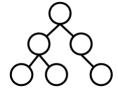
Lecture 2 Basic Data Structures

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DSCI 512

Algorithms & Data Structures

Learning Objectives

- Explain what a data structure is and why it is useful in computing at a high level.
- List Python's built-in data structures and describe their properties (review from 511).
- Explain basic (user-defined) data structures: stacks, queues, linked lists, hash tables, and trees.
- Implement basic data structures in Python.
- Explain the pros and cons of hash tables, and how they work at a high level.

- Explain what recursion is, and why both the base case(s) and recursive step(s) are essential.
- Compare and contrast a binary search tree to a hash table.

```
import numpy as np
import pandas as pd
from collections import defaultdict
import matplotlib.pyplot as plt
import altair as alt
import sklearn.neighbors
```

Introduction to Data Structures:

- A data structure is a way to organize and manage data.
- Data structures help with writing more efficient (both in terms of time and space) code.
- Main operation we consider for data structures:
 - inserting a new element
 - deleting an element
 - checking if an element is present (contain)

Python Built-in Data Structures:

Lists

- inserting a new element: list.append(), list.insert(), etc.
- deleting an element: [list.remove()], [list.pop()], etc.
- checking if an element is present: in

Tuples

- inserting a new element: immutable (but we can still "add" two tuples)
- o deleting an element: immutable
- checking if an element is present: in

Sets

- inserting a new element: set_add(), ^, , |, etc.
- o deleting an element: | set remove() | , | − |, etc.

checking if an element is present: in

Dictionaries

- inserting a new element: dict.update(), etc.
- deleting an element: dict.pop(), etc.
- checking if an element is present: in (for dict.keys(), dict.values())

In the previous lecture, we saw that checking if an element is present in a Python set is very efficient. Let's look into this more.

Hash Tables & Hash Functions

Python's set type supports the following operations in O(1) time:

- inserting a new element
- · deleting an element
- checking if an element is present

How could we implement this using the tools we already have?

- Well, what about using linear search to find elements, e.g. a list?
 - This is too slow
- What about using binary search?
 - Now searching is fast, but insertion/deletion is slow, because we need to maintain an ordered list
- Enter the hash table to save the day!
 - Trees could also work, but hash tables are the most popular.

Hash Functions

Python objects have a hash:

```
hash("mds")
-6961575440847664540
```

hash("")

0

It looks like the hash function returns an integer.

```
hash(5.5)
```

1152921504606846981

hash(5)

5

hash(-9999)

-9999

It looks like the hash function of a Python integer is itself. Or at least small enough integers.

hash(999999999999999999999999)

2003764205207330319

Sometimes it fails?

hash([1, 2, 3])

```
Traceback (most recent call last)
  TypeError
  Cell In[8], line 1
  ----> 1 hash([1, 2, 3])
  TypeError: unhashable type: 'list'
  hash((1, 2, 3))
  529344067295497451
  hash(None)
  -9223372036581166359
If a Python set is a hash table, that means items in it must be hashable (dict has the same
requirement, for keys):
  s = set()
  s.add(5.5)
  s.add("mds")
  S
  {5.5, 'mds'}
  s.add([1, 2, 3])
```

```
TypeError
Cell In[15], line 1
----> 1 s.add([1, 2, 3])

TypeError: unhashable type: 'list'
```

```
s.add((1, 2, 3))
```

```
S
```

```
{(1, 2, 3), 5.5, 'mds'}
```

Hash Function Overview

- Immutable objects (numbers, strings, tuples) are hashable, mutable objects (lists, dicts)
 are not
- Hash functions are deterministic
- Hash functions have a fixed-size output
- Hash function are **collision-resistant**
- Hash functions are extremely broadly useful, beyond what we talk about in this course

Hash Tables

- So, it looks like the hash function maps from an object to an integer.
- And that Python set s use these hash functions.
- How do they work?
- The hash table is basically a list of lists, and the hash function (mod the array size) maps an object to its location in the outer list.
 - But it's a bit more complicated than that.
 - The list typically expands and contracts automatically as needed.
 - \circ These operations may be slow, but averaged or "amortized" over many operations, the runtime is O(1)

- The hash function depends on this array size.
- There's also an issue of collisions: when two different objects hash to the same place.
- Roughly speaking, we can insert, retrieve, and delete things in O(1) time so long as we have a "good" hash function.
 - The hash function will be "good" for default Python objects, and if you end up needing to implement your own one day you should read a bit more about it.

