

Basic Constructs in R

R structures, and the apply class of functions

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 - ▶ Many standard functions in R are written in R, however, more computationally intensive tasks are coded in C++, C, or Fortran. R provides methods for linking these lower level languages into the R framework
 - ▶ R is easily extensible through the use of packages. The primary repository for R packages is CRAN, though there are also many packages geared towards bioinformatics on Bioconductor. There were 7,801 add-on packages available for R as of January 2016

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- ▶ A compiler for R was recently introduced, which apparently can increase speed considerably in certain situations where you may run the same code over and over. (Think R packages, common analytical techniques, etc.)
- ▶ I do not intend to focus on the implementation of R and how it "works", so let's dive into the functionality of R
- ▶ Things I plan to cover:
 - ▶ scalars, vectors, matrices, lists, data frames, functions, and the "apply" class of functions
 - ▶ The "apply" class of functions is very useful for iterating over a list or vector conducting the same operation on each entity in the list/vector

R Data Structures: Scalars

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```

- ▶ The values of y1, y2, and y3 are all set accordingly

R Data Structures: Vectors

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```
v1 <- c(3, 4, 1, 2)
v2 <- c(3.4, 4.16, 7.21, 8.65)
```

R Data Structures: Vectors

- ▶ vectors - a one dimensional list of values, for example: [3,4,1,2], [3.4, 4.16, 7.21, 8.67]

```
v1 <- c(3, 4, 1, 2)
v2 <- c(3.4, 4.16, 7.21, 8.65)
```

- ▶ Now v1, v2 are assigned to the vectors specified above

v1: 3, 4, 1, 2, v2: 3.4, 4.16, 7.21, 8.65

R Data Structures: Cont'd

- ▶ How do we access elements in a vector? We use the usual index notation, which starts at 1 in R. Some languages (C, C++, Fortran, python, javaScript, etc.) start at 0.

```
v1[1]
```

```
## [1] 3
```

```
v2[1]
```

```
## [1] 3.4
```

R Data Structures: Vectorization

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v1 + 2
```

```
## [1] 5 6 3 4
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- ▶ For instance, if we want to add 2 to all elements in the vector `v1` we use:

```
v1 + 2
```

```
## [1] 5 6 3 4
```

- ▶ Or adding two vectors together: (recycled if necessary)

```
v1 + v2
```

```
## [1] 6.40 8.16 8.21 10.65
```

R Data Structures: Matrices

- ▶ matrices: a two dimensional list of values, for example: $\begin{bmatrix} 3 & 4 & 1 & 2 & 3.4 \\ 4.16 & 7.21 & 8.67 \end{bmatrix}$, $\begin{bmatrix} 1 & 0 & 0 & 1 \end{bmatrix}$

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```
m1 <- matrix(c(3, 4, 1, 2, 3.4, 4.16, 7.21, 8.67),  
             nrow = 2, byrow = T)  
m2 <- matrix(c(1, 0, 0, 1), nrow = 2, byrow = T)
```

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```

- ▶ The argument `byrow` tells the `matrix` function whether to create the matrix row by row, from first index to last index. The argument `nrow` specified the number of rows.

m1:

3.0	4.00	1.00	2.00
3.4	4.16	7.21	8.67

Access an element in m1: 4

R Data Structures: Matrices (Recycling)

- ▶ Recycling also applies to Matrices - for instance

```
m1 + c(1, 1)
```

```
##      [,1] [,2] [,3] [,4]  
## [1,]  4.0 5.00 2.00 3.00  
## [2,]  4.4 5.16 8.21 9.67
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- ▶ What happened? the vector was added to each column of m1

```
m1 + c(1, 2)
```

```
##      [,1] [,2] [,3] [,4]  
## [1,]  4.0 5.00 2.00  3.00  
## [2,]  5.4 6.16 9.21 10.67
```

R Data Structures: Lists

- ▶ Lists - I think of lists as a generalized version of a vector, where the type of each index need not be the same. The first index of a list can be a scalar, the second index of a list can be a vector, the third index can be another list, and so on. Examples are below:

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```
l1 <- list(y1, v1, m1)
l2 <- list(first = l1, second = v1,
           third = m1, fourth = function(x) {x ^ 2})
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- Notice that both lists above are valid in R. You can even place functions into a list, as we did in l2.
- Lists are incredibly useful, as we will see later in this lecture. Lists can allow for calculating complicated expressions involved in survival likelihoods, for example.

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- ▶ How do we access elements in lists? It works similar to vectors/matrices...

R Data Structures: Lists (Cont'd)

- ▶ How do we access elements in lists? It works similar to vectors/matrices, but there is more notation

```
l1[[1]]
```

```
## [1] 3
```

```
l1[[2]]
```

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

```
l2$second
```

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

R Data Structures: Lists (Cont'd)

- ▶ One element in a list can be quite complicated!

