Scientific Programming: Part B

Data structures 1

Introduction

Data

In programming languages, data are pieces of information that can be assigned to variables (i.e. **values** that can be assigned to **variables**)

Abstract Data Type (ADT)

A mathematical model, defined by a collection of values and a set of operations that can be performed on them.

Primitive Abstract Data Types

Primitive abstract data types that are **provided directly** by the language



Specification vs. Implementation

Specification

The specification of a type of data is its "manual". It is a **description of the** data that does not provide details

Implementation

The **actual code** (with all the specific details) that **realizes** (i.e. implements) the abstract data type

Example: Real numbers vs IEEE-754

- "a real number is a value of a continuous quantity that can represent a distance along a line"
- IEEE-754 is a standard that defines the format for the representation of floating point numbers

Sometime they differ!

>>> 0.1+0.2 0.3000000000000004

Data structures

Data structures

Data structures are collections of data, characterized more by the organization of the data rather than the type of contained data.

How to describe data structures

- a systematic approach to organize the collection of data
- a set of operators that enable the manipulation of the structure

Data structures can be

- **Linear**: if the position of an element relative to the ones inserted before/after does not change
- Static / Dynamic: depending on if the content or size can change

Data structures

Type	Java	C++	Python
Sequences	List, Queue, Deque LinkedList, ArrayList, Stack, ArrayDeque	list, forward_list vector stack queue, deque	list tuple deque
Sets	Set TreeSet, HashSet, LinkedHashSet	set unordered_set	set, frozenset
Dictionaries	Map HashTree, HashMap, LinkedHashMap	map unordered_map	dict
Trees	E.	E	.
Graphs	T T	=	-

Sequence: description

Sequence

A dynamic data structure representing an "ordered" group of elements

- The ordering is not defined by the content, but by the relative position inside the sequence (first element, second element, etc.)
- Values could appear more than once
- Example: [0.1, "alberto", 0.05, 0.1] is a sequence

Operators

- It is possible to add / remove elements, by specifying their position
 - $s = s_1, s_2, \dots, s_n$
 - the element s_i is in position pos_i
- It is possible to access *directly* some of the elements of the sequence
 - the beginning and/or the end of the list
 - having a reference to the position
- It is possible to sequentially access all the other elements

Sequence: specification

```
SEQUENCE
% Return True if the sequence is empty
boolean isEmpty()
% Returns the position of the first element
Pos head()
% Returns the position of the last element
Pos tail()
\% Returns the position of the successor of p
Pos next(Pos p)
\% Returns the position of the predecessor of p
Pos prev(Pos p)
```

Sequence: specification

```
SEQUENCE (continue)
% Inserts element v of type object in position p.
% Returns the position of the new element
Pos insert(Pos p, object v)
\% Removes the element contained in position p.
% Returns the position of the successor of p, which % becomes successor of
 the predecessor of p
Pos remove(Pos p)
\% Reads the element contained in position p
OBJECT read(Pos p)
% Writes the element v of type OBJECT in position p
write(Pos p, object v)
```

To build our "Sequence" data structure

SEQUENCE (continue)

- % Inserts element v of type object in position p.
- % Returns the position of the new element

Pos insert(Pos p, object v)

- % Removes the element contained in position p.
- % Returns the position of the successor of p, which % becomes successor of the predecessor of p

Pos remove(Pos p)

- % Reads the element contained in position p
- OBJECT read(Pos p)
- % Writes the element v of type OBJECT in position p write(POS p, OBJECT v)

"specifications"

ADT



"implementation"

