# 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	<del>.</del>
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

How the data is organized

#### 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

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 p
Pos next(Pos p)
\% Returns the position of the predecessor of p
Pos prev(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 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

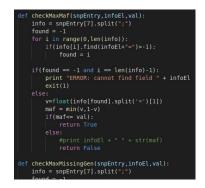
#### Pos insert(Pos p, object v)

- % 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" 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:
           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

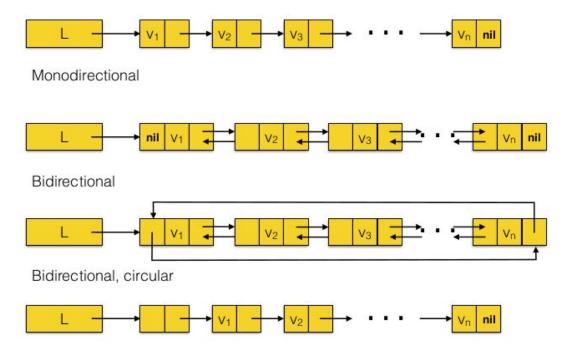
### Note

- 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)
```

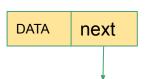
%removes a node n if it is found, does nothing otherwise

```
remove (node n)
```

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

```
__str__()
```

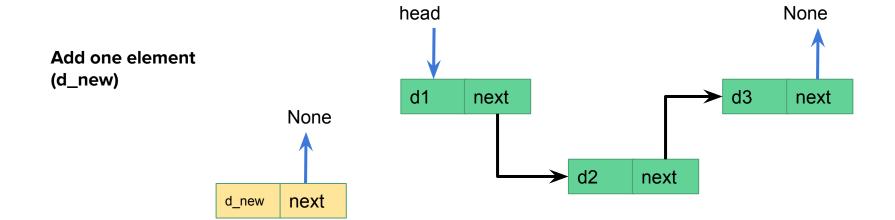




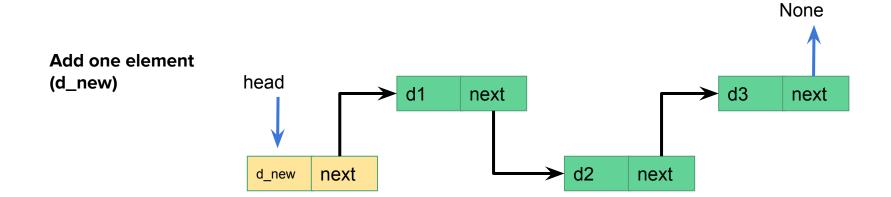
A list is a sequence of nodes, the first of which is the **head.** 

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

### Example: monodirectional list in python

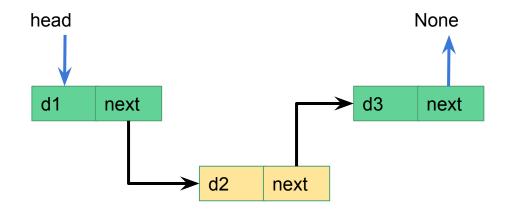


### Monodirectional list in python: add



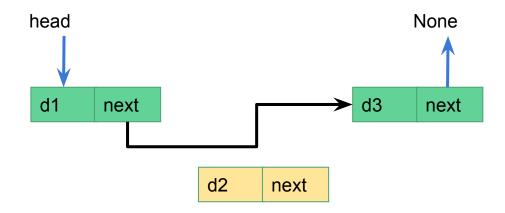
### Monodirectional list in python: remove

Remove one element (d2)



### Monodirectional list in python: remove

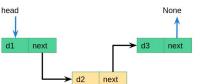
Remove one element (d2)



### 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
```

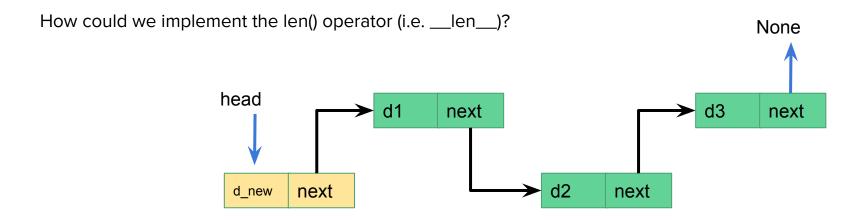
```
class MonodirList:
    def init (self):
        self. head = None #None is the sentinel!
   def add(self.node):
        if type(node) != Node:
            raise TypeError("node is not of type Node")
        else:
           node.set next(self. head)
            self. head = node
   def search(self, 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.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 ""
```