```
l2$first
```

```
## [[1]]  
## [1] 3  
##  
## [[2]]  
## [1] 3 4 1 2  
##  
## [[3]]  
##      [,1] [,2] [,3] [,4]  
## [1,]  3.0 4.00 1.00 2.00  
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R Data Structures: Data Frames

- ▶ Data frames are the fundamental data structure in R. They share many similarities with matrices and lists.
- ▶ A data frame is formally a list of variables with the same number of rows. You can therefore access each variable as you would an element in a list, for instance, with the \$ operator.

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- ▶ A data frame is formally a list of variables with the same number of rows. You can therefore access each variable as you would an element in a list, for instance, with the `$` operator.
- ▶ Data frames are matrix like objects which can have columns of different types. Compare this to lists, where each index can be of different type. For instance, the first column may be numeric, the second may be a factor, the third may be of type string, etc. This can be accomplished with lists, but data frames provide extra convenience, including easier access and other functionality

R Data Structures: Data Frames

► Example:

```
mySeed <- char2seed("Spencer")
set.seed(mySeed) ## So df1 stays the same
df1 <- data.frame(y1 = rnorm(4, 0, 1), y2 = rexp(4, 1),
                  y3 = rbeta(4, 1, 1), ind = c(1,1,0,0))
knitr::kable(df1)
```

y1	y2	y3	ind
0.6322858	0.1558076	0.5478233	1
0.0558107	1.3448398	0.8152160	1
0.8099077	1.5584303	0.6714133	0
0.9714999	1.3880223	0.6401974	0

```
df1$y1
```

```
## [1] 0.63228583 0.05581074 0.80990771 0.97149987
```

R Data Structures: Data Frames

- ▶ It is very simple to calculate new variables in a data set. We will learn dplyr later in this class, but for now I will teach the “old guard” way of doing things

```
df1$y4 <- df1$y1^2 + df1$y2^2 + df1$y3^2  
df1$y4
```

```
## [1] 0.7241718 2.4762859 3.5354515 3.2802706
```

- ▶ You can also look at rows or columns using the following code

```
## Access row 2  
df1[2,]  
## Access column 3  
df1[,3]
```

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- ▶ R Data frames can be viewed as the building blocks for using the R language.
 - ▶ In almost every case, main analysis/modeling function in CRAN packages take data frames as arguments.
 - ▶ Includes the information used to construct design matrices, start the optimization algorithm for estimating model parameters
 - ▶ Using data frames efficiently in your own software can make writing code very efficient. As an example, check out the `model.frame()` and `model.matrix()` functions.

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 - ▶ Any repeated action should be made into a function
 - ▶ Anticipate extending your functions by generalizing the procedure
 - ▶ For instance, make the number of predictors a variable, or better yet let the function take a vector of strings which denotes all predictors

R Data Structures: Function examples

```
fib <- function(number)
{
  ## Simple test for integer value - doesn't really
  ## work if number is VERY close to an integer
  isInt <- all.equal(number, as.integer(number))
  if (number <= 2)
  {
    return(1)
  } else
  {
    return(fib(number-1) + fib(number - 2))
  }
}
```

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Apply class of functions: `apply`

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- ▶ First example function: **`apply(X, MARGIN, FUN, ...)`**
 - ▶ X: an array, including a matrix. MARGIN: 1 (rows) or 2 (columns). FUN: the function to be applied. Returns the result applied to each row or column of X. May return a matrix if results are vectors.

```
## rows  
apply(m1, 1, mean)
```

```
## [1] 2.50 5.86
```

```
## columns  
apply(m1, 2, mean)
```

```
## [1] 3.200 4.080 4.105 5.335
```


The aggregate function

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- ▶ **`aggregate(X, by, FUN)`** - `X`: an R object. `by`: a list of grouping elements, each as long as the variables in the data frame `x`. The elements are coerced into factors before use. `FUN`: a function to compute the summary statistics which can be applied to all data subsets.

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```
aggregate(df1, by = list(df1$ind), mean)
```

##	Group.1	y1	y2	y3	ind	y4
## 1	0	0.8907038	1.4732263	0.6558054	0	3.407861
## 2	1	0.3440483	0.7503237	0.6815196	1	1.600229

Apply class of functions: apply

```
minMax <- function(x) {return(c(min(x), max(x)))}  
## rows  
apply(m1, 1, minMax)
```

```
##      [,1] [,2]  
## [1,]    1 3.40  
## [2,]    4 8.67
```

```
## columns  
apply(m1, 2, minMax)
```

```
##      [,1] [,2] [,3] [,4]  
## [1,]  3.0 4.00 1.00 2.00  
## [2,]  3.4 4.16 7.21 8.67
```

Apply class of functions: `apply`

- ▶ Convenience functions exist for `sum/mean`:
- ▶ `rowSums()`, `rowMeans()`, `colSums()`, `colMeans()`
- ▶ `rowSums() == apply(, 1, sum)`, `colSums() = apply(, 2, sum)`, etc.

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- ▶ **lapply(X, FUN)** - X: a vector (atomic or list). FUN: the function to be applied to each element of X
- ▶ In the below, each element of l3 is a vector of 10000 standard normal deviates