Python code

Sequence: implementation (sketch)

```
class mySequence:
   def init (self):
        #the sequence is implemented as a list
       self. data = []
   #isEmpty returns True if sequence is empty, false otherwise
   def isEmpty(self):
        return len(self. data) == 0
   #head returns the position of the first element
    def head(self):
       if not self.isEmpty():
           return 0
        else:
           return None
   #tail returns the position of the last element
   def tail(self):
       if not self.isEmpty():
           return len(self. data) -1
        else:
            return None
   #next returns the position of the successor of element
   #in position pos
   def next(self, pos):
       if pos <len(self. data)-1:
           return pos +1
        else:
            return None
   #prev returns the position of the predecessor of element
   #in position pos
   def prev(self, pos):
       if pos > 0 and pos < len(self. data):
           return pos - 1
        else:
            return None
```

```
#insert inserts the element obj in position pos
#or at the end
def insert(self, pos, obj):
    if pos <len(self. data):</pre>
        self. data.insert(pos, obj)
        return pos
    else:
        #Not necessary! Already done by list's insert!!!
        self. data.append(obi)
        return len(self. data) -1
#remove removes the element in position pos
#(if it exists in the sequence) and returns the index
#of the element that now follows the predecessor of pos
def remove(self, pos):
    #TODO
    pass
#read returns the element in position pos (if
#it exists) or None
def read(self, pos):
    #TODO
    pass
#write changes the object in position pos to new obj
#if pos is a valid position
def write(self,pos,new obj):
    #TODO
    pass
#converts the data structure into a string
def str (self):
    return str(self. data)
```

Set: description

Set

A dynamic, non-linear data structure that stores an unordered collection of values without repetitions.

• We can consider a total order between elements as the order defined over their abstract data type, if present.

Operators

- Basic operators:
 - insert
 - delete
 - contains
- Sorting operators
 - Maximum
 - Minimum

- Set operators
 - union
 - intersection
 - difference
- Iterators:
 - for x in S:

Set: abstract data type

```
Set
% Returns the size of the set
int len()
\% Returns True if x belongs to the set; Python: x in S
boolean contains(OBJECT x)
\% Inserts x in the set, if not already present
add(OBJECT x)
\% Removes x from the set, if present
discard(OBJECT x)
% Returns a new set which is the union of A and B
SET union (SET A, SET B)
\% Returns a new set which is the intersection of A and B
SET intersection(SET A, SET B)
\% Returns a new set which is the difference of A and B
SET difference(SET A, SET B)
```

Set: implementation (exercise)

```
class MvSet:
    def init (self, elements):
       #HOW are we gonna implement the set?
        #Shall we use a list, a dictionary?
        pass
    #let's specify the special operator for len
    def len (self):
        pass
    #this is the special operator for in
    def contains (self, element):
        pass
    #we do not redefine add because that is for S1 + S2
    #where S1 and S2 are sets
    def add(self,element):
        pass
    def discard(self,element):
        pass
    def iterator(self):
        pass
    def str (self):
        pass
    def union(self, other):
        pass
    def intersection(self, other):
        pass
    def difference(self, other):
        pass
```

Set

% Returns the size of the set int len()

% Returns **True** if x belongs to the set; Python: x in S **boolean** contains(OBJECT x)

% Inserts x in the set, if not already present add(OBJECT x)

% Removes x from the set, if present discard(OBJECT x)

% Returns a new set which is the union of A and BSET union(SET A, SET B)

% Returns a new set which is the intersection of A and BSET intersection(SET A, SET B)

% Returns a new set which is the difference of A and B SET difference(SET A, SET B)

Dictionary

Dictionary

Abstract data structure that represents the mathematical concept of partial function $R: D \to C$, or key-value association

- Set *D* is the domain (elements called keys)
- Set C is the codomain (elements called values)

Operators

- Lookup the value associated to a particular key, if present, None otherwise
- Insert a new key-value association, deleting potential association that are already present for the same key
- Remove an existing key-value association

Dictionary: ADT

DICTIONARY

```
\% Returns the value associated to key k, if present; returns none otherwise
```

```
OBJECT lookup(OBJECT k)
```

- % Associates value v to key k insert(OBJECT k, OBJECT v)
- % Removes the association of key k

```
remove(OBJECT k)
```