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

### Monodirectional list in python: len?



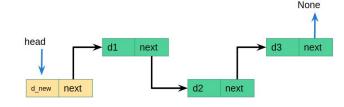
Go from first to last element and sum

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

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

The code:

```
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.

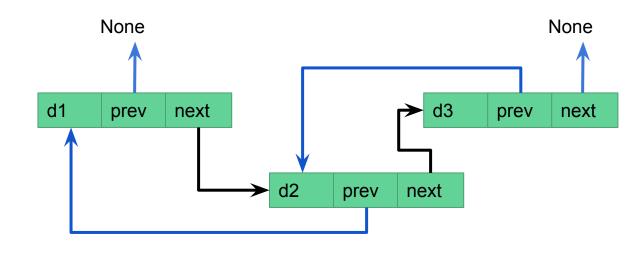
### Bidirectional linked list

#### 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

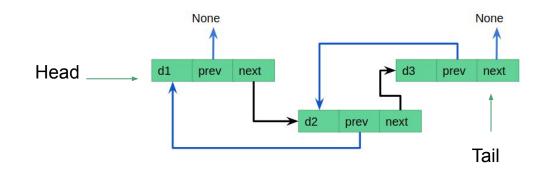
#### Each node now has:

- the data
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prev pointer of the first
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None

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

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

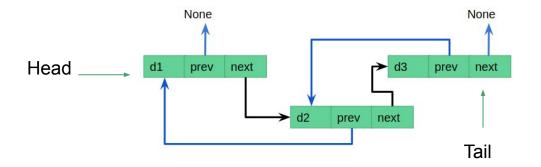


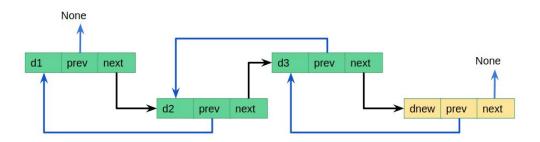
### Bidirectional linked list: append

#### Each node now has:

- the data
- a prev pointer
- a next pointer

**Append:** add a node as next of the current tail





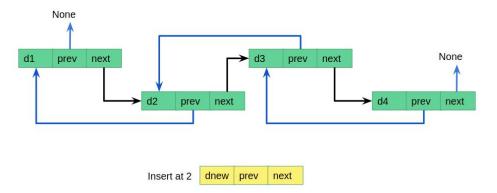
### Bidirectional linked list: insert at/remove

#### Each node now has:

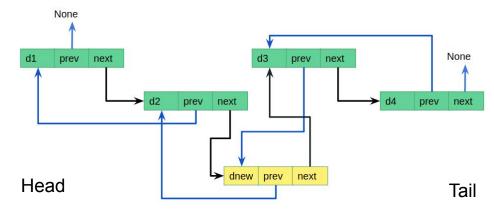
- the data
- a prev pointer
- a next pointer

#### 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:

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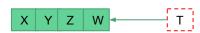
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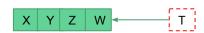
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### Lists in Python implemented through dynamic vectors

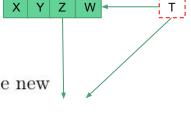
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- When inserting an element at the end (append), the cost is O(1) (just writing the element at first available slot)

#### 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:

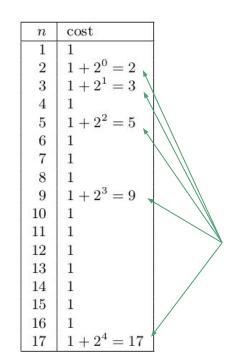
$$c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$$

#### 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.

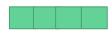
### Actual cost of an append() operation:

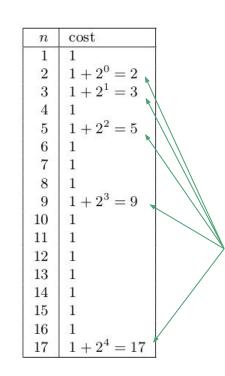
$$c_i = \begin{cases} i & \exists k \in \mathbb{Z}_0^+ : i = 2^k + 1 \\ 1 & \text{otherwise} \end{cases}$$

#### 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.

### 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
İ	1	1
j	2	$1+2^0=2$
1	3	$1+2^1=3$
	4	1
İ	5	$1+2^2=5$
	6	1
	6 7	1
	8	1 \\\
1	9	$1+2^3=9$
	10	1
	11	1
	12	1
1	13	1 /
	14	1 /
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.

### 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.

#### 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	
3	1	
4	1	
5	1 + d = 5	
6	1	
7	1	
7 8 9	1	
9	1 + 2d = 9	
10	1	
11	1	
12	1	Ì
13	1 + 3d = 13	
14	1	
15	1	
16	1	
17	1 + 4d = 17	<b>K</b>

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

lists are dynamic vectors!

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)

### 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):
                                 O(1)
        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):
        D.append(i)
                              O(1)
end = time.time()
print("[deque: append] {:.2f}s elapsed".format(end-start))
start = time.time()
for i in range(len(D)):
    D.popleft()
                              O(1)
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