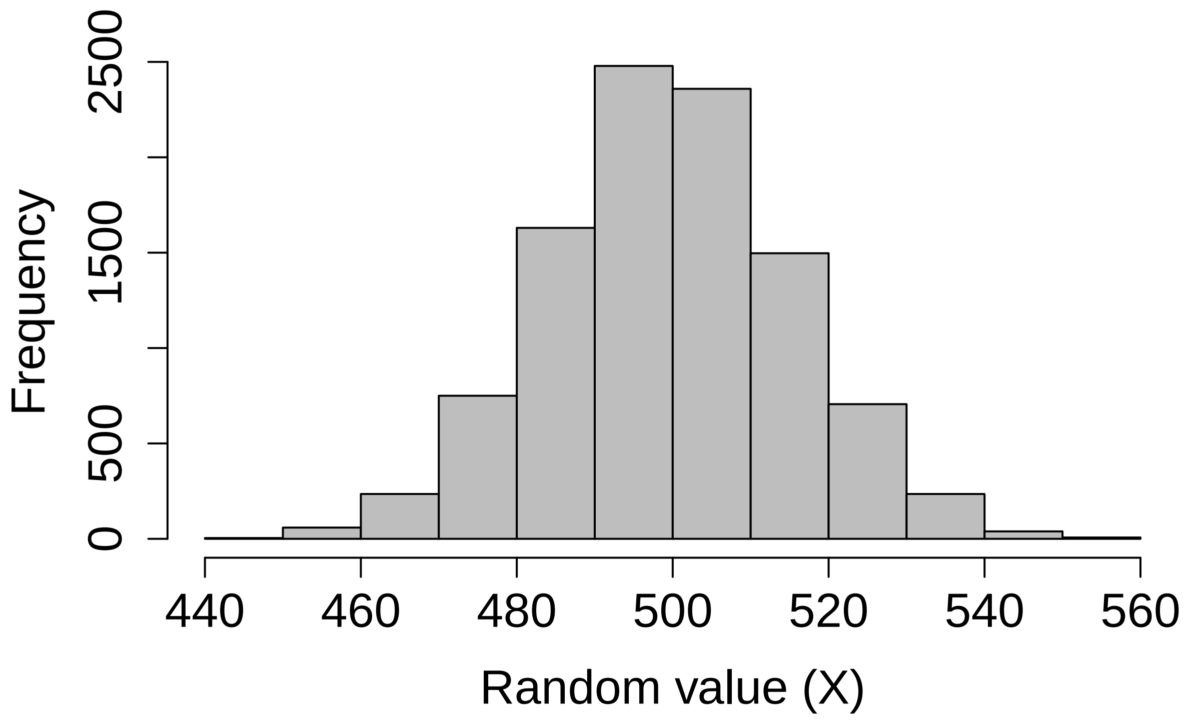
```
## [1] 484 495
```

In the above, a fair coin was flipped 1000 times and returned 484 heads, and then another fair coin was flipped 1000 times and returned 495 heads. As with the `rnorm` and `runif` functions, we can check to see what the distribution of the binomial function looks like if we repeat this process. Suppose, in other words, that we want to see the distribution of the number of times heads comes up after 1000 flips. We can, for example, simulate the process of flipping 1000 times in a row with 10000 different coins using the code below.

```
coin_flips_10000 <- rbinom(n = 10000, size = 1000, prob = 0.5);
```

I have not printed the above `coin_flips_10000` for obvious reasons, but we can use a histogram to look at the results.

```
hist(coin_flips_10000, xlab = "Random value (X)", col = "grey",
     main = "", cex.lab = 1.5, cex.axis = 1.5);
```



As would be expected, most of the time 'heads' occurs around 500 times out of 1000, but usually the actual number will be a bit lower or higher due to chance. Note that if we want to simulate the results of individual flips in a single trial, we can do so as follows.

```
flips_10 <- rbinom(n = 10, size = 1, prob = 0.5);
```

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

In the above, there are `n = 10` trials, but each trial consists of only a single coin flip (`size = 1`). But we can equally well interpret the results as a series of `n` coin flips that come up either heads (`1`) or tails (`0`). This latter interpretation can be especially useful to write code that randomly decides whether some event will happen (`1`) or not (`0`) with some probability `prob`.