Linked lists

List (Linked List)

A sequence of memory objects, containing arbitrary data and 1-2 pointers to the next element and/or the previous one

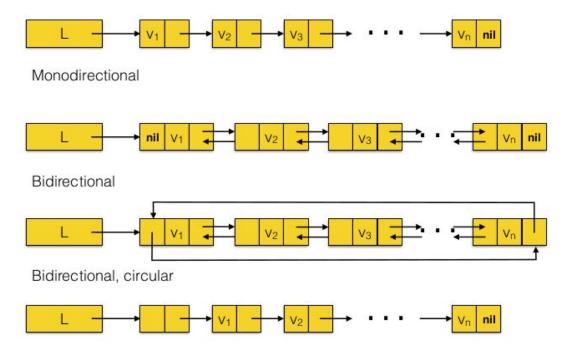
Note

- Contiguity in the list ≠ contiguity in memory
- All the operations require O(1), but in some cases you need a lot of single operations to complete an action

Possible implementations

- Bidirectional / Monodirectional
- With sentinel / Without sentinel
- Circular / Non-circular

Linked lists (types)



Monodirectional, with sentinel

Linked lists are dynamic collections of **objects and pointers** (either 1 or 2) that **point to the next** element in the list **or to both the next and previous** element in the list.

Example: monodirectional list in python

Monodirectional list

%adds a node **n** to the Monodirectional list placing it as the **head** add (node n)

%searches a node n and returns True if it is found, false otherwise

```
boolean search (node n)
```

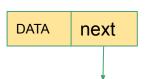
%removes a node n if it is found, does nothing otherwise

```
remove (node n)
```

%produces the string representation of the Monodirectional list as: el1 -> el2 -> ... -> eln

```
__str__()
```

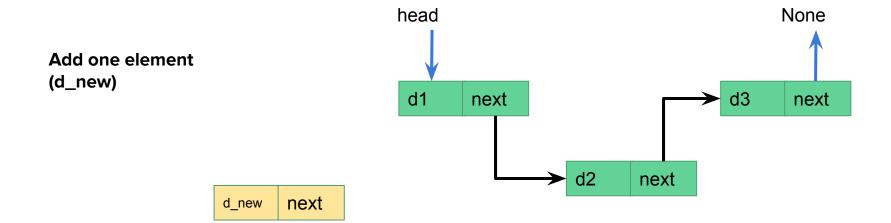




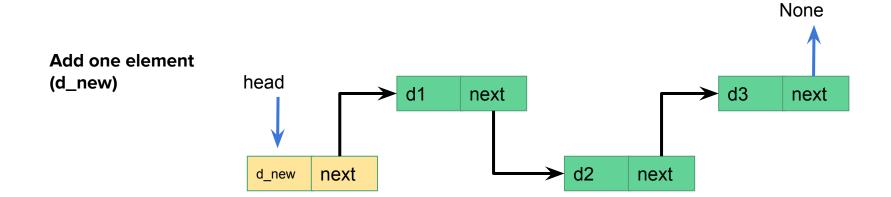
A list is a sequence of nodes, the first of which is the **head.**

Elements are added **at the beginning** and become the new head

Example: monodirectional list in python

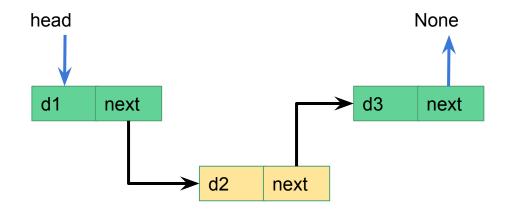


Monodirectional list in python: add



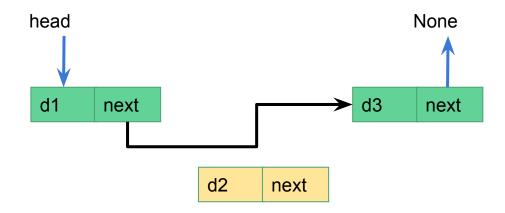
Monodirectional list in python: remove

Remove one element (d2)



