- * A program is a set of instructions for a computer to follow
- Programs are often used to manipulate data (in all type and formats you discussed last week)
- Simple to complex
 - the scripts you wrote last week (simple)
 - instructions to analyze relationships in census data and visualize them
 - a model of global climate

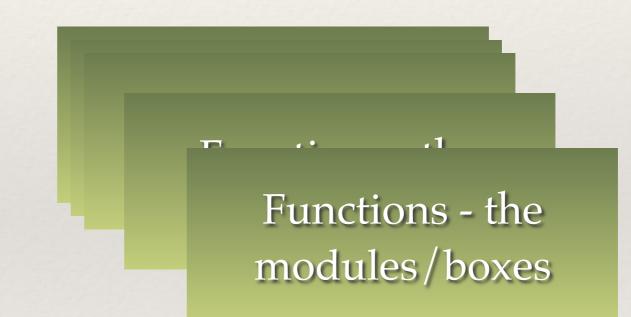
- Programs can be written in many different languages
 (all have their strengths and weakness)
- Languages expect instructions in a particular form (syntax) and then translate them to be readable by the computer
- * Languages have evolved to make it help users write programs that are easy to understand, re-use, extend, test, run quickly, use lots of data...

- Operations (=,+,-,...concatenate, copy)
- Data structures (simple variables, arrays, lists...)
- Control structures (if then, loops)
- * Modules...

Concepts common to all languages through the syntax may be different

Modularity

Main controls the overall flow of program- calls to the functions/ modules/building blocks



- * A program is often multiple pieces put together
- * These pieces or modules can be used multiple times

- Modularity
 - breaking your instructions down into individual pieces
 - identifying instructions that can be reused
 - an ecosystem model might re-use instructions for calculating how a species grows
 - an accounting program might re-use instructions for computing net present value from interest rates
 - modules often become 'black boxes' which hides detail that might make understanding the program overly complex
 - most languages have lots of black boxes already written and most allow you to write your own

Best practices for software development

- Read: Wilson G, Aruliah DA, Brown CT, Chue Hong NP, Davis M, et al. (2014) Best Practices for Scientific Computing. PLoS Biol 12(1): e1001745. doi:10.1371/journal.pbio.1001745
- Blanton, B and Lenhardt, C 2014. A Scientist's Perspective on Sustainable Scientific Software. Journal of Open Research Software 2(1):e17, DOI: http://dx.doi.org/10.5334/jors.ba
- but also
- * <u>http://simpleprogrammer.com/2013/02/17/principles-are-</u> <u>timeless-best-practices-are-fads/</u>

Box 1. Summary of Best Practices

- 1. Write programs for people, not computers.
- (a) A program should not require its readers to hold more than a handful of facts in memory at once.
- (b) Make names consistent, distinctive, and meaningful.
- (c) Make code style and formatting consistent.
- 2. Let the computer do the work.
- (a) Make the computer repeat tasks.
- (b) Save recent commands in a file for re-use.
- (c) Use a build tool to automate workflows.
- 3. Make incremental changes.
- (a) Work in small steps with frequent feedback and course correction.
- (b) Use a version control system.
- (c) Put everything that has been created manually in version control.
- 4. Don't repeat yourself (or others).
- (a) Every piece of data must have a single authoritative representation in the system.
- (b) Modularize code rather than copying and pasting.
- (c) Re-use code instead of rewriting it.

- 5. Plan for mistakes.
- (a) Add assertions to programs to check their operation
- (b) Use an off-the-shelf unit testing library.
- (c) Turn bugs into test cases.
- (d) Use a symbolic debugger.
- 6. Optimize software only after it works correctly.
- (a) Use a profiler to identify bottlenecks.
- (b) Write code in the highest-level language possible.
- 7. Document design and purpose, not mechanics.
- (a) Document interfaces and reasons, not implementation
- (b) Refactor code in preference to explaining how it we
- (c) Embed the documentation for a piece of software in software.
- 8. Collaborate.
- (a) Use pre-merge code reviews.
- (b) Use pair programming when bringing someone new speed and when tackling particularly tricky problem
- (c) Use an issue tracking tool.

Best practices for model (software) development

- Common problems
 - Unreadable code (hard to understand, easy to forget how it works, hard to find errors, hard to expand)
 - Overly complex, disorganized code (hard to find errors; hard to modify-expand)
 - Insufficient testing (both during development and after)
 - Not tracking code changes (multiple versions, which is correct?)

Steps for building model

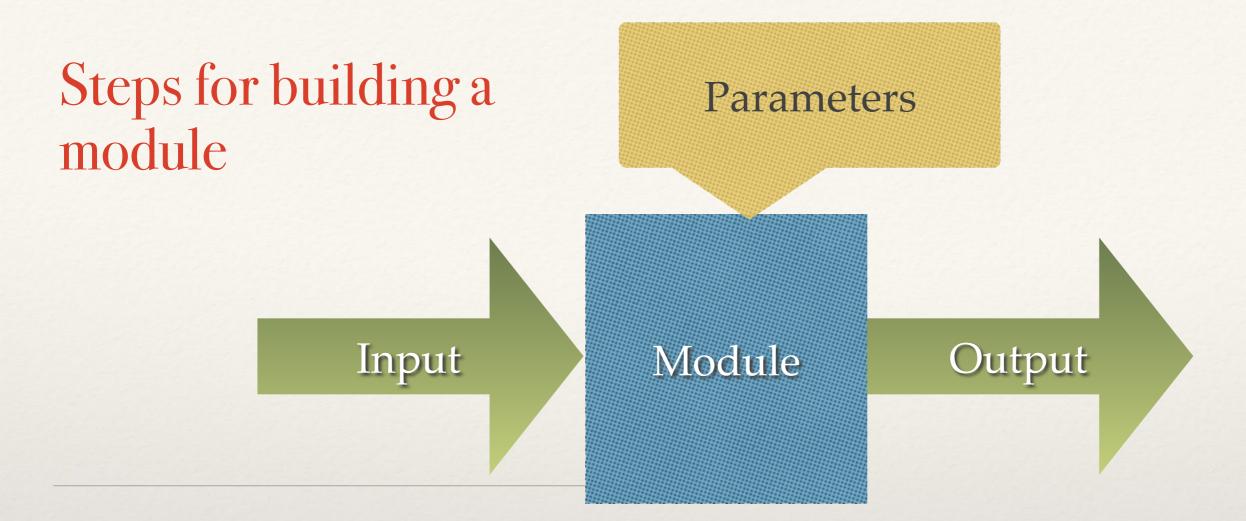
- * We are going to use R; but the basic design of programs are similar across many programming languages
- * Why R?
 - * Free (and open source) software
 - Good (and getting better) visualization tools
 - * Growing user community who make their R code available
 - (currently 2800+ user packages on CRAN R server)
 - * Links with other tools and languages (GIS, Python, C, C++...)
 - * Built in tools to deal with space and time
 - Lots of user support

Steps for building model

- * Why not R?
 - Not particularly computationally efficient (e.g slow for repetitive computations) ; hard to parallelize
 - Not the right tool for developing really complex models (you don't develop GCMs in R!)

STEPS: Program Design

- 1. Clearly define your goal as precisely as possible, what do you want your program to do
 - 1. inputs/parameters
 - 2. outputs
- 2. Implement and document
- 3. Test
- 4. Refine



- 1. Design the program "conceptually" "on paper" in words or figures
- 2. Translate into a step by step representation
- 3. Choose programming language
- 4. Define inputs (data type, units)
- 5. Define output (data type, units)
- 6. Define structure
- 7. Write program
- 8. Document the program
- 9. Test the program
- 10. Refine...

Best practices for model (software) development

- Let us change our traditional attitude to the construction of programs: Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to humans what we want the computer to do. --Donald E. Knuth, Literate Programming, 1984
- Developing readable (by PEOPLE) code and documenting what you are doing is essential
- * "When was the last time you spent a pleasant evening in a comfortable chair, reading a good program?"— Bentley (1986)

Best practices for software development

- * Automated tools (useful for more complex code development
- * (note that GP's often create programs > 100 lines of code)
- Automated documentation
 - http://www.stack.nl/~dimitri/doxygen/
 - http://roxygen.org/roxygen2-manual.pdf
- Automated test case development
 - http://r-pkgs.had.co.nz/tests.html
- * Automated code evolution tracking (Version Control)
 - https://github.com/

Designing Programs

- * Inputs sometimes separated into input data and parameters
 - * input data = the "what" that is manipulated
 - parameters determine "how" the manipulation is done
 - * "sort -n file.txt"
 - * sort is the program set of instructions its a black box
 - * input is file.txt
 - parameters is -n
 - output is a sorted version of file.txt
 - * my iphone app for calculating car mileage
 - * inputs are gallons and odometer readings at each fill up
 - * graph of is miles/gallon over time
 - parameters control units (could be km/liter, output couple be presented as a graph or an average value)

Designing Programs

- What's in the box (the program itself) that gives you a relationship between outputs and inputs
 - * the link between inputs and output
 - breaks this down into bite-sized steps or calls to other boxes)
 - think of programs as made up building blocks
 - * the design of this set of sets should be easy to follow

Building Blocks

- Instructions inside the building blocks/box
 - Numeric data operators
 - * +,-,/,*,%*%
 - * Strings
 - substr, paste..
 - * Math
 - * sin, cos, exp, min, max...
 - these are themselves programs boxes
 - * R-reference card is useful!