A Simple Hash Table

Below is a (very low-quality) hash table implementation, with only 4 buckets by default:

```
class HashTable:
    def __init__(self, num_buckets=4):
        self.stuff = list() # A list of lists
        self.n = num_buckets

        for i in range(num_buckets):
            self.stuff.append([]) # Create the inner lists, one per bucket

    def add(self, item):
        if not self.contains(item):
            self.stuff[hash(item) % self.n].append(item)

    def contains(self, item):
        return item in self.stuff[hash(item) % self.n]

    def __str__(self):
        return str(self.stuff)
```

(Note: The hash function has a random seed that is set at the start of every Python session, so your actual results my vary from mine.)

```
ht = HashTable()
print(ht)
```

```
[[], [], [], []]
```

- So far, all 4 buckets are empty.
- Now let's add something:

```
Lecture 2 Basic Data Structures — DSCI 512: Algorithms and Data Structures
  ht.add("hello")
  print(ht)
  [[], [], [], ['hello']]
"hello" went into this bucket because
  hash("hello")
  590680449708388535
  hash("hello") % 4
  3
Now let's add more things:
  ht.add("goodbye")
  print(ht)
  [[], [], [], ['hello', 'goodbye']]
  ht.add("test")
  print(ht)
  [['test'], [], [], ['hello', 'goodbye']]
  ht.add("item")
  print(ht)
  [['test'], ['item'], [], ['hello', 'goodbye']]
```

```
ht.add("what")
print(ht)
```

```
[['test'], ['item'], ['what'], ['hello', 'goodbye']]
```

If we want to look for something:

```
ht.contains("blah")
```

False

False because

```
hash("blah") % 4
```

3

And "blah" is not found in bucket.

```
ht.contains("item")
```

True

- Same thing here.
- The key idea is that you **only need to look in one bucket** either it's in that bucket, or it's not in the *entire* hash table.

```
print(ht)
```

```
[['test'], ['item'], ['what'], ['hello', 'goodbye']]
```

• Above we have a *collision*: that is, 2 items in the same bucket.

Question: If my hash table has 4 buckets, what is the time complexity of contains?

```
A: O(1)
B: O(n)
C: O(log(n))
D: O(nlog(n))
```

Answer O(n) -> we narrow our search down to one of the 4 buckets, but we still need to search through all the elements in that bucket. Since the size of the bucket is $\frac{n}{4}$, our time complexity is O(n).

- If the main list is able to dynamically grow as the number of items grows, we can keep the number of collisions low.
- This preserves the O(1) operations.

Lookup Tables, Python dict

- Python's dict type is a dictionary (aka symbol table)
- A dictionary should support the following operations:
 - inserting a new element
 - deleting an element
 - finding an element
- It is much like a set except the entries, called "keys", now have some data payload associated with them, which we call "values".
- It is also implemented as a hash table, meaning you can expect O(1) operations.
- Only the keys are hashed, so only the keys have to be hashable.
 - A list can be a value, but not a key.

```
d = dict()
d[5] = "a"
d["b"] = 9
d
```

```
{5: 'a', 'b': 9}
```

```
5 in d
```

True

```
9 in d # it only searches the keys
```

False

```
d[5]
```

'a'

d[6]

```
KeyError
Cell In[35], line 1
----> 1 d[6]

KeyError: 6
```

Hashable types:

```
d[[1,2,3]] = 10
```

```
TypeError
Cell In[36], line 1
----> 1 d[[1,2,3]] = 10

TypeError: unhashable type: 'list'
```

```
d[10] = [1,2,3] \# 0K
```

A reminder of some dictionary syntax:

```
# Comprehensions for dictionaries
f = {i: i*2 for i in range(10)}
f
```

```
{0: 0, 1: 2, 2: 4, 3: 6, 4: 8, 5: 10, 6: 12, 7: 14, 8: 16, 9: 18}
```

```
# Iteration syntax
for key, val in f.items():
    print("key =", key, " val =", val)
```

```
key = 0  val = 0
key = 1  val = 2
key = 2  val = 4
key = 3  val = 6
key = 4  val = 8
key = 5  val = 10
key = 6  val = 12
key = 7  val = 14
key = 8  val = 16
key = 9  val = 18
```

```
# A dictionary can be a value inside another dictionary
g = dict()
g[5] = f
g
```