Random sampling using `sample`

Sometimes it is useful to sample a set of values from a vector or list. The R function `sample` is very flexible for sampling a subset of numbers or elements from some structure (`x`) in R according to some set probabilities (`prob`). Elements can be sampled from `x` some number of times (`size`) with or without replacement (`replace`), though an error will be returned if the `size` of the sample is larger than `x` but `replace = FALSE` (default).

Sampling random numbers from a list

To start out simple, suppose we want to ask R to pick a random number from one to ten with equal probability.

```
rand_number_1 <- sample(x = 1:10, size = 1);
print(rand_number_1);
```

```
## [1] 10
```

The above code will set `rand_number_1` to a randomly selected value, in this case 10. Because we have not specified a probability vector `prob`, the function assumes that every element in `1:10` is sampled with equal probability. We can increase the `size` of the sample to `10` below.

```
rand_number_10 <- sample(x = 1:10, size = 10);
print(rand_number_10);
```

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

Note that all numbers from 1 to 10 have been sampled, but in a random order. This is becaues the default is to sample with replacement, meaning that once a number has been sampled for the first element in `rand_number_10`, it is no longer available to be sampled again. To change this and allow for sampling with replacement, we can change the default.

```
rand_number_10_r <- sample(x = 1:10, size = 10, replace = TRUE);
print(rand_number_10_r);
```

```
##  [1] 8 2 5 9 3 1 2 5 5 7
```

Note that the numbers $\{2, 5\}$ are now repeated in the set of randomly sampled values above. We can also specify the probability of sampling each element, with the condition that these probabilities need to sum to 1. Below shows an example in which the numbers 1-5 are sampled with a probability of 0.05, while the numbers 6-10 are sampled with a probability of 0.15, thereby biasing sampling toward larger numbers.

```
prob_vec      <- c( rep(x = 0.05, times = 5), rep(x = 0.15, times = 5) );
rand_num_bias <- sample(x = 1:10, size = 10, replace = TRUE, prob = prob_vec);
print(rand_num_bias);
```

```
##  [1] 10  7  2  9  5  7 10 10  4  7
```

Note that `rand_num_bias` above contains more numbers from 6-10 than from 1-5.

Sampling random characters from a list

Sampling characters from a list of elements is no different than sampling numbers, but I am illustrating it separately because I find that I often sample characters for conceptually different reasons. For example, if I want to create a simulated data set that includes three different species, I might create a vector of species identities from which to sample.

```
species <- c("species_A", "species_B", "species_C");
```

This gives three possible categories, which I can now use `sample` to draw from. Assume that I want to simulate the sampling of these three species, perhaps with `species_A` being twice as common as `species_B` and `species_C`. I might use the following code to sample 24 times.

```
sp_sample <- sample(x = species, size = 24, replace = TRUE,
                    prob = c(0.5, 0.25, 0.25)
                    );
```

Below are the values that get returned.

```
##  [1] "species_A" "species_A" "species_A" "species_A" "species_A" "species_C"
##  [7] "species_A" "species_B" "species_A" "species_A" "species_B" "species_A"
## [13] "species_A" "species_A" "species_C" "species_A" "species_A" "species_A"
## [19] "species_B" "species_A" "species_B" "species_A" "species_A" "species_A"
```

Simulating data with known correlations

We can generate variables X_1 and X_2 that have known correlations ρ with with one another. The code below does this for two standard normal random variables with a sample size of 10000, such that the correlation between them is 0.3.

```
N   <- 10000;
rho <- 0.3;
x1  <- rnorm(n = N, mean = 0, sd = 1);
x2  <- (rho * x1) + sqrt(1 - rho*rho) * rnorm(n = N, mean = 0, sd = 1);
```