Best practices for software development

- * Structured practices that ensures
 - clear, readable code
 - modularity (organized "independent" building blocks)
 - * testing as you go and after
 - code evolution is documented

Building Blocks

- * Functions (or objects or subroutines)!
- The basic building blocks
- Functions can be written in all languages; in many languages (object-oriented) like C++, Python, functions are also objects
- Functions are the "box" of the model the transfer function that takes inputs and returns outputs
- More complex models made up of multiple functions; and nested functions (functions that call/user other functions)

Functions in R

* Format for a basic function in R

#' documentation that describes inputs, outputs and what the function does
FUNCTION NAME = function(inputs, parameters) {
 body of the function (manipulation of inputs)
 return(values to return)

In R, inputs and parameters are treated the same; but it is useful to think about them separately in designing the model - collectively they are sometimes referred to as arguments

ALWAYS USE Meaningful names for your function, its parameters and variables calculated within the function

A simple program: Example

- * Input: Reservoir height and flow rate
- * Output: Instantaneous power generation (W/s)
- * Parameters: $K_{Efficiency}$, ϱ (density of water), g (acceleration due to gravity)

 $P = \varrho * h * r * g * K_{Efficiency}$

P is Power in watts, ϱ is the density of water (~1000 kg/m3), h is height in meters, r is flow rate in cubic meters per second, g is acceleration due to gravity of 9.8 m/s2, K_{Efficiency} is a coefficient of efficiency ranging from 0 to 1.



```
* Example (power_gen.R)
```

```
power_gen = function(height, flow, rho=1000, g=9.8, Keff=0.8) {
result = rho * height * flow * g * Keff
return(result)
}
```

Building Models

- * Inputs/parameters are height, flow, rho, g, and K
- * For some (particularly parameters) we provide default values by assigning them a value (e.g Keff = 0.8), but we can overwrite these
- * Body is the equations between { and }
- * return tells R what the output is

```
power_gen = function(height, flow, rho=1000, g=9.8, Keff=0.8) {
  result = rho * height * flow * g * Keff
  return(result)
}
```

Building Models: Using the model

```
> power_gen(20,1)
[1] 156800
> power_gen(height=20,flow=1)
[1] 156800
> power.guess = power_gen(height=20,flow=1)
> power.guess
[1] 156800
> power.guess = power_gen(flow=1, height=20)
> power.guess
[1] 156800
```

Arguments to the function follow the order they are listed in your definition Or you can specify which argument you are referring to when you call the program

```
power_gen = function(height, flow, rho=1000, g=9.8, K=0.8) {
# calculate power
result = rho * height * flow * g * K
return(result)
}
```

Building Models

- * Always write your function in a text editor and then copy into R
- * By convention we name files with functions in them by the name of the function.R
 - * so power_gen.R
- you can also have R read a text file by *source("power_gen.R")* make sure you are in the right working directory
- Eventually we will want our function to be part of a package (a library of many functions) - to create a package you must use this convention (name.R)

Building Models: Using the model

```
> power_gen(height=20, flow=1)
[1] 156800
> power_gen(height=20, flow=1, Keff=0.8)
[1] 156800
> power_gen(height=20, flow=1, Keff=0.5)
[1] 98000
> power_gen(height=10, flow=1, Keff=0.5)
[1] 49000
```

Defaults take the value they were assigned in the definition, but can be overwritten

```
power_gen = function(height, flow, rho=1000, g=9.8, K=0.8) {
# calculate power
result = rho * height * flow * g * K
return(result)
```

}



The scope of a variable in a program defines where it can be "seen"

Variables defined inside a function cannot be "seen" outside of that function

There are advantages to this - the interior of the building block does not 'interfere' with other parts of the program

```
> power_gen
function(height, flow, rho=1000, g=9.8, K=0.8) {
```

```
# calculate power
result = rho * height * flow * g * K
return(result)
}
> result
Error: object 'result' not found
> K
Error: object 'K' not found
```

>

One of the equations used to compute automobile fuel efficiency is as follows this is the power required to keep a car moving at a given speed

```
Pb = c_{rolling} * m *g*V + 1/2 A*p_{air}*c_{drag}*V^3
```

where $c_{rolling}$ and c_{drag} are rolling and aerodynamic resistive coefficients, typical values are 0.015 and 0.3, respectively. V: is vehicle speed (assuming no headwind) in m/s (or mps) m: is vehicle mass in kg A is surface area of car (m2) g: is acceleration due to gravity (9.8 m/s2) p_{air} = density of air (1.2kg/m3) Pb is power in Watts

Write a function to compute power, given a truck of m=31752 kg (parameters for a heavy truck) for a range of different highway speeds plot power as a function of speed how does the curve change for a lighter vehicle

Note that 1mph=0.477m/s

Simple Functions

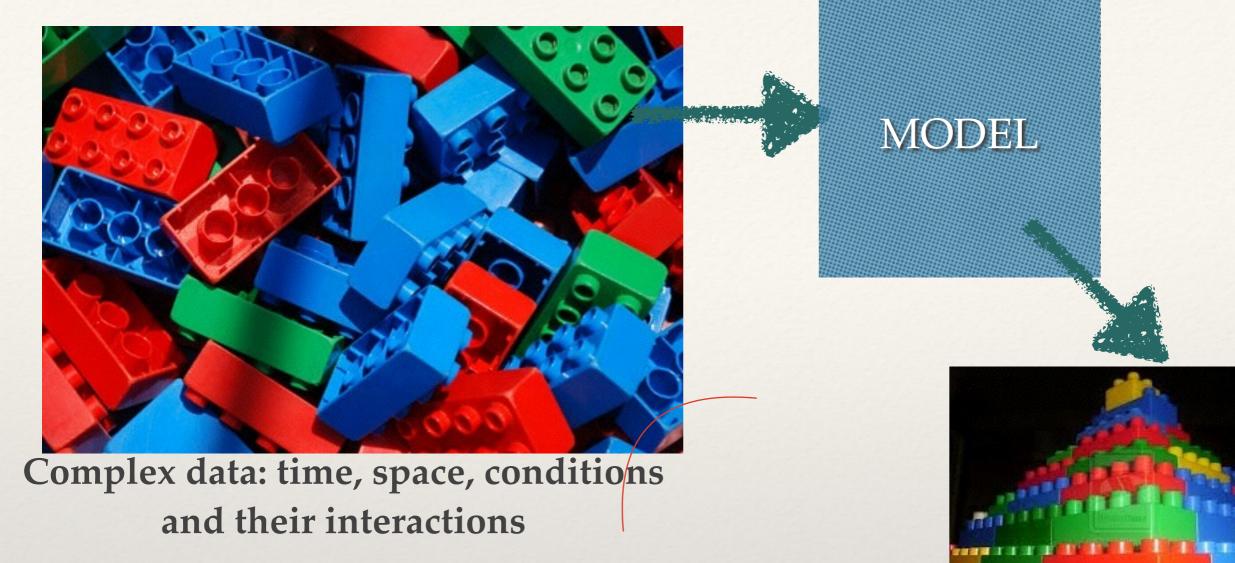
```
power = function(cdrag=0.3, crolling=0.015,pair=1.2,g=9.8,V,m,A) {
P = crolling*m*g*V + 1/2*A*pair*cdrag*V**3
return(P)
}
v=seq(from=0, to=100, by=10)
plot(v, power(V=0.447*v, m=31752, A=25))
```

lines(v, power(V=0.447*v, m=61752, A=25))

Simple Functions

```
Power Required by Speed
#'
#'
  This function determines the power required to keep a vehicle moving
#'
at
#' a given speed
  @param cdrag coefficient due to drag default=0.3
#'
#' @param crolling coefficient due to rolling/friction default=0.015
#' @param v vehicle speed (m/2)
#' @param m vehicle mass (kg)
#' @param A area of front of vehicle (m2)
#' @param g acceleration due to gravity (m/s) default=9.8
#' @param pair (kg/m3) default =1.2
#' @return power (W)
power = function(cdrag=0.3, crolling=0.015,pair=1.2,g=9.8,V,m,A) {
P = crolling*m*g*V + 1/2*A*pair*cdrag*V**3
return(P)
}
v=seq(from=0, to=100, by=10)
plot(v, power(V=0.447*v, m=31752, A=25))
lines(v, power(V=0.447*v, m=61752, A=25))
```

- Understanding data types is important for designing your model I/O; specifying what the model will do
- Data types and data structures are necessary for creating more complex inputs and outputs
- * All programming languages have sets of data types
 - single values: character, integer, real, logical/boolean (Y/N)
 - data structures: arrays, vectors, matrices,
 - * in R core types; dataframes, lists, factors
 - * in R defined types: spatial, date...