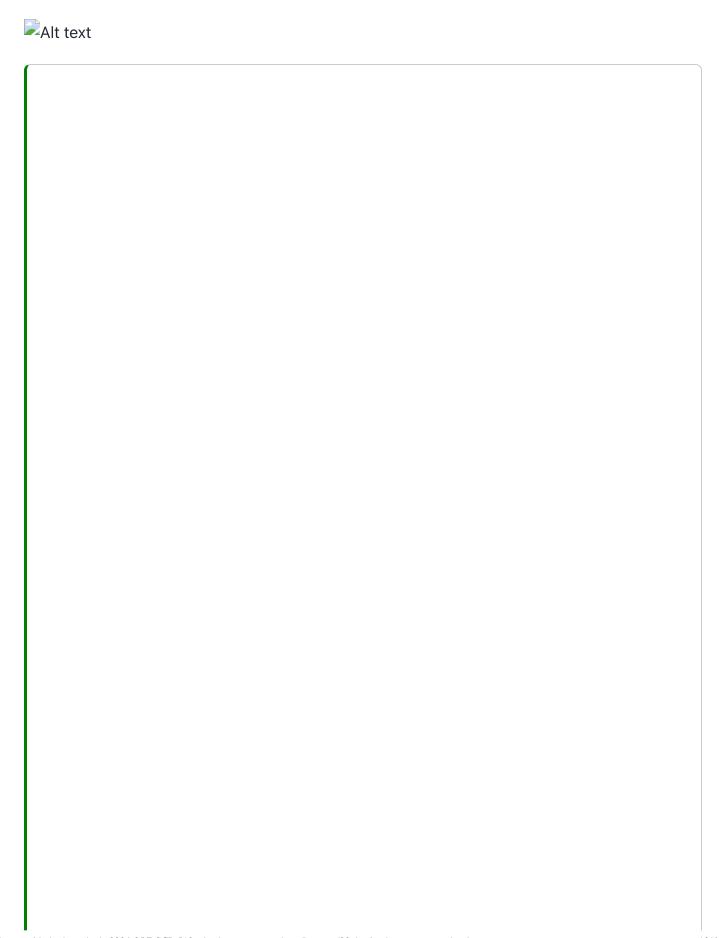
```
{5: {0: 0, 1: 2, 2: 4, 3: 6, 4: 8, 5: 10, 6: 12, 7: 14, 8: 16, 9: 18}}
```

More user-defined data structures

Stacks and queues

• We want a data structure that we can put things into, and then retrieve them later.

• A <u>stack</u> does with with the "last in, first out" (LIFO) mentality - like a stack of books or plates.



```
class Stack:
    """A stack data structure."""
    def __init__(self):
        self.data = list()
    def push(self, item):
        Adds a new item to the top of the stack.
        Parameters
        item : object
           An item added to the stack
        self.data.append(item)
    def pop(self):
        Removes the item that is at the top of the stack and returns the item.
        Returns
        object
             The item that was last added to the stack.
        Examples
        >>> stack = Stack()
        >>> stack.push(1)
        >>> stack.push([1, 2, "dog"])
        >>> stack.push("popcorn")
        >>> stack.pop()
        'popcorn'
        minn'
        return self.data.pop()
    def isEmpty(self):
        Checks to see if the stack is empty.
        Returns
        bool
             True if the stack contains no items, False otherwise.
        Example
        >>> stack = Stack()
        >>> stack.isEmpty()
        True
        return len(self.data) == 0
```

```
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    def __str__(self):
         return self.data.__str__()
s = Stack()
s.push("first")
s.push("second")
print(s)
['first', 'second']
s.pop()
'second'
print(s)
['first']
s.push("third")
s.push("fourth")
print(s)
['first', 'third', 'fourth']
s.pop()
'fourth'
```