Monodirectional list in python: remove

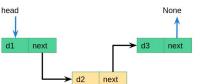
Remove one element (d2)



The code

```
Can place this in Node.py"""
class Node:
   def init (self, data):
       self. data = data
       self. next = None
   def get data(self):
       return self. data
   def set data(self, newdata):
       self. data = newdata
   def get next(self):
       return self. next
   def set next(self, node):
       self. next = node
   def str (self):
       return str(self. data)
   #for sorting
   def lt (self, other):
       return self. data < other. data
```

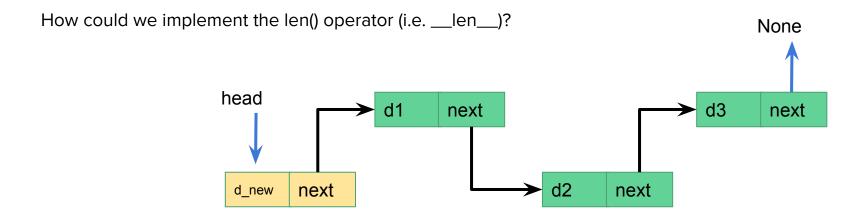
```
class MonodirList:
   def init (self):
       self. head = None #None is the sentinel!
   def add(self,node):
       if type(node) != Node:
           raise TypeError("node is not of type Node")
       else:
           node.set next(self. head)
           self. head = node
   def search(self, item):
       current = self. head
       found = False
       while current != None and not found:
           if current.get data() == item:
                  found = True
            else:
                  current = current.get next()
        return found
   def remove(self,item):
       current = self. head
        prev = None
       found = False
       while not found and current != None:
           if current.get data() == item:
               found = True
           else:
               prev = current
               current = current.get next()
       if found:
           if prev == None:
               self. head = current.get next()
           else:
               prev.set next(current.get next() )
   def str (self):
       if self. head != None:
           dta = str(self. head)
           cur el = self. head.get next()
           while cur el != None:
               dta += " -> " + str(cur el)
               cur el = cur el.get next()
           return str(dta)
       else:
           return ""
```



```
if name == " main ":
   ML = MonodirList()
    for i in range(1,50,10):
        n = Node(i)
        ML.add(n)
    print(ML)
    print("Adding 111")
    new n = Node(111)
   ML.add(new n)
    print("Adding 27")
    new n2 = Node(27)
   ML.add(new n2)
    print(ML)
    print("Removing 1")
    ML. remove(1)
    print(ML)
    print("Removing 1")
   ML. remove(1)
    print("Removing 111")
    print("Removing 31")
   ML.remove(111)
   ML. remove (31)
    print(ML)
```

```
41 -> 31 -> 21 -> 11 -> 1
Adding 111
Adding 27
27 -> 111 -> 41 -> 31 -> 21 -> 11 -> 1
Removing 1
27 -> 111 -> 41 -> 31 -> 21 -> 11
Removing 1
Removing 11
Removing 31
27 -> 41 -> 21 -> 11
```

Monodirectional list in python: min/max?



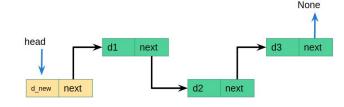
Go from first to last element and accumulate the max_so_far

Monodirectional list in python: ___len___()?

How could we implement the len() operator (i.e. __len__)?

The code:

```
def __len__(self):
    current = self.__head
    length = 0
    while current != None:
        length += 1
        current = current.get_next()
    return length
```



Complexity is **O(n)**. Is it possible to improve this?

Monodirectional list in python: ___len___()?

Faster ___len___().

