# Scientific Programming: Part B

Data structures 1

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### 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 0.30000000000000004

#### 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	$\mathbf{C}++$	Python
Sequences	List, Queue, Deque LinkedList, ArrayList, Stack, ArrayDeque	list, forward_list vector stack queue, deque	list tuple deque
Sets	<mark>Set</mark> TreeSet, HashSet, LinkedHashSet	set unordered_set	set, frozenset
Dictionaries	<mark>Map</mark> HashTree, HashMap, LinkedHashMap	map unordered_map	dict
Trees	<b>H</b>	-	
Graphs	_	-	-

### 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
  - $\bullet\,$  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

# How the data is organized

What we can do with the data

# Sequence: specification (prototype)

#### 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 pPos next(Pos p)

% Returns the position of the predecessor of p Pos $\mathsf{prev}(\mathsf{Pos}\ p)$ 

# Sequence: specification (prototype)

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 pOBJECT read(POS p)

% Writes the element v of type OBJECT in position pwrite(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 pOBJECT read(POS p)

% Writes the element v of type OBJECT in position pwrite(Pos p, OBJECT v)

> "specifications" method prototype 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:</pre> 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):</pre>

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 MySet: 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  $\operatorname{add}(\operatorname{OBJECT} x)$ 

% 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)

### 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 kinsert(OBJECT k, OBJECT v)

% Removes the association of key kremove(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

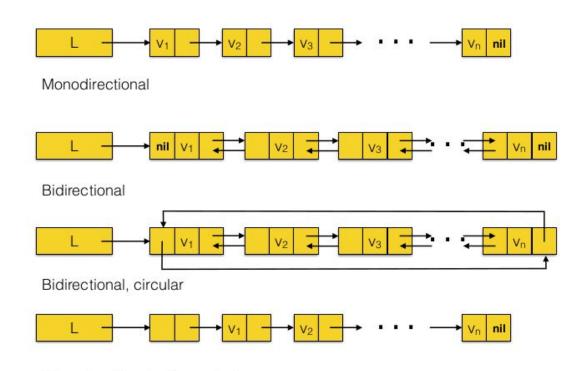
Note

- Contiguity in the list  $\not\Rightarrow$  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

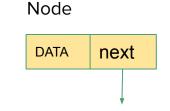
% adds a node **n** to the Monodirectional list placing it as the **head** add (node n)

%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

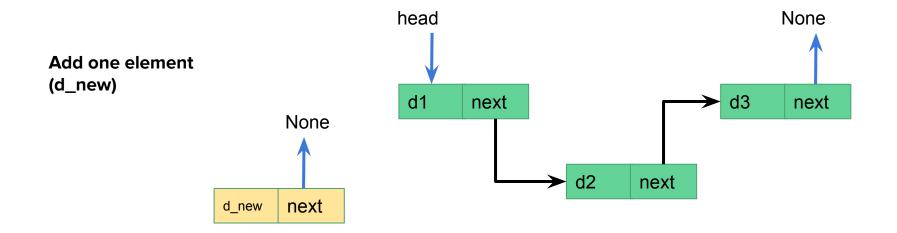
```
___str__()
```



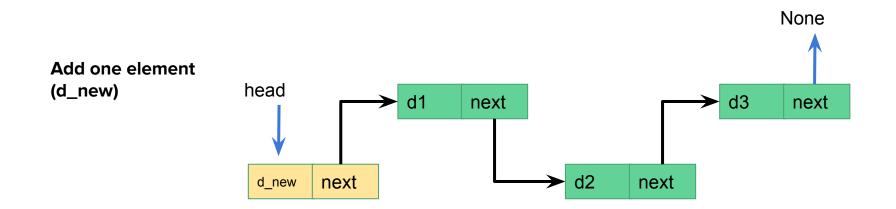
A list is a sequence of nodes, the first of which is the **head.** 