s.pop()

```
'third'
s.pop()
'first'
s.pop()
```

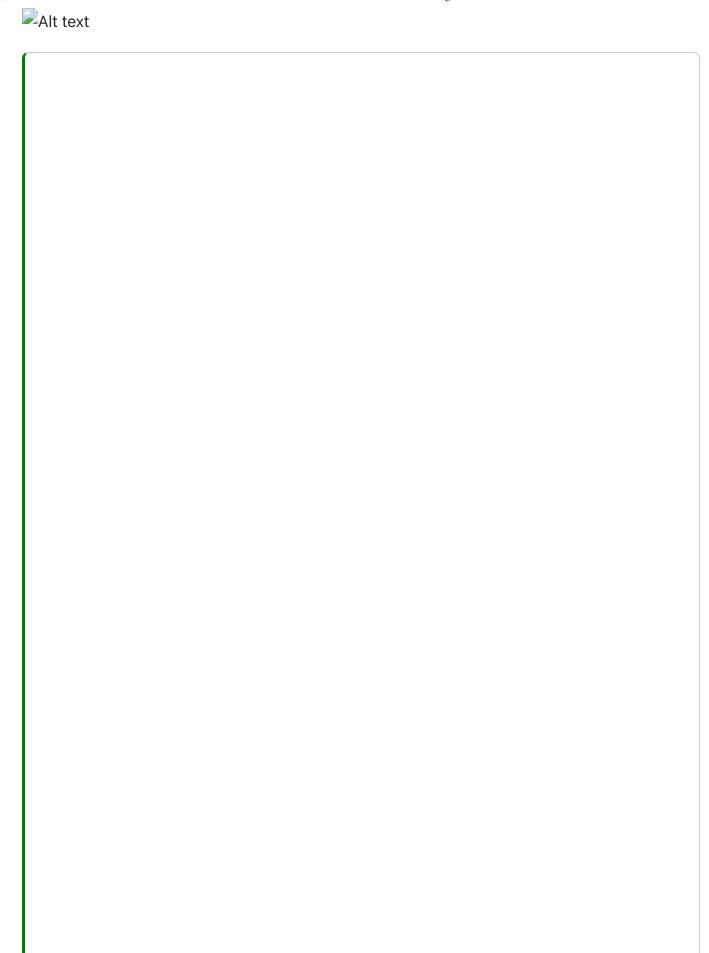
```
IndexError
                                           Traceback (most recent call last)
Cell In[50], line 1
----> 1 s.pop()
Cell In[41], line 36, in Stack.pop(self)
     18 def pop(self):
     19
     20
            Removes the item that is at the top of the stack and returns the i
     21
   (...)
     34
            'popcorn'
     35
---> 36
            return self.data.pop()
IndexError: pop from empty list
```

Question: If I have a stack containing n items, what is the time complexity to retrieve the "bottom" item?

```
A: O(1)
B: O(n)
C: O(\log(n))
D: O(n^2)
E: Not Sure
```

Answer O(n) -> We need to do popping n-1 items before reaching the bottom

- Along with stacks we also have queues, which use "first in, first out" (FIFO) ordering.
 - e.g. an actual queue/lineup



```
class Queue:
    """A Queue data structure."""
    def __init__(self):
        self.data = list()
    def push(self, item):
        Adds a new item to the end of the queue.
        Parameters
        item : object
           An item added to the queue
        self.data.append(item)
    def pop(self):
        Removes the item that is at the front of the queue and returns the ite
        Returns
        object
             The least recent item added to the queue.
        Example
        >>> queue = Queue()
        >>> queue.push(1)
        >>> queue.push([1, 2, "dog"])
        >>> queue.push("popcorn")
        >>> queue.pop()
        111
        .....
        return self.data.pop(0)
    def isEmpty(self):
        Checks to see if the queue is empty.
        Returns
        bool
            True if the stack contains no items, False otherwise.
        Example
        >>> queue = Queue()
        >>> queue.push(1)
        >>> Queue.isEmpty()
        False
        0.00
```

```
return len(self.data) == 0

def __str__(self):
    return self.data.__str__()
```

```
q = Queue()
q.push("first") # often called "enqueue"
q.push("second")
print(q)
```

```
['first', 'second']
```

```
q.pop() # often called "dequeue"
```

```
'first'
```

```
print(q)
```

```
['second']
```

```
q.push("third")
q.push("fourth")
```

```
print(q)
```

```
['second', 'third', 'fourth']
```

```
while not q.isEmpty():
    print(q.pop())
```

second third fourth

Question: If we have a queue [A, B, C, D] with A at the front/head of the queue, what will the queue look like after the following operations:

- push E onto the queue
- push [F] onto the queue
- remove one item from the queue
- push [A] onto the queue

Answer C -> Pushing E gives [A, B, C, D, E], pushing F gives [A, B, C, D, E, F], removing one item gives from the queue removes the first item so [B, C, D, E, F], and finally pushing A just adds it in the end which would give [B, C, D, E, F, A].