Idea: store and update the number of elements present

The code:

```
class MonodirList:
    def __init__(self):
        self.__head = None #None is the sentine!!
        self.__len = 0

def add(self,node):
        if type(node) != Node:
            raise TypeError("node is not of type Node")
    else:
        node.set_next(self.__head)
        self.__head = node
        self.__len += 1
    ...

def __len__(self):
    return self.__len
```

```
def remove(self,item):
    current = self. head
    prev = None
    found = False
    while not found and current != None:
        if current.get data() == item:
            found = True
        else:
            prev = current
            current = current.get next()
    if found:
        if prev == None:
            self. head = current.get next()
        else:
            prev.set next(current.get next() )
        self. len -= 1
```

Complexity is O(1).

Exercise: How about O(1) min/max values? Hint: change again __init__, add, and remove.

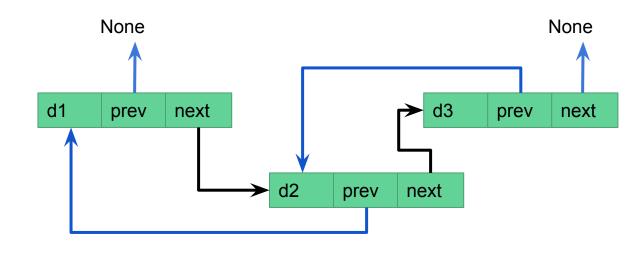
Bidirectional linked list

Each node now has:

- the data
- a prev pointer
- a next pointer

prev pointer of the first
element in the list is
None

next pointer of the **last** element is **None**



Bidirectional linked list

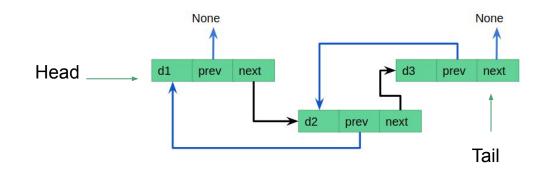
Each node now has:

- the data
- a prev pointer
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prev pointer of the first
element in the list is
None

next pointer of the **last** element is **None**

The list can have a **head** and **tail** pointer

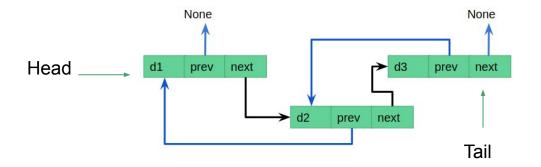


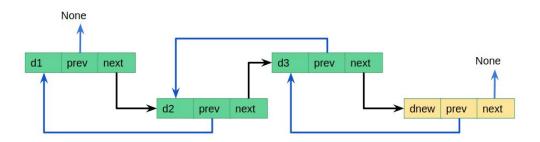
Bidirectional linked list: append

Each node now has:

- the data
- a prev pointer
- a next pointer

Append: add a node as next of the current tail





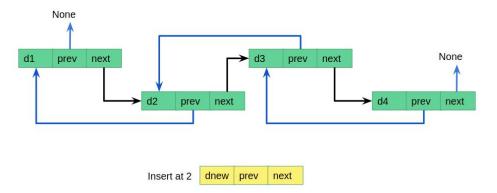
Bidirectional linked list: insert at/remove

Each node now has:

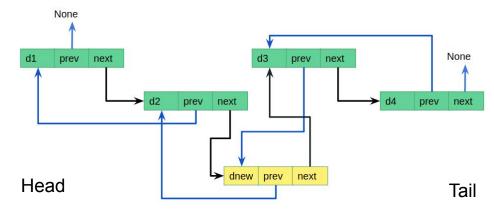
- the data
- a prev pointer
- a next pointer

Insert at/remove:

reach the correct position and update the next/prev pointers of the **three** involved nodes



Insert at 2
First loop until you reach 2 (cur = cur.get_next())



Lists in Python implemented through dynamic vectors

- A vector of a given size (initial capacity) is allocated
- When inserting an element before the end, all elements have to be moved cost O(n)
- When inserting an element at the end (append), the cost is O(1) (just writing the element at first available slot)