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

# Example: monodirectional list in python

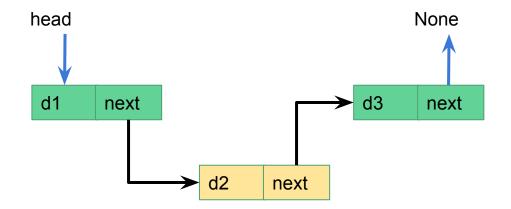


### Monodirectional list in python: add



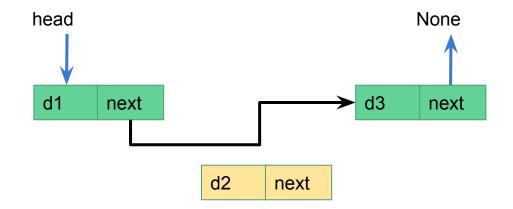
### Monodirectional list in python: remove

Remove one element (d2)



### Monodirectional list in python: remove

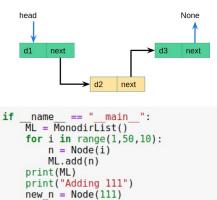
Remove one element (d2)



#### 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
```

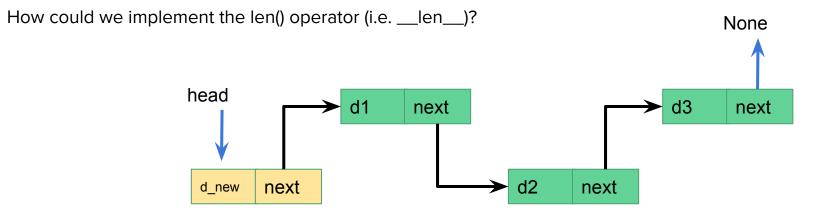
class MonodirList: def init (self): self. head = None #None is the sentinel! def add(self.node): if type(node) != Node: raise TypeError("node is not of type Node") else: node.set next(self. head) self. head = node def search(self, item): current = self. head found = False while current != None and not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



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("Removing 1") ML.remove(1) print("Removing 111") print("Removing 31") ML.remove(31) print(ML)

41 -> 31 -> 21 -> 11 -> 1 Adding 11 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: len?

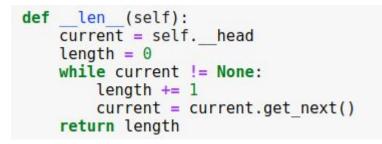


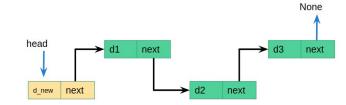
Go from first to last element and sum

# Monodirectional list in python: \_\_len\_\_()?

How could we implement the len() operator (i.e. \_\_len\_\_)?

The code:





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

## Monodirectional list in python: \_\_len\_\_()?

Faster <u>len</u>(). Idea: store and update the number of elements present

The code:

```
class MonodirList:
    def __init__(self):
        self. _ head = None #None is the sentinel!
        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

Complexity is O(1).

```
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
```

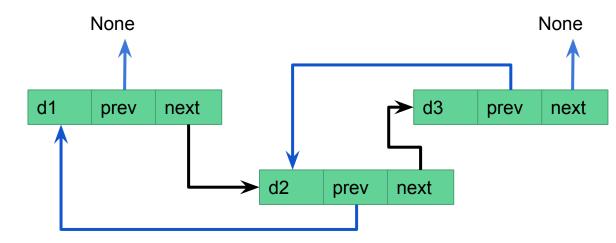
**Exercise:** How about O(1) min/max values? Hint: change again \_\_init\_\_, add, and remove.

