Scientific Programming: Part B

Data structures 1

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[credits: thanks to Prof. Alberto Montresor]

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 (i.e. not in external modules)
Examples:

int : +,-,*, / , ...
boolean: and or, not, ...
strings: [], len(), +, ...

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 (for specific purposes static data structures might be more efficient)

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	-	-	-
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

How the data is organized

Operators

- It is possible to add / remove elements, by specifying their position
  - $s = s_1, s_2, \ldots, s_n$
  - 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)


```python
def checkMaxMaf(snpEntry,infoEl,val):
    info = snpEntry[7].split(";")
    found = -1
    for i in range(0,len(info)):
        if(info[i].find(infoEl+"=")>-1):
            found = i

    if(found == -1 and i == len(info)-1):
        print "ERROR: cannot find field " + infoEl
        exit(1)
    else:
        v=float(info[found].split('=')[1])
        maf = min(v,1-v)
        if(maf<= val):
            return True
        else:
            #print infoEl + " " + str(maf)
            return False

def checkMaxMissingGen(snpEntry,infoEl,val):
    info = snpEntry[7].split(";")
    found = -1
```

"specifications"
method prototype
ADT

"implementation"

Python code

Sequence: implementation (sketch)

```python
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
```

```python
    #insert inserts the element obj in position pos
    #or at the end