Building Programs

A core issue in modeling (both designing and using) are the **data structures** / formats used to hold data that is input and output from programs: In good programs, data structures support organization and program flow and readability Key Programming concepts: Data types and structures

- Good data structures are:
 - * as simple as possible
 - easy understand (readable names, and sub-names)
 - easy to manipulate (matrix operations, applying operations by category)
 - easy to visualize (graphs and other display)

- Vectors a 1-dimensional set of numbers
- * a = c(1,5,8,4,22,33)
- Matrix a 2-dimensional set of numbers (organized in rows and columns)
- * b = matrix(a, nrow=2, ncol=3)

```
> a = c(1,5,8, 4, 22,33)
> 
> b = matrix(a, nrow=2, ncol=3)
> a
[1] 1 5 8 4 22 33
> b
      [,1] [,2] [,3]
[1,] 1 8 22
[2,] 5 4 33
```

- You can also define an "empty" matrix to fill values in later
- think of creating a data structure to store energy production in winter and summer for 6 different power plants)
- * res = matrix(nrow=2, ncol=6)

```
> res = matrix(nrow=2, ncol=6)
> res
     [,1] [,2] [,3] [,4] [,5] [,6]
       NA
           NA
                 NA
                      NA
                           NA
[1,]
                                NA
[2,]
      NA
           NA
                 NA
                      NA
                           NA
                                NA
>
```

- * You can combine vectors into a matrix using
 - * cbind by columns
 - * *rbind* by rows

- * A really useful data structure in R is a data frame
- Dataframe's are like matrices = they have rows and columns but they don't have to be numeric (although they can be)
- * Useful if you have data that is of mixed type

Data Frame Creation Example

```
>
> mth.names = c("Jan", "Feb", "Mar", "Apr", "May",
+ "Jun","Jul","Aug","Sep","Oct","Nov","Dec")
>
> reservoir.operation = data.frame(month=mth.names)
>
> reservoir.operation
   month
1
     Jan
2
     Feb
3
     Mar
4
     Apr
5
     May
6
     Jun
7
     Jul
8
     Aug
9
     Sep
10
     0ct
11
     Nov
12
     Dec
>
```

Data Frame Creation Example

```
>
>
> reservoir.operation$height = c(seq(from=22,to=10, by=-2), seq(from=12,to=20,
by=2))
> \#reservoir.operationheight = c(20, 18, 16, 14, 12, 10, 12, 14, 16, 18, 20)
>
> reservoir.operation$flowrate = rnorm(n=12, mean=3, sd=0.25)
>
> reservoir.operation
   month height flowrate
                                             Adding columns
     Jan
            22 2.967183
1
2
    Feb 20 2.923782
3
    Mar 18 2.891444
4
    Apr
            16 3.048090
                           seq - a sequence of number from to by
5
    May
            14 2.598533
6
    Jun
            12 3.027024
                           rnorm - generate, n numbers from a normal distribution
7
            10 2.906364
    Jul
                           with a given mean and standard deviation
8
    Aug
            12 3.460389
             14 2.965138
9
     Sep
10
    0ct
             16 3.320663
11
    Nov
            18 3.300340
12
             20 2.916503
     Dec
>
```

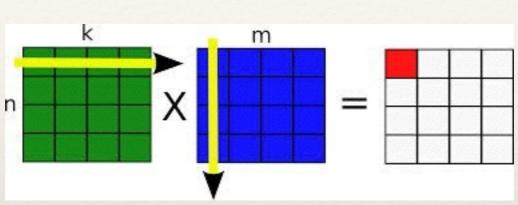
- Of course we can use matrices/data frames as inputs/ output for our models
- Example using our power_gen model from earlier using vectors instead of single values

```
> > power_gen(height=reservoir.operation$height, flow=reservoir.operation$flow)
[1] 511779.6 458449.1 408040.5 382352.4 285215.0 284782.4 227858.9 325553.4
[9] 325453.5 416544.0 465744.0 457307.7
> power_gen
function (height, flow, rho = 1000, g = 9.8, Keff = 0.8)
{
    result = rho * height * flow * g * Keff
    return(result)
}
```

- * Why does this work?
- Because height, flow columns are both from reservoir.operation (a data frame) so they are vectors of the SAME length
- * So when you multiply height* flow, you multiply
 - * height[1]*flow[1],,, and then height[2]*flow[2] etc

```
> > power_gen(height=reservoir.operation$height, flow=reservoir.operation$flow)
[1] 511779.6 458449.1 408040.5 382352.4 285215.0 284782.4 227858.9 325553.4
[9] 325453.5 416544.0 465744.0 457307.7
> power_gen
function (height, flow, rho = 1000, g = 9.8, Keff = 0.8)
{
    result = rho * height * flow * g * Keff
    return(result)
}
```

- * Matrix multiplication is different
- * in R, this would be
 - * k %*% m



 Matrix multiplication is often used within certain types of models...we will get to examples later

Data Frame Creation Example

```
>
>
> reservoir.operation$height = c(seq(from=22,to=10, by=-2), seq(from=12,to=20,
by=2))
> \#reservoir.operationheight = c(20, 18, 16, 14, 12, 10, 12, 14, 16, 18, 20)
>
> reservoir.operation$flowrate = rnorm(n=12, mean=3, sd=0.25)
>
> reservoir.operation
   month height flowrate
                                             Adding columns
            22 2.967183
     Jan
1
2
    Feb 20 2.923782
3
    Mar 18 2.891444
4
    Apr
            16 3.048090
5
    May
            14 2.598533
6
    Jun
            12 3.027024
7
            10 2.906364
    Jul
8
    Aug
            12 3.460389
             14 2.965138
9
     Sep
    0ct
             16 3.320663
10
11
    Nov
            18 3.300340
12
             20 2.916503
     Dec
>
```

* We can also use data frames (or matrices) to store results

> power_gen(height=reservoir.operation\$height, flow=reservoir.operation\$flow)
[1] 511779.6 458449.1 408040.5 382352.4 285215.0 284782.4 227858.9 325553.4
[9] 325453.5 416544.0 465744.0 457307.7

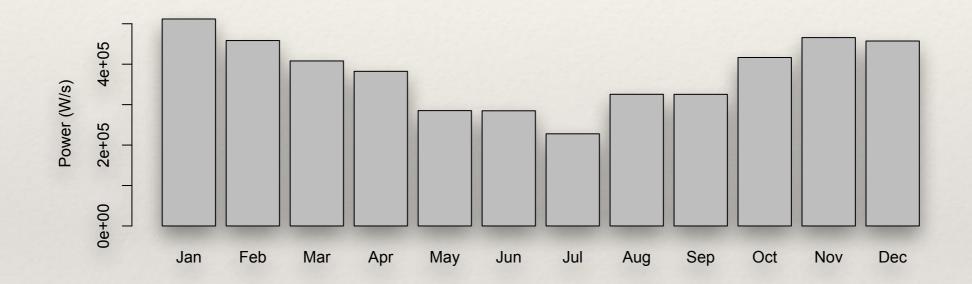
> reservoir.operation\$power = power_gen(height=reservoir.operation\$height,
flow=reservoir.operation\$flow)

> reservoir.operation

	month	height	flowrate	power
1	Jan	22	2.967183	511779.6
2	Feb	20	2.923782	458449.1
3	Mar	18	2.891444	408040.5
4	Apr	16	3.048090	382352.4
5	May	14	2.598533	285215.0
6	Jun	12	3.027024	284782.4
7	Jul	10	2.906364	227858.9
8	Aug	12	3.460389	325553.4
9	Sep	14	2.965138	325453.5
10	0ct	16	3.320663	416544.0
11	Nov	18	3.300340	465744.0
12	Dec	20	2.916503	457307.7

- Some other useful commands
 - *with* allows you to use the names of columns in the data frame directly
 - *summary* summaries of columns (max, min, mean...)

> with(reservoir.operation, barplot(power, names=month, ylab="Power (W/s)"))
>



Summary

>

>

>

>

> summary(reservoir.operation)

month		height	flowrate	power
Apr	:1	Min. :10.0	Min. :2.599	Min. :227859
Aug	:1	1st Qu.:13.5	1st Qu.:2.914	1st Qu.:315394
Dec	:1	Median :16.0	Median :2.966	Median :395196
Feb	:1	Mean :16.0	Mean :3.027	Mean :379090
Jan	:1	3rd Qu.:18.5	3rd Qu.:3.111	3rd Qu.:457593
Jul	:1	Max. :22.0	Max. :3.460	Max. :511780
(Other):6				

- * We can also use other functions and built in R functions (like *mean*, *lm*, *sum*) within our function
- * Lets say we want to commute total annual power generated, given our inputs of average height and flow for each month?
 - * what additional information would we need?