Problem:

- It is not known how many elements have to be stored
- The initial capacity could be insufficient

Solution:

Lists in Python implemented through dynamic vectors

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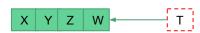
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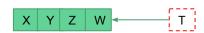
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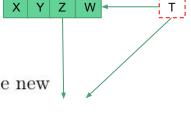
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- When inserting an element before the end, all elements have to be moved cost O(n)
- When inserting an element at the end (append), the cost is O(1) (just writing the element at first available slot)

Problem:

- It is not known how many elements have to be stored
- The initial capacity could be insufficient

Solution:

 A new (larger) vector is allocated, the content is copied in the new vector, the old vector is released



Z

Question

Which is the best approach?

Approach 1

If the old vector has size n, allocate a new vector of size dn. For example, d=2

Approach 2

If the old vector has size n, allocate a new vector of size n+d, where d is a constant. For example, d=16

doubling

increment

Actual cost of an append() operation:

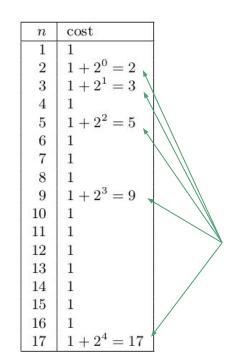
$$c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$$

Assumptions:

- Initial capacity: 1
- Writing cost: $\Theta(1)$

ex. 3 elements in. Append now: 1 operation





Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Doubling

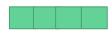
Actual cost of an append() operation:

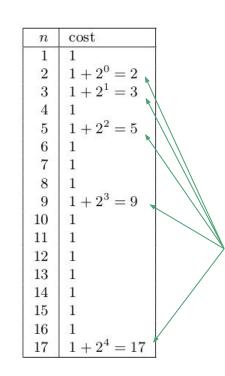
$$c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$$

Assumptions:

- Initial capacity: 1
- Writing cost: $\Theta(1)$

ex. 4 elements in.





Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Doubling

Actual cost of an append() operation:

$$c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$$

Assumptions:

- Initial capacity: 1
- Writing cost: $\Theta(1)$

ex. 4 elements in. Append now: cost 1 + 4 allocations



	n	cost
	1	1
	2	$1+2^0=2$
	3	$1+2^1=3$
	4	1
	5	$1+2^2=5$
	6	1
	6 7	1
	8	1 \\\
	9	$1+2^3=9$
	10	1
	11	1
	12	1
5	13	1
	14	1 /
	15	1 /
	16	1
	17	$1+2^4=17$

Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Doubling

Actual cost of n operations append():

$$T(n) = \sum_{i=1}^{n} c_i$$

$$= n + \sum_{j=0}^{\lfloor \log n \rfloor} 2^j$$

$$= n + 2^{\lfloor \log n \rfloor + 1} - 1$$

$$\leq n + 2^{\log n + 1} - 1$$

$$= n + 2n - 1 = O(n)$$

Amortized cost of a single append():

$$T(n)/n = \frac{O(n)}{n} = O(1)$$

Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Dynamic Vectors: Amortized cost (increment)

Actual cost of an append() operation:

$$c_i = \begin{cases} i & (i \bmod d) = 1\\ 1 & \text{altrimenti} \end{cases}$$

Assumptions

- Increment: d
- Initial size: d
- Writing cost: $\Theta(1)$

Example

• d = 4

n	cost	
1	1	
2	1	
$\frac{2}{3}$	1	
4	1	
5	1 + d = 5	
	1	
7	1	
6 7 8 9	1	
9	1 + 2d = 9	
10	1	
11	1	
12	1	
13	1 + 3d = 13	
14	1	
15	1	
16	1	
17	1 + 4d = 17	Y

Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Increment

Dynamic Vectors: Amortized cost (increment)