    def insert(self, pos, obj):
        if pos <len(self.__data):
            self.__data.insert(pos, obj)
            return pos
        else:
            #Not necessary! Already done by list's insert!!!
            self.__data.append(obj)
            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)

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

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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)

We will get back to this in the next lecture…

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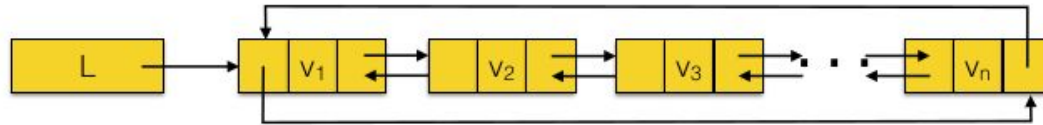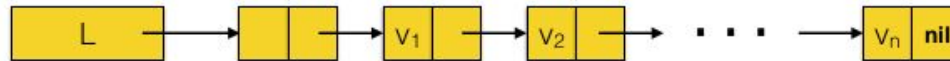- With sentinel / Without sentinel
- Circular / Non-circular

Linked lists (types)
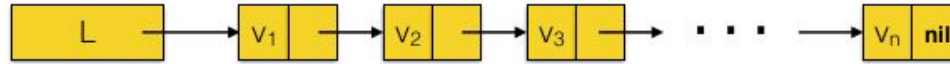
Monodirectional
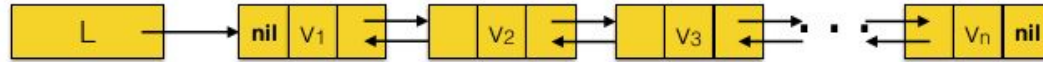
Bidirectional

Bidirectional, circular

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)`

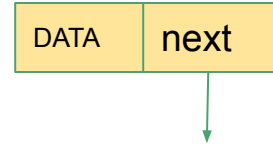%searches for a node n and returns True if it is found, false otherwise
`boolean search(node n)`

%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__()`

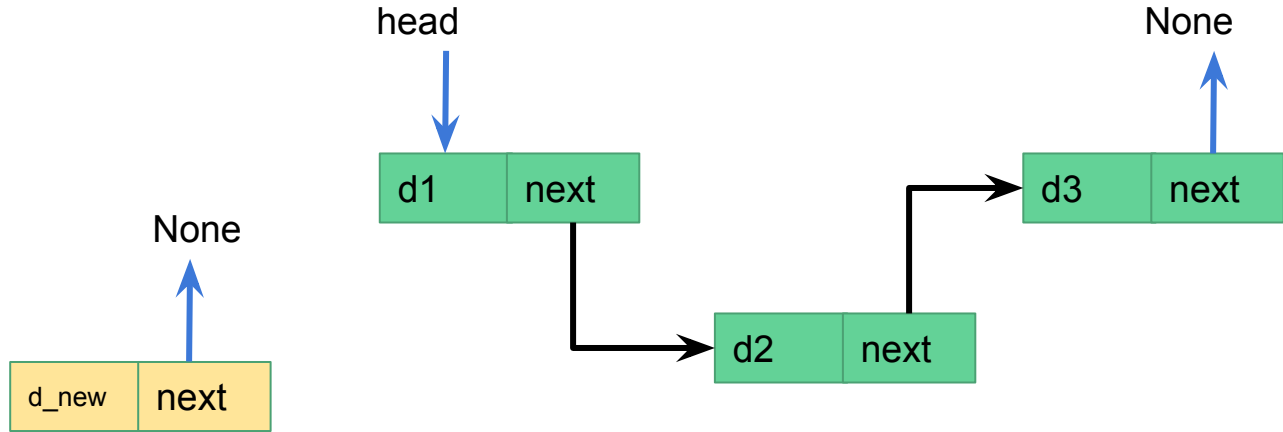---

Node

DATA	next

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
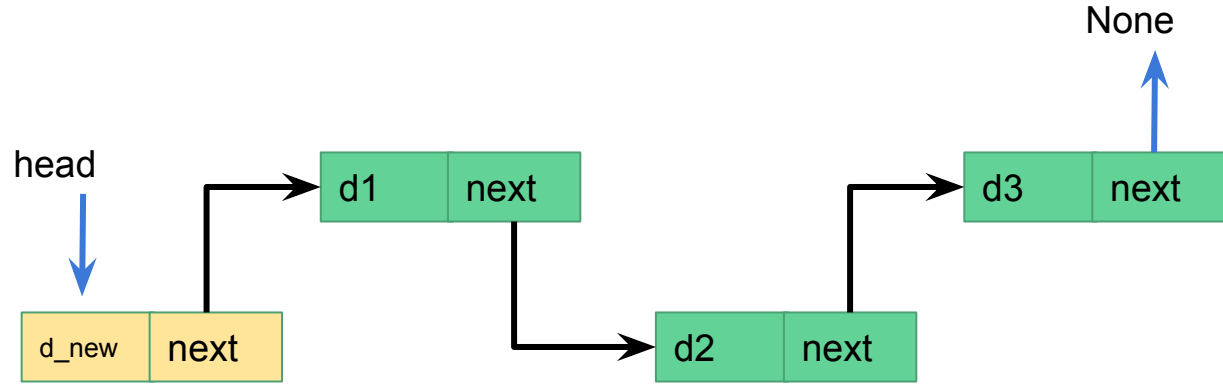
Example: monodirectional list in python
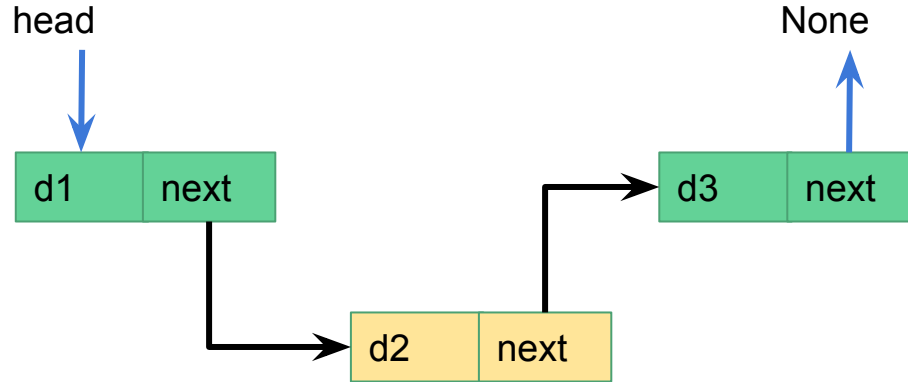
**Add one element
(d_new)**

Monodirectional list in python: add
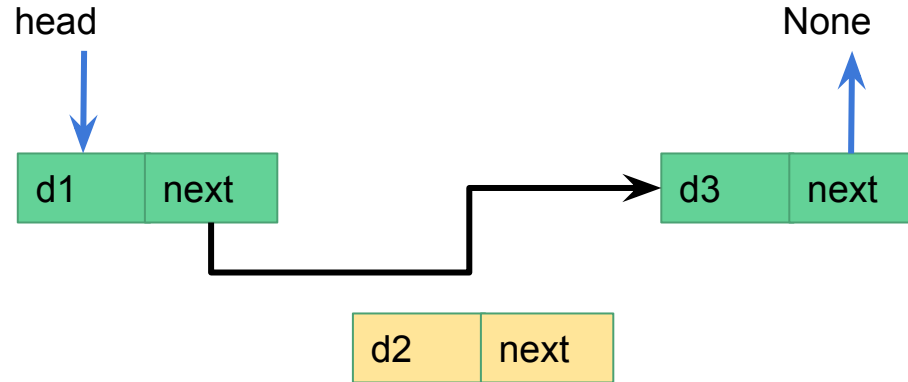
Add one element (d_new)

Monodirectional list in python: remove

Remove one element (d2)

Monodirectional list in python: remove

Remove one element (d2)

The code