>

```
>
> power_gen(height=reservoir.operation$height, flow=reservoir.operation$flow)
[1] 511779.6 458449.1 408040.5 382352.4 285215.0 284782.4 227858.9 325553.4
[9] 325453.5 416544.0 465744.0 457307.7
> power_gen
function (height, flow, rho = 1000, g = 9.8, Keff = 0.8)
{
    result = rho * height * flow * g * Keff
    return(result)
}
```

```
#' Total Power Generation
#'
#' This function computes total power generation from a reservoir given its
height and flow rate into turbines and number of days (and secs) within
those days that the turbines are in operation
#' @param rho Density of water (kg/m3) Default is 1000
#' @param g Acceleration due to gravity (m/sec2) Default is 9.8
#' @param Keff Turbine Efficiency (0-1) Default is 0.8
#' @param height height of water in reservoir (m)
#' @param flow flow rate (m3/sec)
#' @param number of days
#' @param secs in days Default is 86400
#' @author Naomi
#' @examples power_gen(20, 1, 10)
#' @return Power generation (MW)
power gen total = function(height, flow, days, secs=86400, rho=1000, g=9.8,
Keff=0.8) {
result = rho * height * flow * g * Keff
result = result * days * secs
total = sum(result)/1e6
return(total)
}
> power_gen_total(reservoir.operation$height, reservoir.operation$flowrate,
days=30)
[1] 11702915
>
```

In Class example

 Expand your function that computes the power need to compute and return the total power given an input vector of different speeds and the time period over which those speeds are driven (we will ignore acceleration effect)

- * **Arrays** are like matrices but can be multi-dimensional
- *dim* defines the dimensions of an array and gives the number of values in each dimension
- * a matrix is a 2-dimensional array
- * test = array(dim=c(2,5)) this has 2 rows and 5 columns
- * You can have N-dimensional arrays

Data Structures

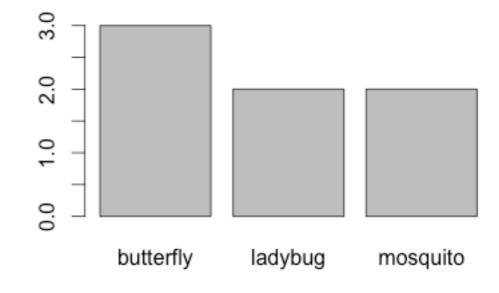
- * vectors (c)
- * matrices, arrays
- data frames
- * lists
- * factors

- * Factors (a bit tricky, basically a vector of "things" that has different levels (classes); not really numeric - so you can't average them!)
- * But can be useful for doing "calculations" with categories

```
>
> a = c(1,5,2.5,9,5,2.5)
> a
[1] 1.0 5.0 2.5 9.0 5.0 2.5
> mean(a)
[1] 4.166667
> a = as.factor(c(1,5,2.5,9,5,2.5))
> mean(a)
[1] NA
Warning message:
In mean.default(a) : argument is not numeric or logical: returning NA
> a
[1] 1 5 2.5 9 5 2.5
Levels: 1 2.5 5 9
> summary(a)
  12.5 5
             9
   2
         2
             1
  1
```

summary can be used with factors to get frequencies in each category (or "level")

```
>
>
> species.recorded = c("butterfly","butterfly","mosquito","butterfly","
ladybug", "ladybug", "mosquito")
> species.recorded = as.factor(species.recorded)
> species.recorded
[1] butterfly butterfly mosquito butterfly ladybug ladybug
                                                                mosquit
0
Levels: butterfly ladybug mosquito
> summary(species.recorded)
butterfly ladybug mosquito
        3
                  2
                            2
> plot(species.recorded)
>
```



```
>
                                              > species.recorded = c("butterfly","butterfly","mosquito","butterfly","
                                              ladybug", "ladybug", "mosquito")
                                              > species.recorded = as.factor(species.recorded)
                                              > species.recorded
                                              [1] butterfly butterfly mosquito butterfly ladybug
                                                                                               ladybug
                                                                                                        mosquit
                                              Levels: butterfly ladybug mosquito
                                              > summary(species.recorded)
> mean(summary(species.recorded))
                                              butterfly ladybug mosquito
                                                      3
                                                               2
                                                                        2
[1] 2.333333
                                              > plot(species.recorded)
> max(summary(species.recorded))
                                              >
[1] 3
> sum(summary(species.recorded))
[1] 7
                                                                            You can "do things" (apply
> sum(species.recorded)
Error in Summary.factor(c(1L, 1L, 3L, 1L, 2L, 2L, 3L), na.rm = FALSE) :
                                                                             functions) to the summary
  sum not meaningful for factors
                                                                             (frequency of each "factor"
> species.recorded
[1] butterfly butterfly mosquito butterfly ladybug
                                                                                          level
                                                        ladybug
[7] mosquito
Levels: butterfly ladybug mosquito
> summary(species.recorded)[1]
butterfly
> summary(species.recorded)[2]
ladybug
      2
> summary(species.recorded)[3]
mosquito
       2
>
```

- * A simple model that takes advantage of factors
- A model to compute an index of species diversity from a list of recorded species

$$D = \Sigma (n / N)^2$$

where n is the number of individuals in each species, and N is total number

```
# '
   Simpson's Species Diversity Index
# '
# '
   Compute a species diversity index
# '
   @param species list of species (names, or code)
# '
   @return value of Species Diversity Index
# '
   @examples
   compute simpson index(c("butterfly","butterfly","mosquito","butterfly",
#' "ladybug", "ladybug")))
#' @references
  http://www.tiem.utk.edu/~gross/bioed/bealsmodules/simpsonDI.html
# '
```

compute_simpson_index = function(species) {

```
species = as.factor(species)
tmp = (summary(species)/sum(summary(species))) ** 2
diversity = sum(tmp)
return(diversity)
}
```

Data Structures

- a bit more on factors; a list of numbers can also be a factor but then they are not treated as actual numbers you could think of them as "codes" or addresses or..
- use *as.numeric* or *as.character* to go back to a regular
 vector from a factor

```
> items = c(1,5,1,5,6,3)
> mean(items)
[1] 3.5
> items = as.factor(c(1,5,1,5,6,3))
> mean(items)
[1] NA
Warning message:
In mean.default(items) : argument is not numeric or logical: returning
NA
> summary(items)
1356
2121
> tmp = as.numeric(items)
> tmp
[1] 1 3 1 3 4 2
> mean(tmp)
[1] 2.333333
>
```

Data Structures

- * vector, (c)
- * matrices, arrays
- * data frames
- * lists
- * factors

- * Lists are the most "informal" data structures in R
- * List are really useful for keeping track of and organizing groups of things that are not all the same
- * A list could be a table where number of rows is different for each column
- A list can have numeric, character, factors all mixed together
- List are often used for returning more complex information from function (e.g. lm)

* A simple list

```
> sale = list(2,"highquality","apple",4)
> sale
[[1]]
[1] 2
[[2]]
[1] "highquality"
[[3]]
[1] "apple"
[[4]]
[1] 4
```

* A simple list: using names to identify elements

```
> sale = list(number=2, quality="high", what="apple", cost=4)
> sale
$number
[1] 2
$quality
[1] "high"
```

\$what [1] "apple"

\$cost [1] 4

```
> costs = c(20,40,22, 32, 5)
> quality = c("G", "G", "F", "G", "B")
> purchased = c(33,5,22,6,7)
> sales = data.frame(costs=costs, quality=quality, purchased=purchased)
> sales
                     >costs = c(73,44)
costs quality purchased
                     >quality = c("G","G")
1
  20
        G
            33
                      >purchased = c(100, 22)
2
     G 5
 40
3
 22 F 22
                      >sales2 = data.frame(costs=costs, quality=quality
                      purchased=purchased)
 32 G 6
4
5
   5
       В
            7
```

With lists we can combine sales data frames from two different places into a single data structure

Lists

```
>
> markets = list(site1=sales, site2=sales2)
> markets
$site1
  costs quality purchased
     20
1
                         33
               G
2
     40
               G
                          5
3
4
               F
   22
                         22
                          6
     32
               G
5
                          7
      5
               В
$site2
  costs quality purchased
1
     73
                        100
               G
2
                         22
     44
               G
> markets[[1]]$costs
[1] 20 40 22 32 5
>
> markets$site1$costs
[1] 20 40 22 32 5
>
```

Lists

>					
>					
>	market	ts[[1]]			
	costs	quality	purchased		
1	20	G	33		
2	40	G	5		
3	22	F	22		
4	32	G	6		
5	5	В	7		
>					
>	market	ts[[2]]			
	costs	quality	purchased		
1	73	G	100		
2	44	G	22		
>					
<pre>> markets[[1]][1,3]</pre>					
[1] 33					
>					