Mathematically, these variables are generated by first simulating the sample x_1 (`x1` above) from a standard normal distribution. Then, x_2 (`x2` above) is calculated as below,

$x_2 = \rho x_1 + \sqrt{1 - \rho^2} x_{rand}$,

Where x_{rand} is a sample from a normal distribution with the same variance as x_1. A simple call to the R function `cor` will confirm that the correlation does indeed equal `rho` (with some sampling error).

```
cor(x1, x2);
```

```
## [1] 0.2799764
```

This is useful if we are only interested in two variables, but there is a much more efficient way to generate any number of variables with different variances and correlations to one another. To do this, we need to use the MASS library, which can be installed and loaded as below.

```
install.packages("MASS");
library("MASS");
```

In the MASS library, the function `mvrnorm` can be used to generate any number of variables for a pre-specified covariance structure.

Suppose we want to simulate a data set of three measurements from a species of organisms. Measurement 1 (M_1) has a mean of $\mu_{M_1} = 159.54$ and variance of $Var(M_1) = 12.68$, measurement 2 (M_2) has a mean of $\mu_{M_1} = 245.26$ and variance of $Var(M_2) = 30.39$, and measurement 3 (M_2) has a mean of $\mu_{M_1} = 25.52$ and variance of $Var(M_3) = 2.18$. Below is a table summarising.

measurement	mean	variance
M1	159.54	12.68
M2	245.26	30.39
M3	25.52	2.18

Further, we want the covariance between M_1 and M_2 to equal $Cov(M_1, M_2) = 13.95$, the covariance between M_1 and M_3 to equal $Cov(M_1, M_3) = 3.07$, and the covariance between M_2 and M_3 to equal $Cov(M_2, M_3) = 4.7$. We can put all of this information into a covariance matrix **V** with three rows and three columns. The diagonal of the matrix holds the variances of each variable, with the off-diagonals holding the covariances (note also that the variance of a variable M is just the variable's covariance with itself; e.g., $Var(M_1) = Cov(M_1, M_1)$).

$$V = \begin{pmatrix} Var(M_1), & Cov(M_1, M_2), & Cov(M_1, M_3) \\ Cov(M_2, M_1), & Var(M_2), & Cov(M_2, M_3) \\ Cov(M_3, M_1), & Cov(M_3, M_2), & Var(M_3) \end{pmatrix}.$$

In R, we can create this matrix as follows.

```
matrix_data <- c(12.68, 13.95, 3.07, 13.95, 30.39, 4.70, 3.07, 4.70, 2.18);
cv_mat      <- matrix(data = matrix_data, nrow = 3, ncol = 3, byrow = TRUE);
rownames(cv_mat) <- c("M1", "M2", "M3");
colnames(cv_mat) <- c("M1", "M2", "M3");
```

Here is what `cv_mat` looks like (note that it is symmetrical along the diagonal).

```
##       M1    M2   M3
## M1 12.68 13.95 3.07
## M2 13.95 30.39 4.70
## M3  3.07  4.70 2.18
```

Now we can add the means to a vector in R.

```
mns <- c(159.54, 245.26, 25.52);
```

We are now ready to use the `mvrnorm` function in R to simulate some number `n` of sampled organisms with these three measurements. We use the `mvrnorm` arguments `mu` and `Sigma` to specify the vector of means and covariance matrix, respectively.

```
sim_data <- mvrnorm(n = 40, mu = mns, Sigma = cv_mat);
```

Here are the example data below.