```
lapply(l3, mean)
```

```
## [[1]]  
## [1] -0.01255568  
##  
## [[2]]  
## [1] -0.009359543  
##  
## [[3]]  
## [1] 0.00768243
```


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```
sapply(l3, mean)
```

```
## [1] -0.012555679 -0.009359543  0.007682430
```

```
sapply(l3, function(x) {sum(x^2) + 10})
```

```
## [1] 10196.602  9673.241  9858.207
```

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```
tapply(df1$y1, df1$ind, mean)
```

```
##           0           1  
## 0.8907038 0.3440483
```

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- ▶ **mapply(FUN, ..., SIMPLIFY = TRUE)** - FUN: function to apply, ...: lists or vectors to iterate over, SIMPLIFY: logical or character string, should R attempt to reduce the result to a vector/matrix, or keep as a list?
- ▶ I almost always use SIMPLIFY = FALSE to keep list structure of answer

Example of using mapply

- ▶ Function mapply is a go-to when you have multiple lists or vectors of the same length and need to use the same operation on each index before gathering your results.

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- ▶ Function mapply is a go-to when you have multiple lists or vectors of the same length and need to use the same operation on each index before gathering your results.
- ▶ Recall the multivariate normal likelihood, i.e. we observe an independent sample (of size n), with i th observation denoted Y_i with dimension $q_i \times 1$, and assume that:

$$Y_{ij} = X_{ij}\beta + b_{oi} + \epsilon_{ij} \quad (1)$$

$$\sim N(X_{ij}\beta, \sigma_b^2 + \sigma^2) \quad (2)$$

- ▶ Where X_{ij} is a vector of covariates for the i th subject at the j th timepoint. This is referred to as a linear mixed model with random subject intercepts.

Example of using mapply

- ▶ Calculation of the log-likelihood requires matrix multiplication of X_i and a current estimate for β , i.e. $\hat{\beta}$, then subtracting this from y_i , and finally, forming a quadratic form with Σ_i^{-1}

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- ▶ The above calculation denotes $(y_i - X_i\beta)' \frac{\Sigma_i^{-1}}{2} (y_i - X_i\beta)$ from the log-likelihood in this problem
- ▶ The following slides show how to use mapply and other base R functions to get this calculation off the ground using a toy data set.

Example of using mapply (Cont'd)

- ▶ Consider the following dataset with y_1 and x_1, x_2, x_3, x_4 included.
- ▶ Example of what one index might look like:

```
dfYSplit[[2]]$y1
```

```
## [1] 5.270686 2.216416 2.081399 6.207842 6.689458 7.177134
```

```
knitr::kable(dfXSplit[[2]][,c("x1", "x2", "x3", "x4")])
```

	x1	x2	x3	x4
9	0.0218036	0.0787564	3.178310	2.5635652
10	1.9215528	2.0730261	3.485042	0.6018452
11	1.1020457	-0.3379613	4.231701	-0.2174204
12	1.4894253	0.5910463	2.763400	2.3932846
13	1.3648414	0.4576341	3.636919	2.4375363
14	1.6343576	1.0716887	2.232086	3.2910254

Example of using mapply (Cont'd)

- ▶ Current beta estimate:

```
beta
```

```
## [1] 0.25 -0.25 0.50 1.25
```

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```
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```

```
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```

- ▶ Current σ^2 and σ_b^2 estimates:

```
sigma2
```

```
## [1] 1.25
```

```
sigma2b
```

```
## [1] 0.25
```

Example of using mapply (Cont'd)

- The below code puts it all together!

```
quadForms <- mapply(function(a, b) {  
  currY <- a[, "y1"]  
  currXM <- b[, c("x1", "x2", "x3", "x4")]  
  fixed <- as.matrix(currXM) %*% beta  
  ni <- dim(currXM)[1]  
  Sigma <- diag(sigma2, ni) + matrix(rep(sigma2b, ni * ni),  
                                     ncol = ni, nrow = ni) - diag(sigma2b, ni)  
  res <- t(currY - fixed) %*% solve(Sigma) %*%  
    (currY - fixed) / 2  
  return(res)  
}, dfYSplit, dfXSplit, SIMPLIFY = FALSE)
```

Example of using mapply (Cont'd)

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}, dfYSplit, dfXSplit, SIMPLIFY = FALSE)
```

- ▶ Mapply provides a convenient way to put our "building blocks" together

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- ▶ Many existing data structures, i.e. vectors, matrices, lists, functions...
- ▶ Apply class of functions very useful for replacing loops which conduct same operation many times
- ▶ Mapply function in particular is very useful when we have many lists
- ▶ Note that lapply can replace mapply if each list element has multiple list entities
- ▶ Ex: `l1[[1]] = list(l11, l12, l13, l14)` (access with the \$ operator)