[[]] is used to get elements from the list

 one of the most useful things to do with list is to use them to return multiple 'items' from a function

```
#' computes profit from price for forest plot and Mg/C in that plot
#' @param price ($)
#' @param carbon (MgC)
#' @return list with mean, min, and max prices
compute_carbonvalue = function(price, carbon) {
  cost.per.carbon = price/carbon
  a = mean(cost.per.carbon)
  b = max(cost.per.carbon)
  c = min(cost.per.carbon)
  result = list(avg=a, min=c, max=b)
  return(result)
}
```

* example: returning lists from a function

```
>
> obs = data.frame(prices=c(23,44,60,4,2,33,59),
forestC=c(59,88,100,10,8,79,300))
> obs
  prices forestC
      23
               59
1
2
      44
               88
3
      60
             100
4
               10
       4
5
       2
               8
6
      33
               79
7
      59
             300
> forest.res = compute_carbonvalue(obs$prices, obs$forestC)
> forest.res
$avg
[1] 0.3934598
$min
[1] 0.1966667
$max
[1] 0.6
```

>

example: returning lists from a function

```
> obs=data.frame(prices=c(18,2,12,5), grassC=c(22,3,19,8))
```

```
> grass.res=compute_carbonvalue(obs$prices, obs$grassC)
```

> grass.res
\$avg
[1] 0.6853569

\$min [1] 0.625

>

\$max [1] 0.8181818

- * Many functions that you use in R, return lists
- *names* (to see what is in a list)
- * *attributes* (to see what is in a list)

```
> names(forest.res)
[1] "avg" "min" "max"
> attributes(forest.res)
$names
[1] "avg" "min" "max"
```

lm is an
 example of a function that
 returns a list >> res = lm(obs\$prices~obs\$forestC) > names(res) [1] "coefficients" "residuals" "effects" [4] "rank" "fitted.values" "assign" [7] "qr" "df.residual" "xlevels" [10] "call" "terms" "model" > res\$coefficients (Intercept) obs\$forestC 14.9789368 0.1865644 > res\$model obs\$prices obs\$forestC 23 59 1 2 44 88 3 60 100 4 10 4 5 2 8 33 79 6 7 59 300

>

* example: returning lists from a function

```
#' Describe diversity based on a list of species
#'
#' Compute a species diversity index
#' @param species list of species (names, or code)
#' @return list with the following items
#' \describe{
#' \item{num}{ Number of distinct species}
#' \item{simpson}{Value of simpson diversity index}
#' \item{dominant}{Name of the most frequently occuring species}
#'}
#'
  @examples
#'
compute_diversity(c("butterfly","butterfly","mosquito","butterfly","ladybug",
"ladybug")))
#' @references
#' http://www.tiem.utk.edu/~gross/bioed/bealsmodules/simpsonDI.html
compute_diversity = function(species) {
species = as.factor(species)
tmp = (summary(species)/sum(summary(species))) ** 2
diversity = sum(tmp)
nspecies = length(summary(species))
tmp = which.max(summary(species))
dominant = names(summary(species)[tmp])
return(list(num=nspecies, simpson=diversity, dominant=dominant))
}
```

- * to your function that computes power, also return
 - * an array that contains both power for each input speed
 - total power

Key Programming concepts: Review of data typessd

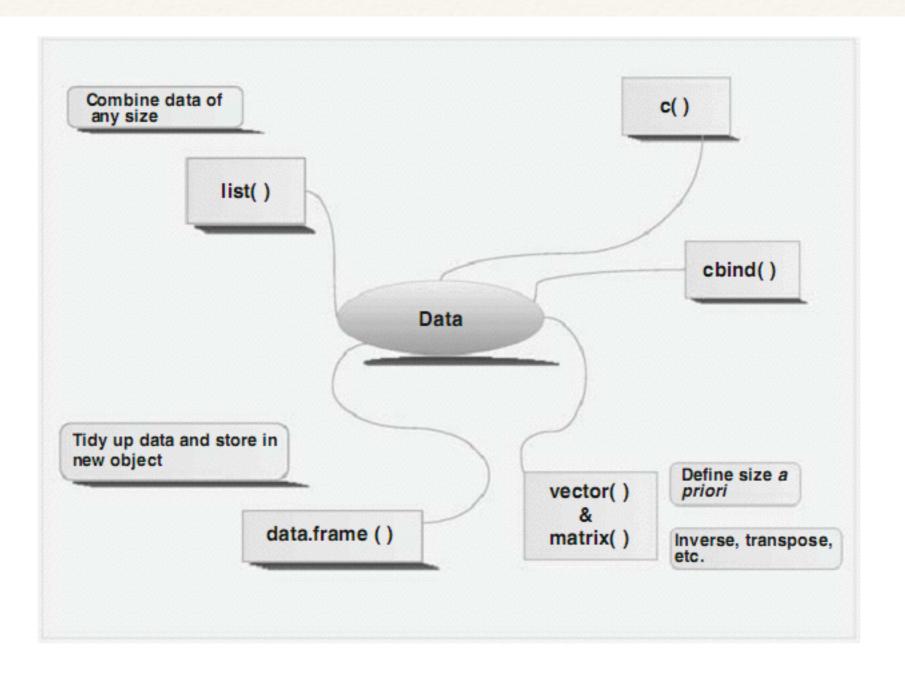
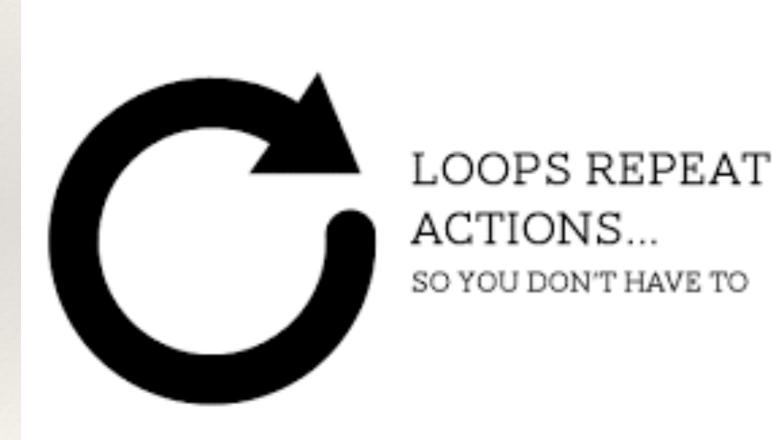
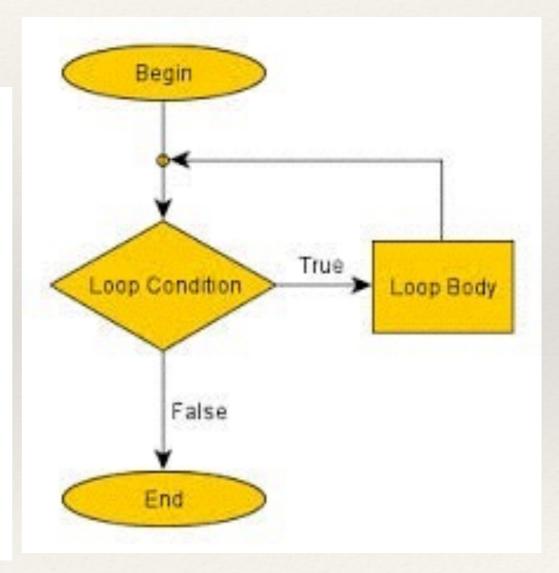


Fig. 2.1 Overview of various methods of storing data. The data stored by cbind, matrix, or data.frame assume that data in each row correspond to the same observation (sample, case)

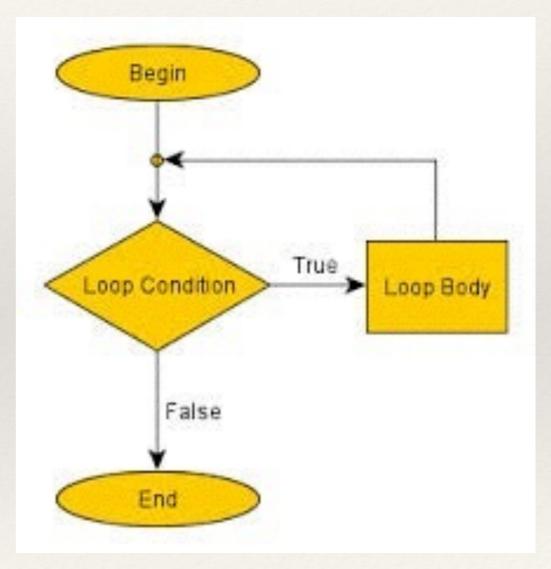
http://www.simonqueenborough.com/R/basic/figure/data-types.png

 Loops are fundamental in all programming languages: and are frequently used in models