M1	M2	M3
160.3626	243.3549	25.23192
162.7822	249.5737	25.37819
166.3443	249.8801	25.07985
154.7679	240.9511	24.31659
155.2488	240.6471	24.64598
159.1804	247.7235	25.46442

M1	M2	M3
165.5023	254.0871	25.78475
167.3832	252.0561	28.78178
158.6888	247.2276	27.15461
159.2239	247.1460	25.49968
158.3559	243.7494	25.55654
158.9630	236.6612	22.57456
160.8147	244.5186	25.96574
166.1307	250.8496	26.96263
165.5635	250.8109	27.31443
161.4523	245.0603	25.65987
162.6332	250.7438	27.02312
155.9435	238.6337	25.27251
160.9691	245.2572	25.67335
162.1673	246.2041	26.70684
157.6781	239.9921	27.10495
160.4469	241.1811	24.14159
162.0948	241.7324	25.61436
151.5944	237.2404	23.70996
161.2231	245.8584	25.65664
162.2703	251.3218	26.01222
162.3657	249.5309	28.25750
160.1144	244.6785	24.48259
158.1074	246.8832	25.60986
162.7700	245.0326	26.74400
156.7904	244.9419	24.08294
157.6474	242.0578	22.93666
155.3287	247.7704	25.53643
164.4344	245.2851	26.73227
164.1483	255.5635	26.93515
162.3423	248.2778	25.64527
164.8902	252.9837	24.82725
157.5340	248.9831	25.69448
161.6361	247.5924	25.52118
161.5356	240.0215	25.36886

We can check to confirm that the mean values of each column are correct using `apply`.

```
apply(X = sim_data, MARGIN = 2, FUN = mean);
```

```
##        M1        M2        M3 
## 160.68576 246.05162  25.66654
```

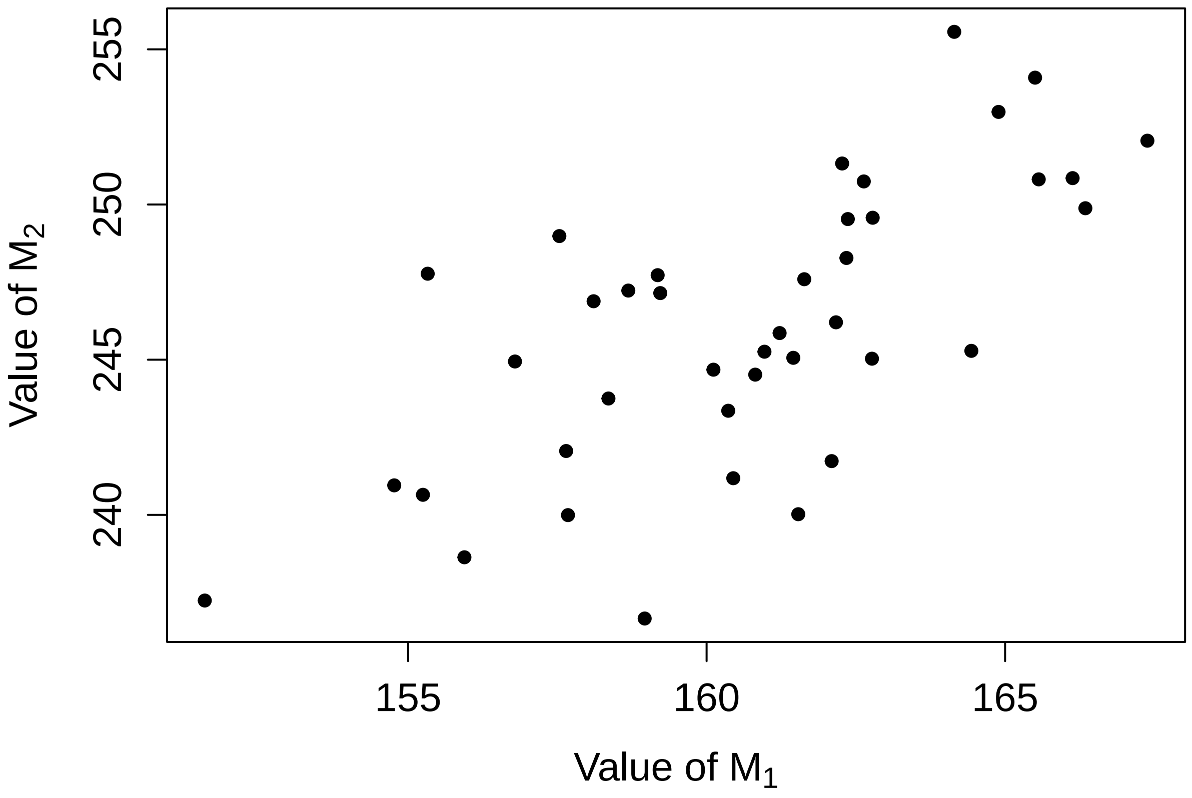
And we can check to confirm that the covariance structure of the data is correct using `cov`.

```
cov(sim_data);
```

```
##           M1        M2       M3
## M1 12.573128 11.216471 2.480759
## M2 11.216471 21.219021 3.346267
## M3  2.480759  3.346267 1.635349
```