Actual cost of n operations append():

$$T(n) = \sum_{i=1}^{n} c_i$$

$$= n + \sum_{j=1}^{\lfloor n/d \rfloor} d \cdot j$$

$$= n + d \sum_{j=1}^{\lfloor n/d \rfloor} j$$

$$= n + d \frac{(\lfloor n/d \rfloor + 1) \lfloor n/d \rfloor}{2}$$

$$\leq n + \frac{(n/d + 1)n}{2} = O(n^2)$$

Amortized cost of a single append():

$$T(n)/n = \frac{O(n^2)}{n} = O(n)$$

Amortized analysis tells how the average of the performance of a set of operations on a large data set scales.

We consider a block of operations.

Dynamic vectors: growth factor

Language	Data structure	Expansion factor
GNU C++	std::vector	2.0
Microsoft VC++ 2003	vector	1.5
Python	list	1.125
Oracle Java	ArrayList	2.0
OpenSDK Java	ArrayList	1.5

Performance of Python's data structures

The choice of the data structure has implications on the performances

It is important to know the properties of built-in structures to use them properly!



Performance of Python's lists

Operator		Worst case	Worst case
	1227		amortized
L.copy()	Copy	O(n)	O(n)
L.append(x)	Append	O(n)	O(1)
L.insert(i,x)	Insert	O(n)	O(n)
L.remove(x)	Remove	O(n)	O(n)
L[i]	Index	O(1)	O(1)
for x in L	Iterator	O(n)	O(n)
L[i:i+k]	Slicing	O(k)	O(k)
L.extend(s)	Extend	O(k)	O(n+k)
x in L	Contains	O(n)	O(n)
min(L), max(L)	Min, Max	O(n)	O(n)
len(L)	Get length	O(1)	O(1)

Reality check

```
import time
from collections import deque
N = 750
L = []
start = time.time()
for i in range(N):
    for j in range(N):
        L.insert(0, i)
end = time.time()
print("[list: insert] {:.2f}s elapsed".format(end-start))
L=[]
start = time.time()
for i in range(N):
    for j in range(N):
        L.append(i)
                              O(1)
end = time.time()
print("[list: append] {:.2f}s elapsed".format(end-start))
start = time.time()
for i in range(len(L)):
                              O(n)
    L.pop(0)
end = time.time()
print("[list: remove] {:.2f}s elapsed".format(end-start))
 [list: insert] 88.90s elapsed
 [list: append] 0.04s elapsed
 [list: remove] 30.33s elapsed
```

Operator		Worst case	Worst case amortized
L.copy()	Copy	O(n)	O(n)
L.append(x)	Append	O(n)	O(1)
L.insert(i,x)	Insert	O(n)	O(n)
L.remove(x)	Remove	O(n)	O(n)
L[i]	Index	O(1)	O(1)
for x in L	Iterator	O(n)	O(n)
L[i:i+k]	Slicing	O(k)	O(k)
L.extend(s)	Extend	O(k)	O(n+k)
x in L	Contains	O(n)	O(n)
min(L), max(L)	Min, Max	O(n)	O(n)
len(L)	Get length	O(1)	O(1)

```
D = deque()
start = time.time()
for i in range(N):
    for j in range(N):
        D.insert(0, i)
end = time.time()
print("[deque: insert] {:.2f}s elapsed".format(end-start))
D = deque()
start = time.time()
for i in range(N):
    for j in range(N):
                                O(1)
        D.append(i)
end = time.time()
print("[deque: append] {:.2f}s elapsed".format(end-start))
start = time.time()
for i in range(len(D)):
    D.popleft()
end = time.time()
print("[deque: remove] {:.2f}s elapsed".format(end-start))
[deque: insert] 0.06s elapsed
[deque: append] 0.04s elapsed
[deque: remove] 0.04s elapsed
```

collections.deque

https://docs.python.org/3.7/library/collections.html#collections.degue