# **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

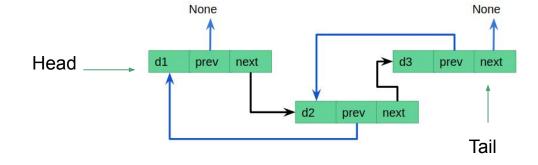


next pointer of the last element is None

### **Bidirectional linked list**

Each node now has:

- the data
- a prev pointer
- a next pointer



# **prev pointer** of the **first** element in the list is **None**

next pointer of the last element is None

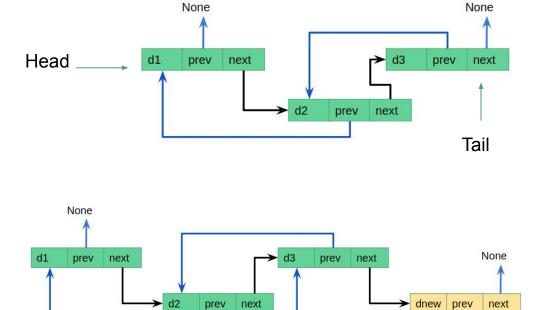
The list can have a **head** and **tail** pointer

# 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



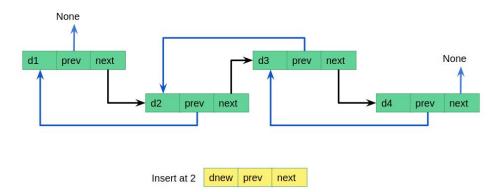
# Bidirectional linked list: insert at/remove

Each node now has:

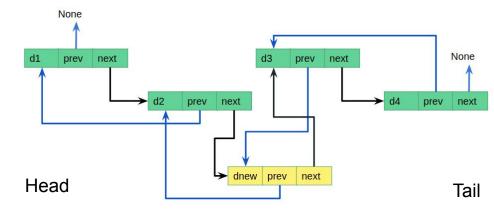
- the data
- a prev pointer
- a next pointer



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







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:

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#### X Y Z W

#### Solution:

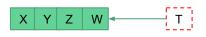
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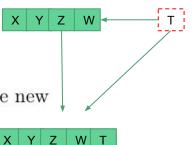
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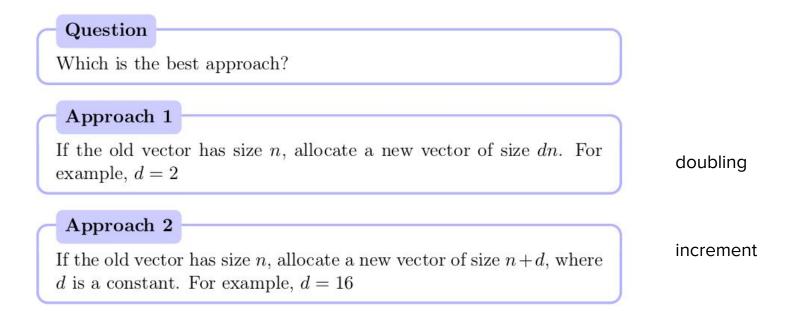
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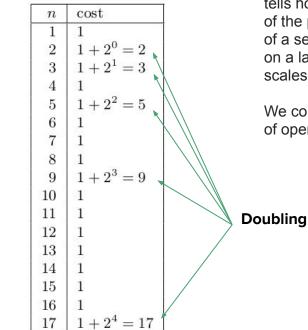


Actual cost of an append() operation:  $c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$ 

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.

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.

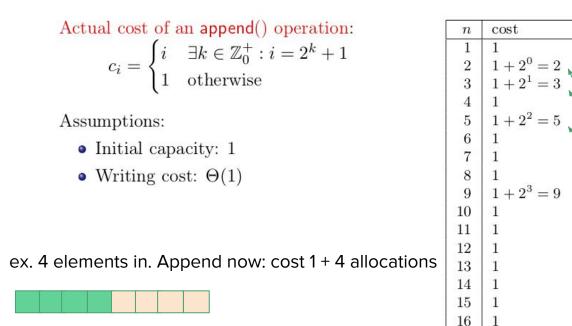


n	cost	1	tells ho
1	1	1	of the p
2	$1+2^0=2$		of a set on a la
3	$ \begin{array}{c} 1 + 2^0 = 2 \\ 1 + 2^1 = 3 \end{array} $		scales.
4	1	$\Lambda$	scales.
5	$1+2^2=5$	$\mathbb{N}$	We cor
6	1	$\langle \rangle \rangle$	of oper
6 7 8	1	$\langle \rangle \rangle$	or oper
8	1		
9	$1+2^3=9$		
10	1		
11	1		Doubling
12	1	7	
13	1		
14	1		
15	1		
16	1		
17	$1+2^4=17$	ſ	