Note that the values are not exact, but should become closer to the specified values as increase the sample size `n`. We can visualise the data too; for example, we might look at the close correlation between M_1 and M_2 using a scatterplot, just as we would for data sampled from the field.

```r
par(mar = c(5, 5, 1, 1));
plot(x = sim_data[,1], y = sim_data[,2], pch = 20, cex = 1.25, cex.lab = 1.25,
     cex.axis = 1.25, xlab = expression(paste("Value of ", M[1])),
     ylab = expression(paste("Value of ", M[2])));
```



We could even run an ordination on these simulated data. For example, we could extract the principle components with `prcomp`, then plot the first two PCs to visualise these data. We might, for example, want to compare different methods of ordination using a data set with different, pre-specified properties (e.g., Minchin 1987). We might also want to use simulated data sets to investigate how different statistical tools perform. I show this in the next section, where I put a full data set together and run linear models on it.

Simulating a full data set

Putting everything together, here I will create a data set of three different species from which three different measurements are taken. We can just call these measurements 'length', 'width', and 'mass'. For simplicity, let us assume that these measurements always covary in the same way that we saw with **V** (i.e., `cv_mat`) above. But let's also assume that we have three species with slightly different mean values. Below is the code that will build a new data set of $N = 20$ samples with four columns: species, length, width, and mass.

```r
N           <- 20;
matrix_data <- c(12.68, 13.95, 3.07, 13.95, 30.39, 4.70, 3.07, 4.70, 2.18);
cv_mat      <- matrix(data = matrix_data, nrow = 3, ncol = 3, byrow = TRUE);
mns_1       <- c(159.54, 245.26, 25.52);
```

```r
sim_data_1  <- mvrnorm(n = N, mu = mns, Sigma = cv_mat);
colnames(sim_data_1) <- c("Length", "Width", "Mass");
# Below, I bind a column for indicating 'species_1' identity
species     <- rep(x = "species_1", times = 20); # Repeats 20 times
sp_1        <- data.frame(species, sim_data_1);
```

Let us add one more data column. Suppose that we can also sample the number of offspring each organism has, and that the mean number of offspring that an organism has equals one tenth of the organism's mass. To do this, we can use `rpois`, and take advantage of the fact that the argument `lambda` can be a vector rather than a single value. So to get the number of offspring for each organism based on its body mass, we can just insert the mass vector `sp_1$Mass` times 0.1 for `lambda`.

```r
offspring   <- rpois(n = N, lambda = sp_1$Mass * 0.1);
sp_1        <- cbind(sp_1, offspring);
```

I have also bound the offspring number to the data set `sp_1`. Here is what it looks like below.

species	Length	Width	Mass	offspring
species_1	159.0113	250.7984	24.83656	5
species_1	154.1571	233.4577	22.45595	2
species_1	158.5285	246.0929	24.25284	4
species_1	159.2640	244.0639	24.77818	1
species_1	166.0649	253.3350	27.97753	3
species_1	158.9404	250.7135	25.36085	4
species_1	164.2185	245.0743	25.36301	2
species_1	163.7161	245.9773	27.21383	7
species_1	162.2245	249.8570	28.75093	2
species_1	161.8746	250.2403	26.83533	3
species_1	162.6754	256.1094	27.21100	5
species_1	159.5476	246.7478	26.46932	3
species_1	161.5611	240.0040	25.90780	2
species_1	164.4103	244.9234	25.48097	4
species_1	163.4710	246.9149	25.18949	2
species_1	162.2044	248.9505	30.03781	2
species_1	158.0328	247.2494	26.91347	1
species_1	160.0725	249.4608	28.23195	6
species_1	164.4510	247.3645	27.35433	3
species_1	156.8111	246.1763	24.57261	3