Recursive Data Structures

Recursion Introduction

Setting the Stage

- Writing software is largely about breaking down problems into smaller, more manageable pieces
 - Complex applications are broken down into packages or modules
 - Modules are broken down into functions and sub-functions

o etc.

- Some divisions of a problem are easier to work with than others
- Recursion is a tool for breaking down problems in a different way

Factorial: Iterative Definition

$$n! = n(n-1)(n-2)...(2)(1)$$

Useful for counting permutations and computing probabilities.

For example, if you have 5 books on a shelf, how many different ways can you organize them?

$$5! = 5 \times 4 \times 3 \times 2 \times 1 = 120$$

Let's look at an iterative implementation.

```
print("5! =", factorial(5))
```

```
5! = 120
```

How are we breaking down this problem?

- each step is a multiplication operation
- we keep track of the "working result" at each step

This is the iterative approach.

Execution Schematic

```
factorial(5):

Execution
------
Step 1: result=5
Step 2: result=result*4
Step 3: result=result*3
Step 4: result=result*2
Step 5: result=result*1
Step 6: return result
```

Factorial: Recursive Definition

Another way to break up the problem

We first defined factorial as follows:

Definition 1:

$$n!=n(n-1)(n-2)\dots(2)(1)$$

Another way to define the factorial is:

Definition 2:

$$n! = n(n-1)!$$

We can define the problem in terms of itself! This is the recursive approach.

 Rather than write out all the steps or the algorithm, we define the nth step in terms of the (n-1)th step • This is called the **inductive step** or **recursive step**

(We're calling a function from within itself here, which might seem weird at first. We will talk about what is going on in more detail here a little later on. For now, just think of it in terms of the mathematical definition 2.)

```
def factorial_recursive(n):
    """
    Computes the factorial of the input n (n!).

    Parameters
    -----
    n : int
        The value to compute factorial of. Must be a positive integer.

    Returns
    -----
    integer
        The value of n!
    """
    return n * factorial_recursive(n-1) # n(n-1)!
```

```
print("5! =", factorial_recursive(5))
```

```
RecursionError
                                            Traceback (most recent call last)
Cell In[61], line 1
----> 1 print("5! =", factorial_recursive(5))
Cell In[60], line 15, in factorial recursive(n)
      1 def factorial recursive(n):
            .....
      2
      3
            Computes the factorial of the input n (n!).
      4
   (\ldots)
     13
                The value of n!
     14
---> 15
            return n * factorial_recursive(n-1)
Cell In[60], line 15, in factorial_recursive(n)
      1 def factorial recursive(n):
      2
      3
            Computes the factorial of the input n (n!).
      4
   (\ldots)
     13
                The value of n!
     14
---> 15
            return n * factorial recursive(n-1)
    [... skipping similar frames: factorial recursive at line 15 (2970 times)]
Cell In[60], line 15, in factorial_recursive(n)
      1 def factorial recursive(n):
      2
      3
            Computes the factorial of the input n (n!).
      4
   (\ldots)
     13
                The value of n!
            .....
     14
  -> 15
            return n * factorial_recursive(n-1)
RecursionError: maximum recursion depth exceeded
```

Oops, we are missing something important!

We've found a problem in our recursion.

Aside: Stack overflow



(Image source: Wikipedia)

- A stack overflow error most commonly occurs when a recursive function makes an
 exceedingly large numbers of calls to itself (usually because of not properly setting up a
 base case), causing the memory allocated for a function's call stack to overflow.
- Python prevents this from happening by throwing a [RecursionError] when a certain number of recursive calls are made (this number is system-dependent)

Revise Recursive Definition to Include Base Case

Let's revise **Definition 2** to define when to stop:

$$n! = egin{cases} n(n-1)! \;, & n>1 \ 1 \;, & n=1 \end{cases}$$

Now we have the two essential parts to any recursive algorithm:

- Inductive Step ("how do we call the function from within itself")
- Base Case ("when do we stop")





(Image attribution to Jake Clark, edited from source)

Now, let's adjust the implementation to include the second part of **Definition 2**.

```
def factorial_recursive(n):
    """
    Computes the factorial of the input n (n!).

    Parameters
------
n: int
        The value to compute factorial of. Must be a positive integer.

    Returns
-----
integer
        The value of n!
"""
if n == 1:
        return 1
return n * factorial_recursive(n-1)
```

```
print("5! =", factorial_recursive(5))
# print("5! =", factorial_recursive(5000))
```

```
5! = 120
```

How are we breaking up this problem?

- each step is a factorial operation
- at the base case, we return a constant (end the recursion)
- Don't need to keep track of an intermediary result

What happens when we call a function

recursively?

Execution Schematic

Time & Space Complexity

Question: What is the time complexity of factorial?

```
def factorial(n):
    result = n
    while n > 1:
        result = result * (n-1)
        n = n-1
    return result
```

Answer: O(n)

Question: What is the time complexity of [factorial_recursive]?

```
def factorial_recursive(n):
    if n == 1:
        return 1
    return n * factorial_recursive(n-1)
```

A: O(1)

B: O(n)

C: O(log(n))

D: O(nlog(n)) \

Answer: O(n)

Question: What is the space complexity of factorial?

A: O(1)

B: O(n)

C: O(log(n))

 $\operatorname{D}:O(n^2)$

Answer: O(1)

Question: What about the space complexity of factorial_recursive?

```
def factorial_recursive(n):
    if n == 1:
        return 1
    return n * factorial_recursive(n-1)
```

A: O(1)

B: O(n)

C: O(log(n))

D: $O(n^2)$

Answer: O(n)

Why is this? Each time we make a recursive function call, we enter a new "stack frame" (or "level" in our execution schematic). Each stack frame takes up space in memory.

Linked lists

We have talked about nested data structures, like:

```
x = [[1, 2, 3], ["a", "b", "c"]]
x
```

```
[[1, 2, 3], ['a', 'b', 'c']]
```

- This is a list of lists.
- We can also have a doll within a doll:



(Image attribution to Fanghong, from Wikipedia article)

- Consider that you wanted to store items, one inside each doll.
- How would you add a new item? Describe it in words.
 - To the outside?
 - To the inside?

```
class TreasureBox:
    A linked list, aka treasure box. The user add and retrive items from it.
    def __init__(self, treasure):
        self.next = None # data type: TreasureBox
        self.treasure = treasure # data type: whatever
    def append_outer(self, treasure):
        """Add a new treasure box to the outside by putting lastest box inside
        Parameters
        _____
        treasure : object
           the label designated to the newly covered treasure box
        Returns
        new box : TreasureBox
             new treasure box object containing previous boxes inside
        Example
        >>> box = box.append outer(10)
        new box = TreasureBox(treasure)
        new box.next = self
        return new box
    def append inner(self, treasure):
        """Add a new treasure box inside the innermost current box.
        Parameters
        treasure : object
           the label designated to the newly inserted treasure box
        Returns
        new box : TreasureBox
             new treasure box object contained within innermost box of
             the last treasure box
        Example
        >>> box.append_inner(55)
        if self.next is None:
            self.next = TreasureBox(treasure)
        else:
            self.next.append_inner(treasure)
        return self
```

```
def get(self, depth):
    """Get the treasure by going depth levels deep into the treasure boxes
    Parameters
    depth : int
       the depth of which to unwrap the treasure box
    Returns
    object:
         the treasure retrieved after recursing the specified depth.
    Example
    >>> box = TreasureBox(12)
    >>> box = box.append_outer(9)
    >>> box = box.append_inner(55)
    >>> box.get(0)
    >>> box.get(2)
    if depth == 0:
        return self.treasure
    if self.next is None:
        return None # Index out of bounds
    return self.next.get(depth-1)
```

```
box = TreasureBox("$5")
box = box.append_outer("$100")
box = box.append_outer("$20")
```

```
box.get(0)
```

```
'$20'
```

```
box.get(1)
```

```
'$100'
```

```
box.get(2)
  '$5'
  box.get(3)
  box = TreasureBox("Initial box")
  box = box.append_inner("Box in initial box")
  box = box.append_inner("Box in the second box")
  box.get(0)
  'Initial box'
  box.get(1)
  'Box in initial box'
  box.get(2)
  'Box in the second box'
  box.get(3)
Activity: without running the code, what will this return?
```

```
box = TreasureBox("A")

box = box.append_inner("B")
box = box.append_outer("C")
box = box.append_outer("D")
box = box.append_inner("E")

box.get(3)
```

```
'B'
[D [C [A [B [E]] ]]]
```

