Class06: Writing functions in R

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Introduction

 \mathbf{R} code

```
add <- function(x, y=10, z=0){
    x + y + z
}
```

I can just use this function

```
add (1,100)
```

[1] 101

```
add(x=c(1,2,3,4), y=100)
```

```
[1] 101 102 103 104
```

Functions can have "required" input arguments and "optional" input arguments. The optional arguments are defined with an equals default value (y=0) in the function definition.

```
add(x=1, y=100, z=10)
```

[1] 111

Generate DNA sequence

Q. Write a function to return a DNA sequence of a user specifed length. Call it generate_dna()

The sample() can help here.

```
#generate_dna() <- function(size=5){ }
students <- c("jeff", "jeremy", "peter")
sample(students, size = 5, replace=TRUE)</pre>
```

```
[1] "jeremy" "jeff" "peter" "jeff" "peter"
```

Now work with bases rather than students

```
bases <- c("A", "C", "G", "T")
sample(bases, size=10, replace=TRUE)</pre>
```

```
[1] "T" "G" "A" "T" "C" "T" "G" "G" "T" "G"
```

Now I have a working 'snippet' of code, so I can use this as the body of my first function version here:

```
generate_dna <- function(size=5){
  bases <- c("A", "C", "G", "T")
  sample(bases, size=size, replace=TRUE)
}</pre>
```

```
generate_dna(size=100)
```

```
generate_dna()
```

```
[1] "T" "G" "C" "C" "C"
```

I want the ability to return a sequence like "AGTACCTG" string, i.e. a one element vector where the bases are all together.

```
generate_dna <- function(size=5, together=TRUE){
  bases <- c("A", "C", "G", "T")
  sequence <- sample(bases, size=size, replace=TRUE)
  if (together){
    sequence <- paste(sequence, collapse = "")
  }
  return(sequence)
}</pre>
```

```
generate_dna(together=FALSE)
```

```
[1] "C" "T" "G" "G" "T"
```

3. Generate Protein function

we can get the set of 20 natural amino-acids from the bio3d package

q. Write a protein sequence generating function that will return sequences of a user-specified length?

```
generate_protein <- function(size=5, together=TRUE){
   aa <- bio3d::aa.table$aa1[1:20]
   sequence <- sample(aa, size=size, replace=TRUE)

## Optionally return a single string
   if (together){
       sequence <- paste(sequence, collapse = "")
   }
   return(sequence)
}</pre>
```

Q. Generate random protein sequences of length 6 to 12 amino acids.

```
#errored code
#generate_protein(size=6:12)
```

We can fix this inability to generate multiple sequences by either editing and adding to the function body code (eg. for a for loop) or by using the R **apply** family of utility functions

```
ans <- sapply(6:12, generate_protein)
ans

[1] "HNQGAE" "QMAHYCH" "HSDMDTGM" "QEIVAAVGL" "CGEEKMAPPF"
[6] "NDCPQHHSSLL" "NTGQRIDDTFKC"</pre>
```

It would be cool and useful if I could get FASTA format output.

```
cat(ans, sep="\n")
```

HNQGAE

QMAHYCH

HSDMDTGM

QEIVAAVGL

CGEEKMAPPF

NDCPQHHSSLL

NTGQRIDDTFKC

I want this to look like

>ID.6 CNSTRV >ID.7 NGCVYMV >ID.8 QATSNMQI

```
with.id <- paste(">ID.",6:12,"\n", ans, sep="")
cat(with.id, sep="\n")
```

>ID.6 HNQGAE

>ID.7

QMAHYCH

>ID.8

 ${\tt HSDMDTGM}$

>ID.9

QEIVAAVGL

>ID.10

CGEEKMAPPF

>ID.11

NDCPQHHSSLL

>ID.12

NTGQRIDDTFKC

Q. Determine if these sequences can be found in nature or are they unique? Why or why not?

I BLASTp searched by FAFST format sequences against the sequences with length 6, 7, 8, were not unique with 100% coverage and 100% identity.

sequences with length 9,10,11,12 are unique and can't be found in the databases.