To add two more species, let us repeat the process two more times, but change the expected mass just slightly each time. The code below does this, and puts everything together in a single data set.

```r
# First making species 2
mns_2       <- c(159.54, 245.26, 25.52 + 3); # Add a bit
sim_data_2  <- mvrnorm(n = N, mu = mns, Sigma = cv_mat);
colnames(sim_data_2) <- c("Length", "Width", "Mass");
species     <- rep(x = "species_2", times = 20); # Repeats 20 times
offspring   <- rpois(n = N, lambda = sim_data_2[,3] * 0.1);
sp_2        <- data.frame(species, sim_data_2, offspring);
# Now make species 3
mns_3       <- c(159.54, 245.26, 25.52 + 4.5); # Add a bit more
```

```
sim_data_3  <- mvrnorm(n = N, mu = mns, Sigma = cv_mat);
colnames(sim_data_3) <- c("Length", "Width", "Mass");
species     <- rep(x = "species_3", times = 20); # Repeats 20 times
offspring   <- rpois(n = N, lambda = sim_data_3[,3] * 0.1);
sp_3        <- data.frame(species, sim_data_3, offspring);
# Bring it all together in one data set
dat <- rbind(sp_1, sp_2, sp_3);
```

Our full data set now looks like the below.

species	Length	Width	Mass	offspring
species_1	159.0113	250.7984	24.83656	5
species_1	154.1571	233.4577	22.45595	2
species_1	158.5285	246.0929	24.25284	4
species_1	159.2640	244.0639	24.77818	1
species_1	166.0649	253.3350	27.97753	3
species_1	158.9404	250.7135	25.36085	4
species_1	164.2185	245.0743	25.36301	2
species_1	163.7161	245.9773	27.21383	7
species_1	162.2245	249.8570	28.75093	2
species_1	161.8746	250.2403	26.83533	3
species_1	162.6754	256.1094	27.21100	5
species_1	159.5476	246.7478	26.46932	3
species_1	161.5611	240.0040	25.90780	2
species_1	164.4103	244.9234	25.48097	4
species_1	163.4710	246.9149	25.18949	2
species_1	162.2044	248.9505	30.03781	2
species_1	158.0328	247.2494	26.91347	1
species_1	160.0725	249.4608	28.23195	6
species_1	164.4510	247.3645	27.35433	3
species_1	156.8111	246.1763	24.57261	3
species_2	159.0888	249.4359	26.51284	3
species_2	154.6772	241.8155	24.50630	1
species_2	163.0354	250.1498	23.51754	5
species_2	158.7639	252.9078	27.01738	5
species_2	159.4987	249.0553	24.96255	5
species_2	161.3078	245.0385	26.40047	2
species_2	158.7134	240.3947	25.04027	0
species_2	162.6335	246.0098	27.64063	2
species_2	160.8309	247.8036	23.16477	1
species_2	158.3227	245.1763	25.22077	4
species_2	158.1422	245.1502	22.92787	2
species_2	158.6302	247.4524	22.77116	1
species_2	157.2669	248.1639	25.26655	0
species_2	156.9296	249.3084	26.59826	2
species_2	156.1447	239.7409	25.21606	3
species_2	153.2131	235.6938	25.39891	1
species_2	160.8431	241.7733	24.34945	2
species_2	163.1760	249.6963	25.35015	0
species_2	153.8687	243.6540	23.95292	5
species_2	156.4811	245.7730	24.82242	4
species_3	163.1477	247.8090	27.57055	4
species_3	160.8497	253.5204	27.32570	2

