

COMP 204

Functions II

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based on material from Mathieu Blanchette and Carlos Oliver
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Quiz 12 password

Getting help

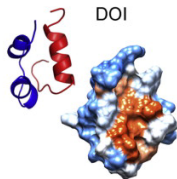
- ▶ TAs and I are available to help, and not just for assignments!
- ▶ The Computer Science Undergraduate Student (CSUS) association has a help desk where you can drop in with questions any time 10am-5pm in Trottier 3090.

Quiz 11 review: order the functions get executed

```
1 import math # this imports the math module
2
3 def euclid(xHome, yHome, xAcc, yAcc):
4     return math.sqrt((xHome - xAcc)**2 + (yHome - yAcc)**2)
5
6 def pregnantQuestion():
7     if (input("Are you pregnant? (yes/no) ") == "yes"):
8         print("You must evacuate")
9     else:
10        print("Evacuation is recommended")
11
12 def evaluateRisk(distance):
13     if distance <= 20:
14         print("You must evacuate")
15     elif distance <= 40:
16         pregnantQuestion()
17     else:
18         print("No need to evacuate")
19
20 def evacuateAssessmentMain():
21     xAcc = 20; yAcc = 30
22     xHome = 40; yHome = 50
23     evaluateRisk(float(euclid(xHome, yHome, xAcc, yAcc)))
24
25 evacuateAssessmentMain()
```

Example: Hydrophobic patches

- ▶ Protein sequences are made of amino acids.
- ▶ Some amino acids (G, A, V, L, I, P, F, M, W) are hydrophobic (i.e. they don't like to interact with water molecules).
- ▶ Some proteins contain *hydrophobic patches*, which are portions of the sequence that start and end with an hydrophobic amino acid and where at least 80% of the amino acid are hydrophobic.



- ▶ For example, in the sequence EDAYQIALEGAASTE, the longest hydrophobic patch is IALEGAA.

Goal: Write a function that identifies the *longest* hydrophobic patch in a given protein sequence.

Find longest hydrophobic patch by *divide-and-conquer*

findLongestHydrophobicPatch



isHydrophobicPatch



isHydrophobic

```
findLongestHydrophobicPatch(protein)
isHydrophobicPatch(sequence)?
EDAYQIALEGAASTE
outer for loop: start position from start = 0
inner for loop end position from end = start + 1
```

```
isHydrophobicPatch(sequence)?
isHydrophobic('E') # (1) first a.a.
isHydrophobic('L') # (2) last a.a.
EDAYQIAL
for-loop patchLen += isHydrophobic(s[aa])
# (3) length of hydrophobic amino acids (min 80%)
```

```
isHydrophobic(aa)?
aa in ["G", "A", "V", "L", "I", "P", "F", "M", "W"]?
```

Not the most efficient way (discussed a bit later)

Example: Hydrophobic patches

Divide-and-Conquer (bottom up approach): Break it down into small, manageable tasks and start with the lowest tasks

1. Write a function that checks if a given amino acid is hydrophobic
2. Write a function that checks if a given sequence is a hydrophobic patch:
 - ▶ Starts and ends with a hydrophobic amino acid
 - ▶ Made at 80% or more of amino acids (i.e. count hydrophobic amino acids; see if count is at least $0.8 \cdot \text{length}$)
3. Use nested for or while loop to iterate over all possible start and end points of a candidate patch. Use function above to test if it is a patch. If it is, calculate length and update the variable that keeps track of the longest patch found so far.
4. Report longest patch found

isHydrophobic function

```
1 # This function returns True if aa is a hydrophobic amino
  acid
2 def isHydrophobic(aa):
3     hydrophobic = ["G", "A", "V", "L", "I", "P", "F", "M", "W"]
4
5     # This checks if aa is equal to an object in the list
  hydrophobic
6     if aa in hydrophobic:
7         return True
8     else:
9         return False
10
11 # This is a shorter way to do the same thing
12 def isHydrophobic2(aa):
13     return (aa in ["G", "A", "V", "L", "I", "P", "F", "M", "W"])
```


isHydrophobicPatch function

```
1 # This function tests whether a given sequence
2 # contains at least 80% of hydrophobic amino acids
3 def isHydrophobicPatch(sequence):
4     # test if sequence starts and ends with a hydrophobic aa
5     # If not, it is not a hydrophobic patch, so return False
6     if isHydrophobic(sequence[0]) == False or isHydrophobic(
7         sequence[-1]) == False:
8         return False
9     # Count the fraction of hydrophobic amino acids
10    hydrophobicCount = 0
11    for aa in sequence:
12        if isHydrophobic(aa):
13            hydrophobicCount += 1
14    # See if we have enough hydrophobic amino acids
15    if hydrophobicCount >= 0.8 * len(sequence):
16        return True
17    else:
18        return False
```

```
1 # shorter way to do the same with one boolean expression
2 def isHydrophobicPatch2(sequence):
3     return isHydrophobic(sequence[0]) and \
4            isHydrophobic(sequence[-1]) and \
5            len([aa for aa in sequence if isHydrophobic(aa)]) >
6            0.8 * len(sequence)
```

findLongestHydrophobicPatch function

```
1 # This returns the longest hydrophobic patch found in a
  sequence
2 def findLongestHydrophobicPatch(protein):
3     longestPatch="" # the longest patch found so far
4
5     # for every possible starting point
6     for start in range(0, len(protein)):
7
8         # and every possible end point
9         for end in range(start+1, len(protein)+1):
10            # get the sequence
11            candidate = protein[start:end]
12
13            # test hydrophobicity
14            if isHydrophobicPatch(candidate):
15
16                # if longer than longest seen so far, update
17                if len(candidate)>len(longestPatch):
18                    longestPatch = candidate
19
20    return longestPatch
```

This is an exhaustive search and not the most efficient algorithm.
How do we improve it? How much can we improve?