#### Amortized analysis

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

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#### Amortized analysis

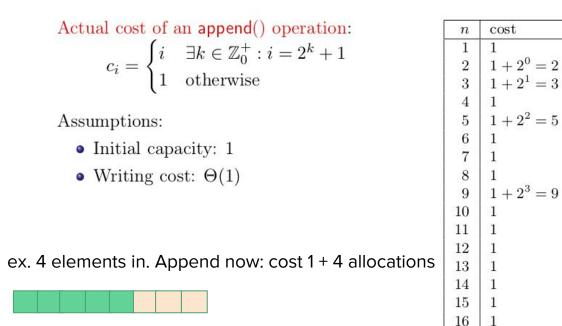
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Doubling

 $1+2^4=17$ 

17



#### Amortized analysis

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We consider a block of operations.

Doubling

 $1+2^4=17$ 

17

Actual cost of *n* operations append():

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

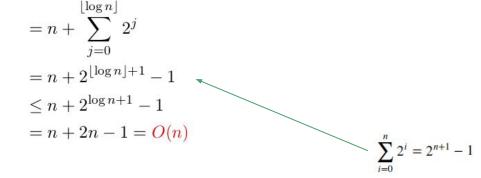
Amortized cost of a single append():

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

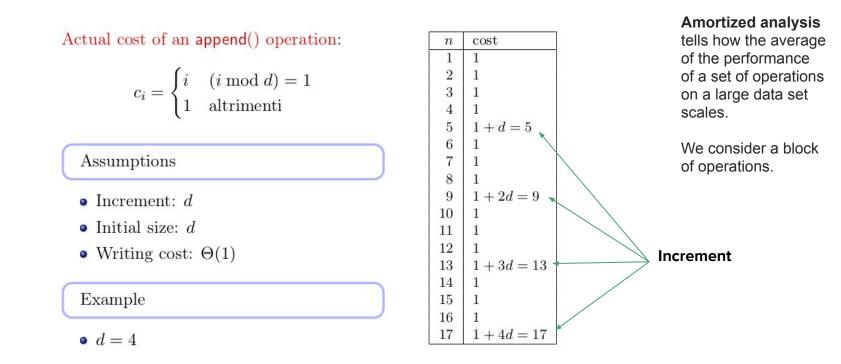
#### Amortized analysis

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We consider a block of operations.



### Dynamic Vectors: Amortized cost (increment)



### Dynamic Vectors: Amortized cost (increment)

Amortized cost of a single

Actual cost of n operations append():

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

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

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

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

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

$$\sum_{i=1}^{n} i = \frac{n \cdot (n+1)}{2}$$

#### 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++	<pre>std::vector</pre>	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

lists are dynamic vectors!

Operator		Worst case	Worst case
	1222		$\operatorname{amortized}$
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)
<pre>min(L), max(L)</pre>	Min, Max	O(n)	O(n)
len(L)	Get length	O(1)	O(1)

# Reality check

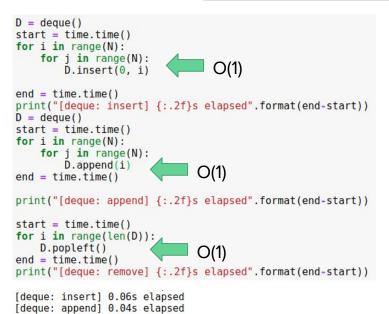
#### import time

from collections import deque

```
N = 750
L = [1]
start = time.time()
for i in range(N):
    for j in range(N):
        L.insert(0, i)
                                O(n)
end = time.time()
print("[list: insert] {:.2f}s elapsed".format(end-start))
L = [1]
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)



#### [deque: remove] 0.04s elapsed

#### collections.deque

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