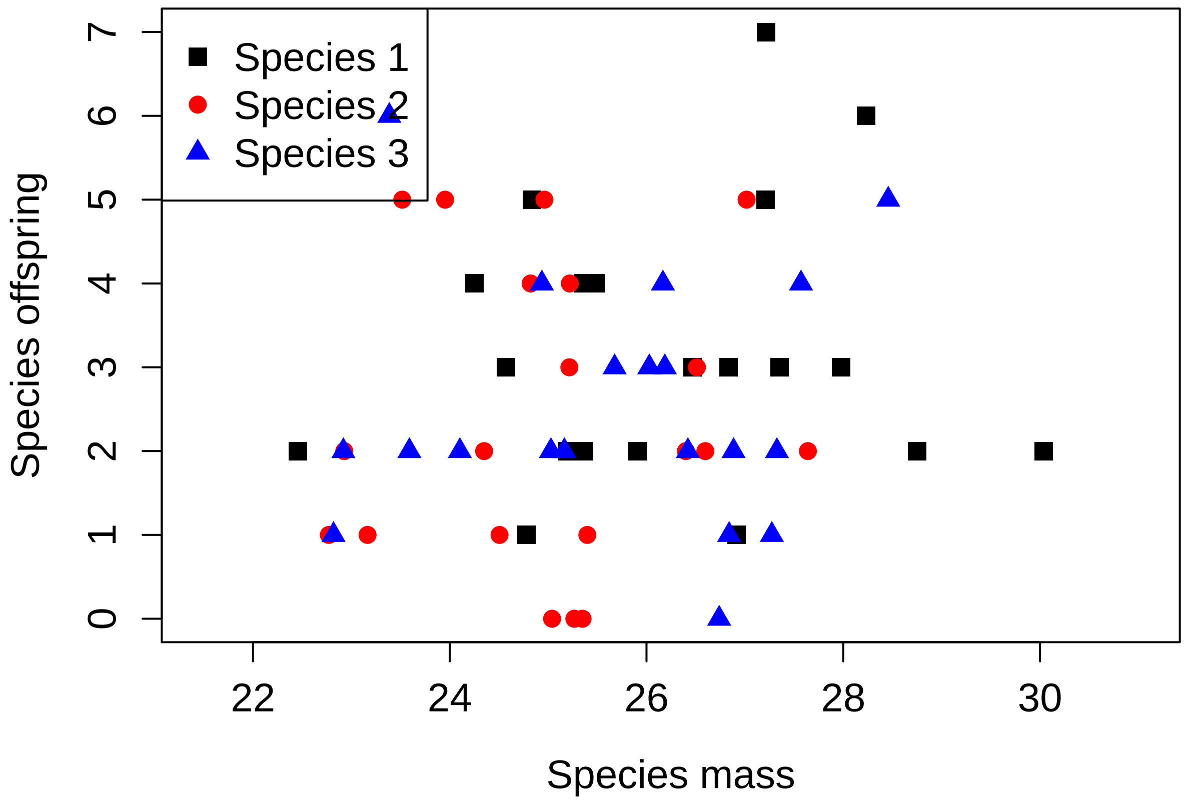
species	Length	Width	Mass	offspring
species_3	154.2328	241.2828	25.02871	2
species_3	155.0204	235.9476	26.16691	4
species_3	155.9114	239.0644	22.81872	1
species_3	166.2133	258.0434	26.88514	2
species_3	155.7555	245.4111	25.16524	2
species_3	167.6971	257.5420	27.27423	1
species_3	151.2289	241.9858	23.38577	6
species_3	154.4216	239.7416	22.91903	2
species_3	163.6301	245.3597	26.84020	1
species_3	163.1049	249.3539	26.18650	3
species_3	160.9147	250.3723	26.73870	0
species_3	159.0499	247.6844	25.67611	3
species_3	151.6900	238.1012	23.58986	2
species_3	157.1262	241.9523	26.02859	3
species_3	163.8989	250.3643	26.42061	2
species_3	162.9526	251.2700	28.45734	5
species_3	153.2313	238.6517	24.10297	2
species_3	157.8031	250.6427	24.93638	4