Recursion version (advanced): findLongestHydrophobicPatch_recur

```
1 def findLongestHydrophobicPatch_recur(protein, start, end):
2
3     if start < end and end <= len(protein):
4         if isHydrophobicPatch(protein[start:end]):
5             return protein[start:end]
6         else:
7             patch1 = findLongestHydrophobicPatch_recur(
8                 protein, start+1, end)
9             patch2 = findLongestHydrophobicPatch_recur(
10                protein, start, end-1)
11         else:
12             return ""
13
14         if len(patch1) > len(patch2):
15             return patch1
16         else:
17             return patch2
18
19 # code to test our function
20 protein = input("Enter protein sequence: ")
21 patch = findLongestHydrophobicPatch_recur(protein, 0, len(
22     protein))
23 print("Longest hydrophobic patch is ", patch)
```

Positional arguments

The functions we have seen so far take as input *positional arguments*.

Arguments are passed in the same order as the function definition

Example:

```
1 def inputInRange(message, minVal, maxVal):
```

Notes:

- ▶ Every call to the function *must* provide exactly three objects as arguments
- ▶ The order of the arguments matter:
inputInRange("Enter age", 0, 150)
is not the same thing as
inputInRange("Enter age", 150, 0)

Optional arguments

Another way to pass arguments to functions is to use *keyword arguments*. Example:

```
1 # The function takes two keyword arguments
2 def inputInRange(message, minVal = 0, maxVal = 100):
3     while True: # loops until return statement is executed
4         n = int(input(message))
5         if n >= minVal and n <= maxVal:
6             return n
7         else:
8             print("Number outside of range", minVal, maxVal)
9
10 age = inputInRange("Enter age:")
11 height = inputInRange("Enter height (in cm):", maxVal = 250)
12 weight = inputInRange("Enter weight:", maxVal=250, minVal=20)
```

Notes:

- ▶ Keyword arguments are optional when calling the function. If the caller does not provide them, they are set to their default value specified in the function header.
- ▶ Keyword arguments must come *after* positional arguments.
- ▶ Keyword arguments can be specified in any order.
- ▶ Useful when a function can take a large number of optional

Returning multiple outputs

A function can only return one object. What if a function needs to return multiple pieces of information? Idea: The object returned can be a compound object (list, tuple).

```
1 # This returns a tuple made of the longest hydrophobic patch
2 # found in a sequence, along with its start and end
   positions
3 def findLongestHydrophobicPatch(protein):
4     longestPatch=""
5     for start in range(0, len(protein)):
6         for end in range(start+1, len(protein)):
7             candidate = protein[start:end]
8             if isHydrophobicPatch(candidate):
9                 if len(candidate)>len(longestPatch):
10                    longestPatch = candidate
11                    longestPatchStart = start
12                    longestPatchEnd = end
13     # this returns a tuple
14     return (longestPatch, longestPatchStart, longestPatchEnd)
15
16 # code to test our function
17 protein = input("Enter protein sequence: ")
18 patch, s, e = findLongestHydrophobicPatch(protein)
19 print("Longest hydrophobic patch is ", patch)
20 print("It goes from position", s, "to position", e)
```

Recursion version 2: findLongestHydrophobicPatch_recur2

```
1 def findLongestHydrophobicPatch_recur2(protein, start, end):
2
3     if start < end and end <= len(protein):
4         if isHydrophobicPatch(protein[start:end]):
5             return (protein[start:end], start, end)
6         else:
7             patch1, patch1_start, patch1_end =
findLongestHydrophobicPatch_recur2(protein, start+1, end
8
9             patch2, patch2_start, patch2_end =
findLongestHydrophobicPatch_recur2(protein, start, end
10            -1)
11
12            else:
13                return ("", 0, 0)
14
15            if len(patch1) > len(patch2):
16                return patch1, patch1_start, patch1_end
17            else:
18                return patch2, patch2_start, patch2_end
```

The scope of variables

When inside a function, the only variables that are available are:

- ▶ Local variables: The function's arguments, and all the variables defined within that function.
 - ▶ When we return from a function, all local variables are discarded.
 - ▶ It is possible for a function to have a local variable called `x`, even if a global variable `x` already exists. Those are considered two different variables, and only the local version is used.
- ▶ Global variables: Those defined outside any function. Their value can be accessed within a function, but not changed.

Notes:

- ▶ Avoid referring to global variables within functions. It makes code very confusing.
- ▶ It is actually possible for a function to change the value of global variables, but this is rarely a good thing to do, so we will not explain it here.


```
1 def fun1():
2     x=53 # is local to fun1
3     print("Within fun1, x = ",x)
4
5 def fun2(x):
6     x=2 # is local to fun2
7     print("Within fun2, x = ",x)
8
9 def fun3(): # x is not defined within fun3,
10            # so we use the global variable
11     print("Within fun3, x = ",x)
12
13 x=17
14 print("To start , x = " ,x)
15 fun1()
16 print("After fun1, x = " ,x)
17 fun2(x)
18 print("After fun2, x = " ,x)
19 fun3()
20 print("After fun3, x = " ,x)
```

Output:

```
To start, x = 17
Within fun1, x = 53
After fun1, x = 17
Within fun2, x = 2
After fun2, x = 17
Within fun3, x = 17
After fun3, x = 17
```