- In computer science, this is called a linked list.
- It's not just a nested data structure (list of lists); the definition of the data type itself is recursive.
 - What is a list? It contains stuff (including possibly lists).
 - What is a treasure box? It contains one thing, and another treasure box.

Recursive algorithms vs. data structures

- We have a relationship between recursive function calls (see append_inner and get) and recursive data types (see <a href="mit_").
- Recursion is an important idea in understanding algorithms and data structures.

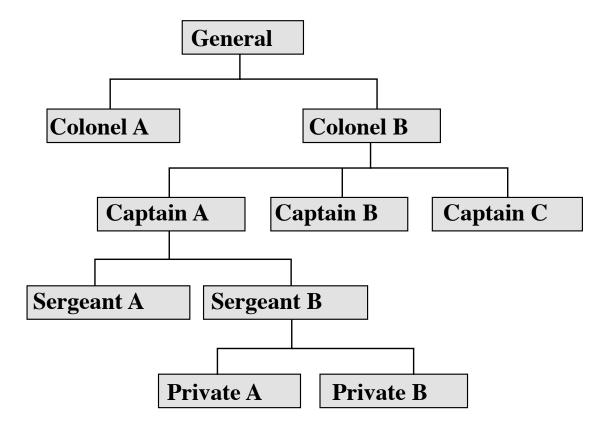
Could we just implement this with lists?

- Yes, if we decide each list contains 2 elements, an item and another list.
- But using OOP we can make it more clear / less buggy.

Trees, binary search trees

- Trees are recursive data structures, like the linked lists.
- In lab, you will implement a set based on trees instead of a hash table.
 - In particular this data structure is called a binary search tree.

- We will talk about them a bit to help with the lab.
- Below we have a generic tree:



(Image attribution to TotoBaggins, from Wikipedia article)

Tree terminology:

- A tree is either empty or a node with zero or more *children* that are themselves trees (or "subtrees").
- If X is the child of Y, then Y is the parent of X (e.g. Captain A is a child of Colonel B; Colonel B is the parent of Captain A).
- The *root* is the only node without a parent (e.g. General).
- A leaf is a node that does not have children (e.g. Private A).
- An internal node is a node that is not a leaf (e.g. Captain A).
- The *height* (aka *depth*) of the tree is the largest number of edges connecting the root to a leaf (here, 4).

Let's build a simple binary tree class using Python. A binary tree is a tree where each node has at most 2 children (the above is not a binary tree). So each tree node will have a label and two children.

```
class BinaryTree:

def __init__(self, label):
    self.label = label
    self.left = None # type = BinaryTree
    self.right = None # type = BinaryTree

def contains(self, target):
    if self.label == target:
        return True

    leftContains = False if self.left is None else self.left.contains(tar rightContains= False if self.right is None else self.right.contains(tar return leftContains or rightContains

# We would want some more functions here, e.g. to add/remove things from t
```

Let's manually build a binary tree containing some of the information in the example above:

```
root = BinaryTree("General")
root.left = BinaryTree("Colonel A")
root.right = BinaryTree("Colonel B")
root.right.left = BinaryTree("Captain A")
root.right.right = BinaryTree("Captain B")
```

```
root.contains("Clown")
```

False

```
root.contains("Captain B")
```

True

```
type(root)
```

```
__main__.BinaryTree
```

```
type(root.left)
```

```
__main__.BinaryTree
```

- The key idea here is that, like TreasureBox, the BinaryTree object stores more binary tree objects.
- However, each TreasureBox only stores one TreasureBox, whereas each BinaryTree stores **two** BinaryTree s.