```python
""" 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
```

```python
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 ""
```
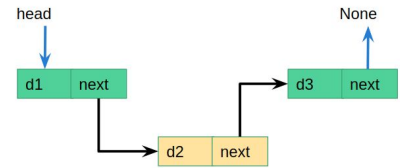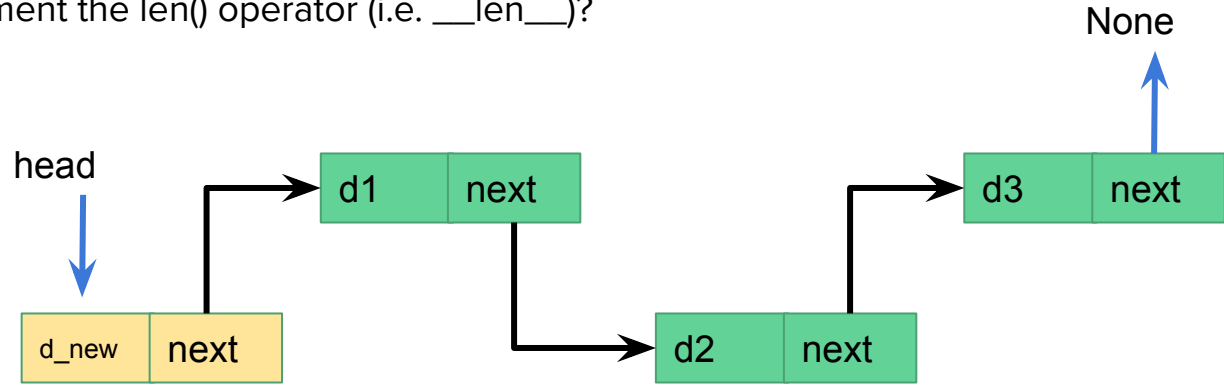


```python
if __name__ == "__main__":
    ML = MonodirList()
    for i in range(1,50,10):
        n = Node(i)
        ML.add(n)
    print(ML)
    print("Adding 111")
    new_n = Node(111)
    ML.add(new_n)
    print("Adding 27")
    new_n2 = Node(27)
    ML.add(new_n2)
    print(ML)
    print("Removing 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 111
Removing 31
27 -> 41 -> 21 -> 11
```

Monodirectional list in python: len?

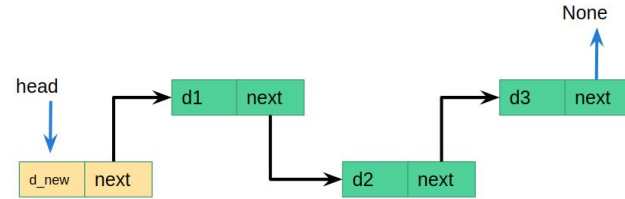How could we implement the len() operator (i.e. __len__)?

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:

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


Complexity is **Θ(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:

```python
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
```

```python
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**

None

None

| d1 | prev | next |

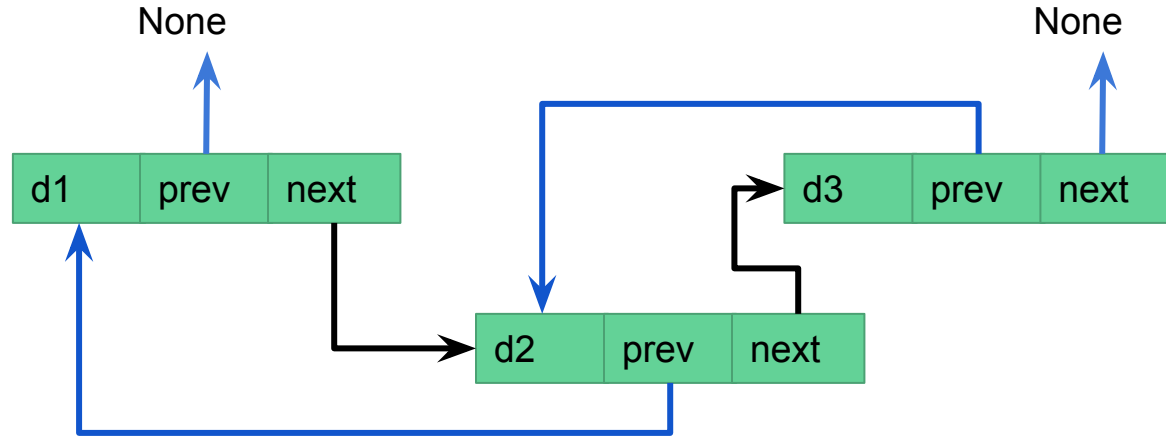| d2 | prev | next |

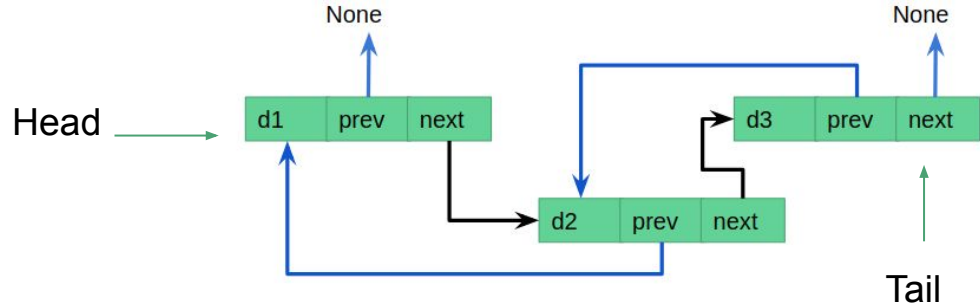| d3 | prev | next |

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**

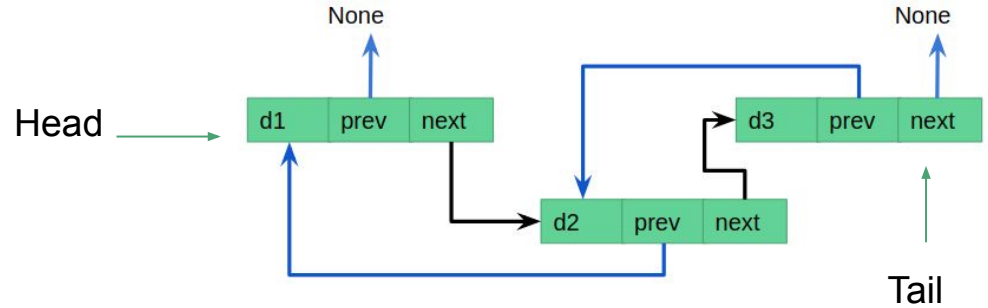**next pointer** of the **last** element is **None**

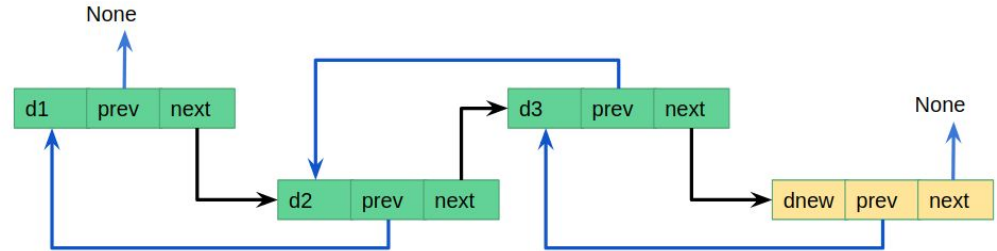The list can have a **head** and **tail** pointer

Bidirectional linked list: append

Each node now has:
- the data
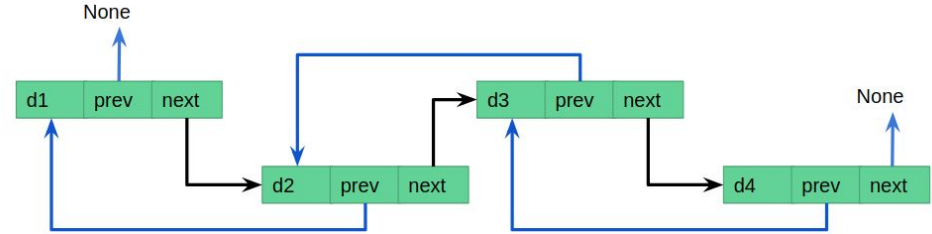- a prev pointer
- a next pointer