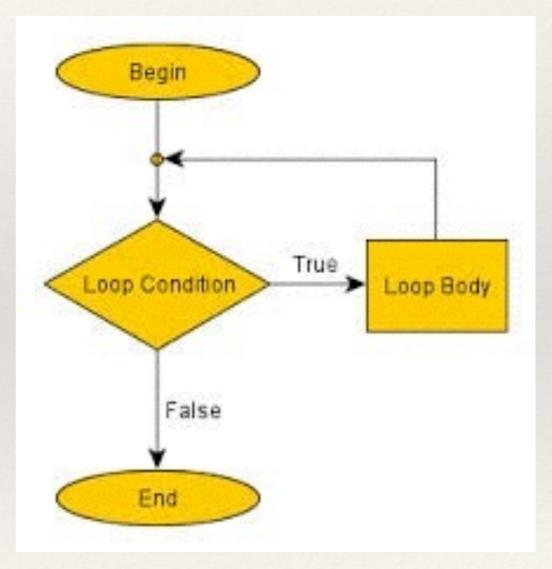




- * Two distinctive reasons for looping
- Apply the same equations (e.g for power generation) over a range of parameter values
- Evolve a variable through time (or space), when the variable's value at the next time step depends on the previous one (e.g growing a population)



 All loops have this basic structure - repeat statements (loop body) until a condition is true



- * In R, the most commonly used loop is the *For* loop
- * for (i in 1:n) { statements }
- * In "for" loops the i (or whatever variable you want to use as the counter, is automatically incremented each time the loop is gone through; and the looping ends when i (the counter) reaches n
- * What is x? alpha? after this loop is run

>x=0> for (alpha in 1:4) { x = x+alpha} >
>
>
x=0
> for (alpha in 1:4) { x = x+alpha}
>
>
> alpha
[1] 4
> x
[1] 10

- * Loops can be "nested" one loop inside the other
- * For example, if we want to calculate NPV for a range of different interest rates and a range of damages that may be incurred 10 years in the future
 - * using a function called compute_npv
- * Steps
 - define inputs (interest rates, damages)
 - define a data structure to store results
 - define function/model (already available)
 - * use looping to run model for all inputs and store in data structure

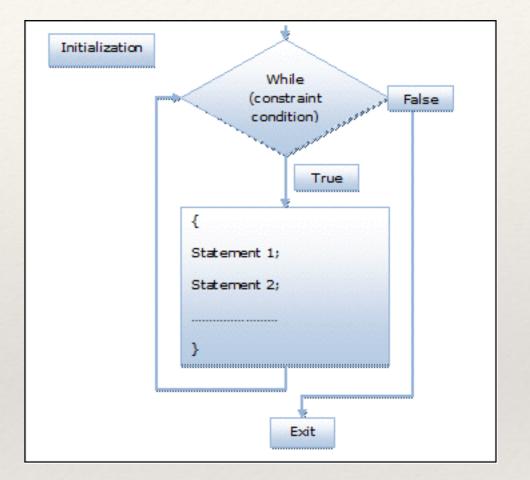
```
>
> damages = c(25,33,91,24)
> discount.rates = seq(from=0.01, to=0.04, by=0.005)
> yr=10
> npvs = as.data.frame(matrix(nrow=length(damages), ncol=length(discount.rates)))
> for (i in 1:length(damages)) {
      for (j in 1:length(discount.rates)) {
+
      npvs[i,j]= compute_npv(net=damages[i], dis=discount.rates[j],yr )
+
+
+
> npvs
    V1
           V2
                 V3
                        V4
                              V5
                                     V6
                                            V7
1 22.63217 21.54168 20.50871 19.52996 18.60235 17.72297 16.88910
2 29.87447 28.43502 27.07149 25.77955 24.55510 23.39432 22.29362
3 82.38111 78.41172 74.65170 71.08905 67.71255 64.51161 61.47634
4 21.72689 20.68001 19.68836 18.74876 17.85825 17.01405 16.21354
> colnames(npvs)=discount.rates
> rownames(npvs)=damages
>npvs
   0.01
                 0.02 0.025
                               0.03
                                     0.035
         0.015
                                             0.04
25 22.63217 21.54168 20.50871 19.52996 18.60235 17.72297 16.88910
```

33 29.87447 28.43502 27.07149 25.77955 24.55510 23.39432 22.29362 91 82.38111 78.41172 74.65170 71.08905 67.71255 64.51161 61.47634 24 21.72689 20.68001 19.68836 18.74876 17.85825 17.01405 16.21354

>

>

- Another useful looping construct is the While loop
- keep looping until a condition is met
- Useful when you don't know what "n" in the for 1 in to "n" is
- often used in models where you are evolving
 - accumulate something until a threshold is reached (population, energy, biomass?



* A simple *while* loop example

>
>
> alpha = 0
> x = 0
> while (alpha < 100) { alpha = alpha + x; x = x+1}
> x
[1] 15
> alpha
[1] 105
>

* alpha = (1+2+3+4+5+6+7+8+9+10+11+12+13+14) = 105

- * A more useful *while* loop example
- A question: if a metal toxin in a lake increases by 1% per year, how many years will it take for the metal level to be greater than 30 units, if toxin is current at 5 units
- there are other ways to do this, but a while loop would do it

why won't this work?

> pollutant.level = 5
> while (pollutant.level < 30) {
+ pollutant.level = pollutant.level + 0.01* pollutant.level
+ yr = yr + 1
+ }
>

```
> yr=1
> pollutant.level = 5
> while (pollutant.level < 30 ) {
+ pollutant.level = pollutant.level + 0.01* pollutant.level
+ yr = yr + 1
+ }
> > yr
[1] 182
> pollutant.level
[1] 30.2788
```

* Most programming languages have For and while loops

File Loops

```
# average5.py
# Computes the average of numbers listed in a file.

def main():
    fileName = raw_input("What file are the numbers in? ")
    infile = open(fileName,'r')
    sum = 0.0
    count = 0
    for line in infile.readlines():
        sum = sum + eval(line)
        count = count + 1
    print "\nThe average of the numbers is", sum / count
```

mcsp.wartburg.edu/zelle/python/ppics1/.../Chapter08.p

Python Programming, 1/e

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Key Programming concepts: Control Structures

* if(cond) expression

> > a=4 > b=10 > if(a > b) win = "a" > if(b > a) win = "b" > win [1] "b"

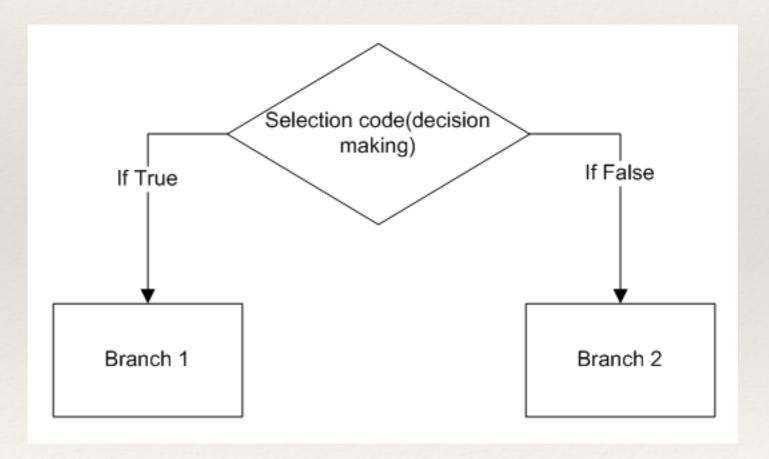
>

* ifelse(cond, true, false)
>
> win = ifelse(a > b, "a", "b")
> win
[1] "b"
>

Conditions: == equal > greater than >= greater than or equal to < less than <= less than or equal to %in% is in a list of something

&& AND || OR is.null()

- * Inside functions if(cond) {expression} else {expression}
- * the expression can always have multiple statements using {}
- * *If* can be useful for branching in your model



Key Programming concepts: Control Structures

```
#'
  compute annual yield
#'
  Function to compute yeild of different fruits as a function of annual temperature and precipitation
#'
#' @param T annual temperature (C)
#' @param P annual precipitation (mm)
#' @param ts slope on temperature
#' @param tp slope on precipitation
#' @param intercept (kg)
#' @param irr Y or N (default N)
#' @return yield in kg
compute_yield = function(T, P, ts, tp, intercept, irr="N") {
if (irr=="N"){
yield = tp*P + ts*T + intercept
else {
yield = ts*T + intercept
                                                       > compute_yield(32,200, 0.2, 0.4, 500)
return(yield)
                                                        [1] 586.4
}
                                                       > compute_yield(32,200, 0.2, 0.4, 500, "N")
                                                       [1] 586.4
                                                       > compute_yield(32,200, 0.2, 0.4, 500, "Y")
                                                        [1] 506.4
```

If can also be useful for creating classes of variables

Lets say we want to build a function that will compute mean spring, winter, summer, streamflow - from a dataset that looks something like this