To summarise, we now have a simulated data set of measurements from three different species, all of which have known variances and covariances of length, width, and mass. Each species has a slightly different mean mass, and for all species, each unit of mass increases the expected number of offspring by 0.1. Because we know these properties of the data for certain, we can start asking questions that might be useful to know about our data analysis. For example, given this covariance structure and these small differences in mass, is a sample size of 20 really enough to even get a significant difference among species masses using an ANOVA? What if we tried to test for differences among masses using some sort of randomisation approach Instead? Would this give us more or less power? Let us run an ANOVA to see if the difference between group means (which we know exists) is recovered.

```
aov_result <- aov(Mass ~ species, data = dat);
summary(aov_result);
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## species      2  15.09   7.544   2.948 0.0605 .
## Residuals   57 145.88   2.559
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

It appears not! What about the relationship between body mass and offspring production that we know exists? Below is a scatterplot of the data for the three different species.



This looks like there might be a positive relationship, but it is very difficult to determine just from the scatterplot. We can use a generalised linear model to test it with species as a random effect, as we might do if these were data sampled from the field (do not worry about the details of the model here; the key point is that we can use the simulated data with known properties to assess the performance of a statistical test).

```
library(lme4);
```

```
## Loading required package: Matrix
```

```
mod <- glmer(offspring ~ Mass + (1 | species), data = dat, family = "poisson");
```

```
## boundary (singular) fit: see help('isSingular')
```

```
summary(mod);
```

```
## Generalized linear mixed model fit by maximum likelihood (Laplace
##   Approximation) [glmerMod]
##  Family: poisson  ( log )
## Formula: offspring ~ Mass + (1 | species)
##    Data: dat
##
##      AIC      BIC   logLik deviance df.resid
##    228.7    234.9   -111.3    222.7       57
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -1.6878 -0.5817 -0.2498  0.8039  2.3954
##
## Random effects:
##  Groups  Name        Variance Std.Dev.
##  species (Intercept) 0        0
## Number of obs: 60, groups:  species, 3
##
## Fixed effects:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -0.19573    1.23093  -0.159    0.874
## Mass         0.04647    0.04765   0.975    0.329
##
## Correlation of Fixed Effects:
##      (Intr)
## Mass -0.998
## optimizer (Nelder_Mead) convergence code: 0 (OK)
## boundary (singular) fit: see help('isSingular')
```

There does not appear to be any effect here either! To get one, it appears that we will need to simulate a larger data set (or a bigger effect size – or just get lucky when re-simulating a new data set).

Note that I have run a linear model that might be reasonable given the structure of our data. But the advantage of working with simulated data and knowing for certain what the relationship is between the underlying variables is that we can explore different statistical techniques. For example, we know that our response variable `offspring` is count data, so we are supposed to specify a Poisson error structure using the `family = "poisson"` argument above, right? But what would happen if we just used a normal error structure anyway? Would this really be so bad? Now is the opportunity to test because we *know* what the correct answer is supposed to be! Trying statistical methods that are normally ill-advised can actually be useful here, as it can help us see for ourselves when a technique is bad – or perhaps when it really is not (e.g., Ives 2015).

Conclusions

Simulating data can be a powerful tool for learning and investigating different statistical analyses. The main benefits of using simulated data are flexibility and certainty. Simulation gives us the flexibility to explore any number of hypotheticals, including different sample sizes, effect sizes, relationships between variables, and error distributions. It also works from a point of certainty; we know what the real relationship is between variables, and what the actual effect sizes are because we define them when generating random samples. So if we want to better understand what would happen if we were unable to sample an important variable in our system, or if we were to use a biased estimator, or if we we were to violate key model assumptions, simulated data is a very useful tool.

Literature cited

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