Append: add a node as next of the current tail

Bidirectional linked list: insert at/remove

Each node now has:
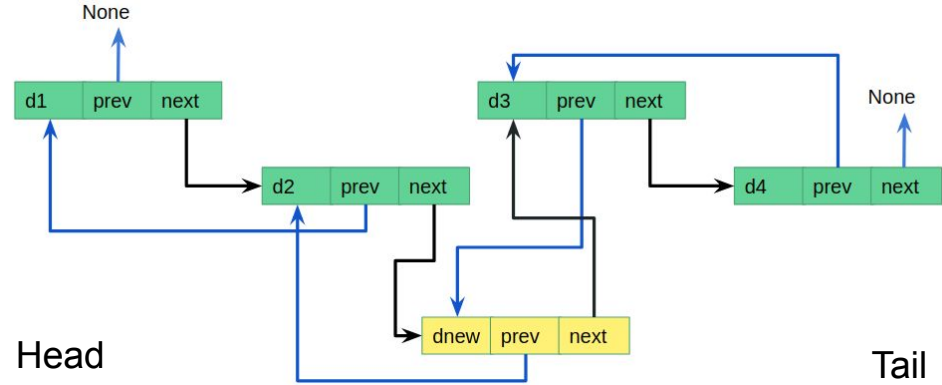- the data
- a prev pointer
- a next pointer

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())

Head

Tail

Dynamic Vectors

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)

L.insert(p, x)

L.append(x)

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

Dynamic Vectors

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X	Y	Z	W

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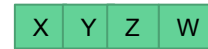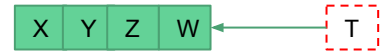
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| X | Y | Z | W | ← | T |

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Dynamic Vectors

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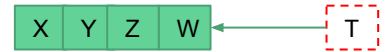
| X | Y | Z | W |

| T |

| X | Y | Z | W | T |

Dynamic Vectors

Question

Which is the best approach?

Approach 1

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

doubling

Approach 2

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

increment

Dynamic Vectors: Amortized cost (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. 3 elements in. Append now: 1 operation

n	cost
1	1
2	$1 + 2^0 = 2$
3	$1 + 2^1 = 3$
4	1
5	$1 + 2^2 = 5$
6	1
7	1
8	1
9	$1 + 2^3 = 9$
10	1
11	1
12	1
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 (we have to pay the cost of copying already inserted elements)

Note: starting with an initial capacity bigger than 1 is a good idea!

Dynamic Vectors: Amortized cost (doubling)

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

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

ex. 4 elements in.

n	cost
1	1
2	$1 + 2^0 = 2$
3	$1 + 2^1 = 3$
4	1
5	$1 + 2^2 = 5$
6	1
7	1
8	1
9	$1 + 2^3 = 9$
10	1
11	1
12	1
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 (we have to pay the cost of copying already inserted elements)

Dynamic Vectors: Amortized cost (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
7	1
8	1
9	$1 + 2^3 = 9$
10	1
11	1
12	1
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 (we have to pay the cost of copying already inserted elements)

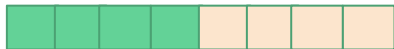# Dynamic Vectors: Amortized cost (doubling)

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. For next 4 elements the cost of insertion is 1

n	cost
1	1
2	$1 + 2^0 = 2$
3	$1 + 2^1 = 3$
4	1
5	$1 + 2^2 = 5$
6	1
7	1
8	1
9	$1 + 2^3 = 9$
10	1
11	1
12	1
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.

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Doubling (we have to pay the cost of copying already inserted elements)

Dynamic Vectors: Amortized cost (doubling)

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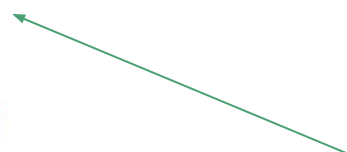
Actual cost of n operations append():

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

$$= n + \sum_{j=0}^{\lfloor \log n \rfloor} 2^j \qquad = n + 1 + 2 + 4 + \dots + n$$

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

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

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

Amortized cost of a single append():

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

$$\sum_{i=0}^{n} 2^i = 2^{n+1} - 1$$

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
8	1
9	$1 + 2d = 9$
10	1
11	1
12	1
13	$1 + 3d = 13$
14	1
15	1
16	1
17	$1 + 4d = 17$

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 (have to pay the cost of copying already inserted values)

Dynamic Vectors: Amortized cost (increment)

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

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():

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

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

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++	`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	$O(1)$	$O(1)$

https://wiki.python.org/moin/TimeComplexity

Notes

[1] These operations rely on the "Amortized" part of "Amortized Worst Case". Individual actions may take surprisingly long, depending on the history of the container.

Reality check

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	$O(1)$	$O(1)$

```python
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)          # O(n)

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)):
    L.pop(0)                    # O(n)
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
```

```python
D = deque()
start = time.time()
for i in range(N):
    for j in range(N):
        D.insert(0, i)          # O(1)

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.deque