> summary(streamflow)

year month day mm Min. :1953 Min. :1.000 Min. :1.00 Min. :0.08996 1st Qu.:1967 1st Qu.: 4.000 1st Qu.: 8.00 1st Qu.: 0.24290 Median :1981 Median : 7.000 Median :16.00 Median : 0.38685 Mean :1981 Mean : 6.542 Mean :15.73 Mean : 1.07800 3rd Qu.:1995 3rd Qu.:10.000 3rd Qu.:23.00 3rd Qu.: 0.98961 Max. :2010 Max. :12.000 Max. :31.00 Max. :71.97168

> head(streamflow)
year month day mm
1 1953 10 1 0.2608973

2 1953 10 2 0.2608973

>

> streamflow\$season = ifelse(streamflow\$month %in%)

c(1,2,3,10,11,12),"winter","summer")

> head(streamflow)

year month day mm season

- 1 1953 10 1 0.2608973 winter
- 2 1953 10 2 0.2608973 winter
- 3 1953 10 3 0.2608973 winter
- 4 1953 10 4 0.2608973 winter
- 5 1953 10 5 0.2608973 winter
- 6 1953 10 6 0.2608973 winter

> plot(streamflow\$season)

Error in plot.window(...) : need finite 'ylim' values

In addition: Warning messages:

1: In xy.coords(x, y, xlabel, ylabel, log) : NAs introduced by coercion

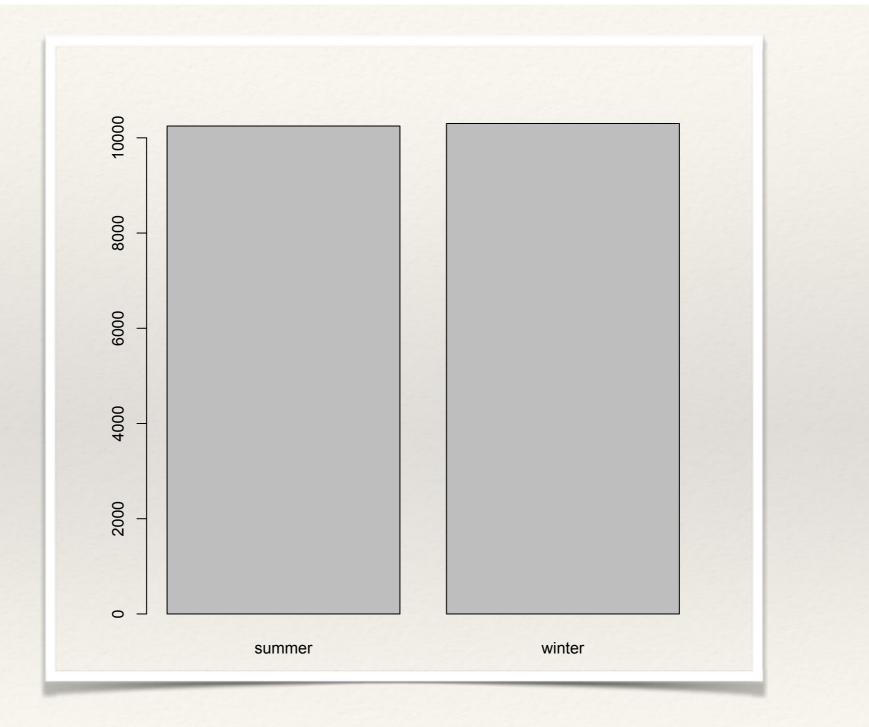
2: In min(x) : no non-missing arguments to min; returning Inf

3: In max(x) : no non-missing arguments to max; returning -Inf

> plot(as.factor(streamflow\$season))

>

> plot(as.factor(streamflow\$season)) >



>

```
#' @param str data frame with columns month and mm (mm is daily streamflow)
compute_seasonal_meanflow = function(str) {
```

```
str$season = ifelse( str$month %in% c(1,2,3,10,11,12),"winter","summer")
```

```
tmp = subset(str, str$season=="winter")
mean.winter = mean(tmp$mm)
```

```
tmp = subset(str, str$season=="summer")
mean.summer = mean(tmp$mm)
return(list(summer=mean.summer, winter=mean.winter))
}
```

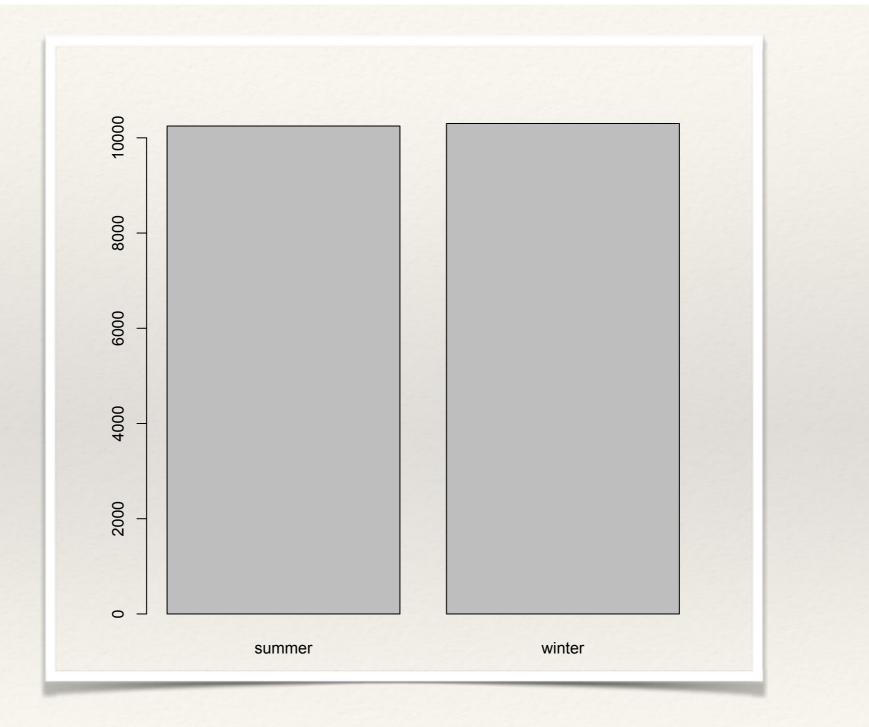
> compute_seasonal_meanflow(streamflow)
\$summer
[1] 1.538304
\$winter
[1] 0.6200728
>

Key Programming concepts: Control Structures

If can also be used to choose what you return from a function

```
compute_seasonal_flow = function(str,kind) {
  str$season = ifelse( str$month %in% c(1,2,3,10,11,12),"winter","summer")
  tmp = subset(str, str$season=="winter")
  if(kind=="mean") winter= mean(tmp$mm)
  if(kind=="min") winter=min(tmp$mm)
  tmp = subset(str, str$season=="summer")
  if(kind=="mean") summer= mean(tmp$mm)
  if(kind=="mean") summer= max(tmp$mm)
  if(kind=="min") summer=max(tmp$mm)
  if(kind=="min") summer=min(tmp$mm)
  if(kind=="min") summer=min(tmp$min")
  if(kind=="mi
```

> plot(as.factor(streamflow\$season)) >



>

```
#' @param str data frame with columns month and mm (mm is daily streamflow)
compute_seasonal_meanflow = function(str) {
```

```
str$season = ifelse( str$month %in% c(1,2,3,10,11,12),"winter","summer")
```

```
tmp = subset(str, str$season=="winter")
mean.winter = mean(tmp$mm)
```

```
tmp = subset(str, str$season=="summer")
mean.summer = mean(tmp$mm)
return(list(summer=mean.summer, winter=mean.winter))
}
```

> compute_seasonal_meanflow(streamflow)
\$summer
[1] 1.538304
\$winter
[1] 0.6200728
>

Key Programming concepts: Control Structures

If can also be used to choose what you return from a function

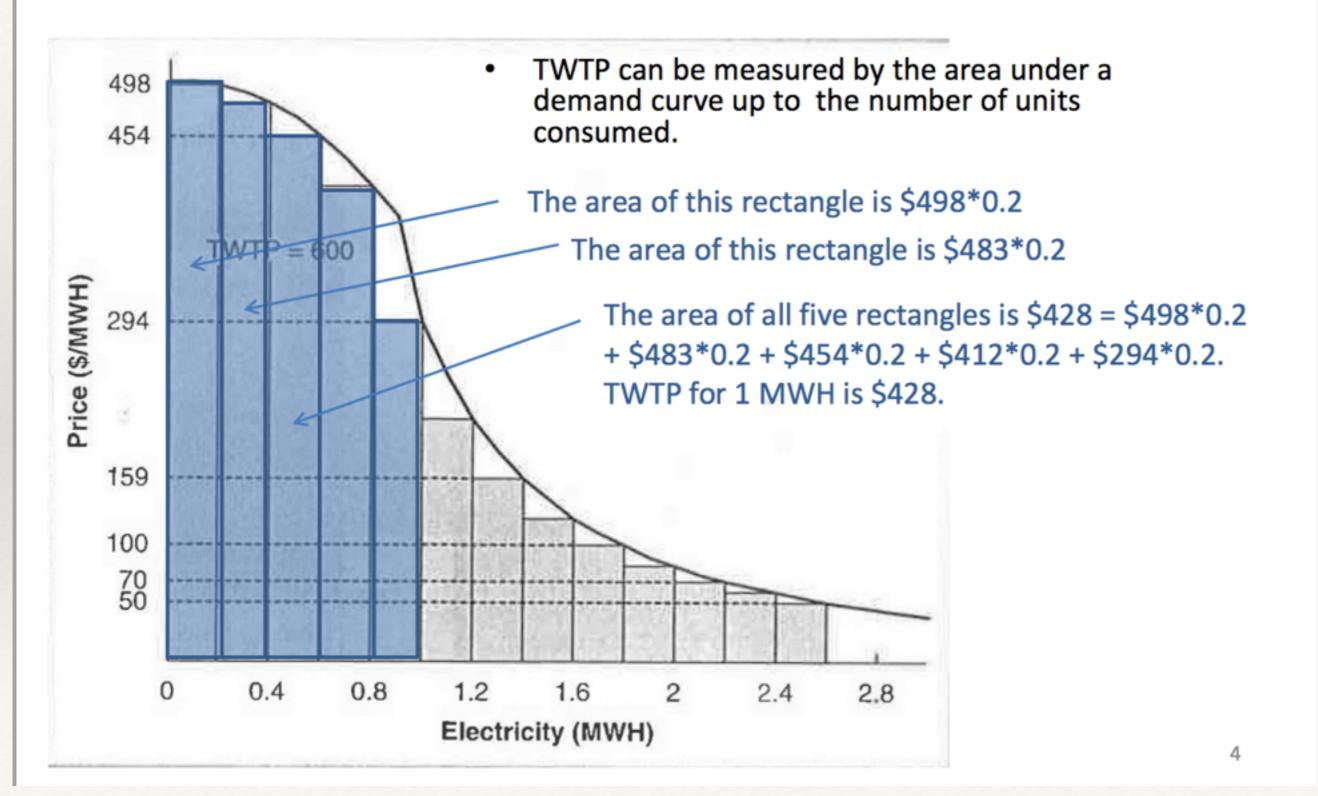
```
compute_seasonal_flow = function(str,kind) {
  str$season = ifelse( str$month %in% c(1,2,3,10,11,12),"winter","summer")
  tmp = subset(str, str$season=="winter")
  if(kind=="mean") winter= mean(tmp$mm)
  if(kind=="min") winter=min(tmp$mm)
  tmp = subset(str, str$season=="summer")
  if(kind=="mean") summer= mean(tmp$mm)
  if(kind=="mean") summer= max(tmp$mm)
  if(kind=="min") summer=max(tmp$mm)
  if(kind=="min") summer=min(tmp$mm)
  if(kind=="min") summer=min(tmp$min")
  if(kind=="mi
```

Key Programming concepts: Control Structures

If can also be used to choose what you return from a function

> compute_seasonal_flow(streamflow,"mean") \$summer [1] 1.538304 \$winter [1] 0.6200728 > compute_seasonal_flow(streamflow,"max") \$summer [1] 23.66069 \$winter [1] 71.97168

Measuring TWTP

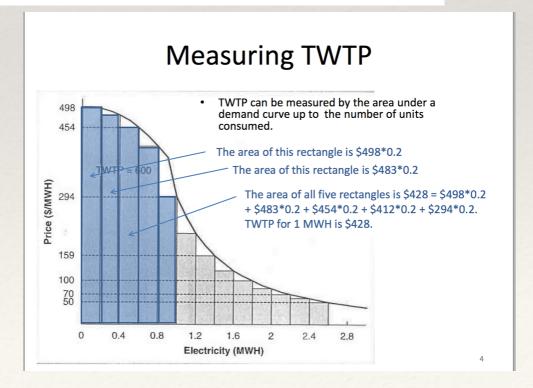


Example

- * Lets say our demand curve is as follows:
- * Electricity = c(0.1, 0.2, 0.4, 0.5, 0.6) MW
- * Marginal willingness to pay = c(300,250,200,50, 20) \$/MW
- Write a function that takes as input a data frame with values for marginal willingness to pay for different electricity values and returns total willingness to pay for a given electricity requirement (in MW)
- Take as input to the function a data frame called curve that has two columns elect, mwtop (electricity and marginal willingness to pay), and the electricity requirement

Key Programming concepts: Control Structures

```
compute_TWP = function(curve, req) {
total = 0
i=1
prev.elect = 0
while (( curve$elect[i] <= req) && (i < length(curve$elect))) {
total = total + (curve$elect[i]-prev.elect)*curve$mwtop[i]
prev.elect = curve$elect[i]
i = i+1
}
return(total)
}</pre>
```



```
compute_TWP = function(curve, req) {
total = 0
i=1
prev.elect = 0
while (( curve$elect[i] <= req) && (i < length(curve$elect))) {</pre>
total = total + (curve$elect[i]-prev.elect)*curve$mwtop[i]
prev.elect = curve$elect[i]
i = i+1
return(total)
}
>
> example.curve = data.frame(elect = c(0.1,0.2,0.4,0.5,0.6), mwtop=c(300,250,200,50,20))
> example.curve
elect mwtop
  0.1 300
1
  0.2 250
2
  0.4 200
3
  0.5 50
4
5
  0.6 20
> compute_TWP(example.curve, req=0.2)
[1] 55
>(0.1*300)+(0.1*250)
[1] 55
>
```

```
compute_TWP = function(curve, req) {
total = 0
i=1
prev.elect = 0
while (( curve$elect[i] <= req) && (i < length(curve$elect))) {</pre>
total = total + (curve$elect[i]-prev.elect)*curve$mwtop[i]
prev.elect = curve$elect[i]
i = i+1
                                                                > example.curve
                                                                  elect mwtop
return(total)
                                                                    0.1 300
                                                                    0.2
                                                                         250
                                                                    0.4 200
                                                                3
                                                                          50
                                                                    0.5
                                                                4
                                                                5
                                                                   0.6
                                                                          20
                                                                >> compute_TWP(example.curve, req=0.7)
              Measuring TWTP
                                                                [1] 100
                                                                > compute_TWP(example.curve, req=0.6)
                   TWTP can be measured by the area under a
    498
                    demand curve up to the number of units
                    consumed.
    454
                                                                [1] 100
                    The area of this rectangle is $498*0.2
                     The area of this rectangle is $483*0.2
   Price ($/MWH)
                                                                > compute_TWP(example.curve, req=0.9)
                      The area of all five rectangles is $428 = $498*0.2
                      + $483*0.2 + $454*0.2 + $412*0.2 + $294*0.2.
                                                                [1] 100
                      TWTP for 1 MWH is $428.
    159
                                                                > compute_TWP(example.curve, req=0.3)
    100
     70
50
                                                                [1] 55
      0
         0.4
             0.8
                            2.4
                 1.2
                    1.6
                        2
                               2.8
                Electricity (MWH)
                                                                > compute_TWP(example.curve, req=0.4)
                                                                 [1] 95
                                                                >>
```

Example

- If the user asks for an electricity requirement beyond what was described by the demand curve, return NA from the function
- * How would you implement that

```
compute_TWP = function(curve, req) {
  total = 0
  i=1
  prev.elect = 0
  while (( curve$elect[i] <= req) && (i < length(curve$elect))) {
  total = total + (curve$elect[i]-prev.elect)*curve$mwtop[i]
  prev.elect = curve$elect[i]
  i = i+1
  }
  return(total)
  }</pre>
```

Example

```
compute_TWP = function(curve, req) {
highest.elect = max(curve$elect)
if (req <= highest.elect) {</pre>
total = 0
i=1
prev.elect = 0
while (( curve$elect[i] <= req) && (i < length(curve$elect))) {</pre>
total = total + (curve$elect[i]-prev.elect)*curve$mwtop[i]
prev.elect = curve$elect[i]
i = i+1
                                                    > example.curve
}
}
                                                     elect mwtop
else { total="NA" }
                                                    1
                                                       0.1 300
return(total)
                                                    2
                                                       0.2 250
}
                                                    3
                                                       0.4 200
                                                    4
                                                       0.5
                                                             50
                                                    5
                                                       0.6 20
                                                    >
                                                    > compute_TWP(example.curve, req=0.4)
                                                    [1] 95
                                                    > compute_TWP(example.curve, req=0.9)
                                                    [1] "NA"
```

Assignment 2

In your group, write a simple function (that involves at least two data types and a control structure) Enter this function in your organization's github space Read/create some data to test your function Also include that in github Submit the link the repository