Binary search trees (BSTs)

- A binary tree is a tree where each node has at most 2 children.
- A binary tree is a *binary search tree* if, for all nodes, all keys in its left subtree are smaller than its key, and all keys in its right subtree are larger than its key.

```
"abc" < "zzz"

True
```

To do in class: draw out a binary search tree, show the process of adding nodes.

```
8
/ \
1 13
/ \
9 5942
```

```
1
2
3
4
5
```

- Requirement to use BSTs: we must be able to compare keys.
- Compare this to a hash table: we need to be able to hash the keys.

Computational complexity:

- Binary search trees (BSTs) can be slow if they become very unbalanced (think of adding numbers in increasing order).
- Industrial strength implementations stay balanced and are still efficient.
- Deletion is more tricky and we won't cover it here.
- But the take-home message is that search/insert/delete all run in $O(\log n)$ time, which is pretty fast.

Could we do this with lists/dictionaries?

• Again, yes. But here the python data type best reflects the conceptual structure best.

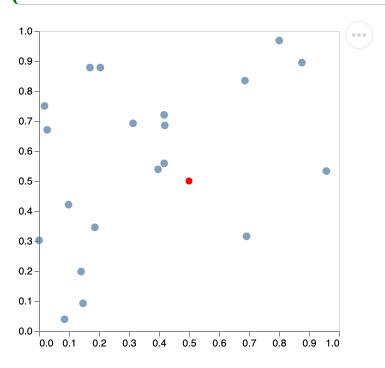
Nearest neighbours intro (Optional)

- A common problem (DSCI 571, 563, more) is to find the nearest neighbours of a point.
- We can start in 2D:

```
# You can ignore the code - we'll just look at the plot
###

# Creating Data
n = 20
np.random.seed(1)
X = np.random.rand(n, 2)
```

```
# Creating Dataframe
data = pd.DataFrame({'x0': X[:, 0], "x1" : X[:, 1]})
data['m0'] = .5
data['m1'] = .5
# Creating Plot
chart1 = alt.Chart(data).mark_circle(size=60).encode(
    x = alt.X('x0',
             axis=alt.Axis(grid=False)),
    y = alt.Y('x1',
             axis=alt.Axis(grid=False)))
chart2 = alt.Chart(data).mark_circle().encode(
    x= alt.X('m0',
              axis=alt.Axis(title = "")),
    y = alt.Y('m1',
               axis=alt.Axis(title = "")),
    color = alt.value('red'),
    size = alt.value(50)
)
chart1 + chart2
```



- Which blue points are nearest to the red ("query") point?
 - To define "nearest" we need a notion of distance.
 - For now, we'll use Euclidean distance (the one you're used to from day-to-day life).
 - In future courses, this might change.
 - Choosing a distance metric is actually important in machine learning.

The algorithmic approach is:

- 1. Find the distance from the red point to all the blue points.
- 2. Find the smallest distances.

```
# It's OK if you don't understand this code, especially during lecture
def nearest_neighbour(data, query):
    Find the point in the data that is nearest to the query point.
    Parameters
    data : numpy.ndarray
        a 2D array containing the points as rows
    query : numpy.ndarray
        a 1D array containing the guery point
    Returns
    int
        the index of the nearest point
    Example
    >>> array = np.array([[1, 1], [2, 5], [5, 6], [3, 0], [9, 9]])
    >>> nearest_neighbour(array, [10, 10])
    .....
    if query.ndim == 1:
        query = query[None]
    return np.argmin(np.sum((data - query)**2, axis=1))
```

```
print(X)
```

```
[[4.17022005e-01 7.20324493e-01]
[1.14374817e-04 3.02332573e-01]
[1.46755891e-01 9.23385948e-02]
[1.86260211e-01 3.45560727e-01]
[3.96767474e-01 5.38816734e-01]
[4.19194514e-01 6.85219500e-01]
[2.04452250e-01 8.78117436e-01]
[2.73875932e-02 6.70467510e-01]
[4.17304802e-01 5.58689828e-01]
[1.40386939e-01 1.98101489e-01]
[8.00744569e-01 9.68261576e-01]
[3.13424178e-01 6.92322616e-01]
[8.76389152e-01 8.94606664e-01]
 [8.50442114e-02 3.90547832e-02]
[1.69830420e-01 8.78142503e-01]
[9.83468338e-02 4.21107625e-01]
[9.57889530e-01 5.33165285e-01]
[6.91877114e-01 3.15515631e-01]
[6.86500928e-01 8.34625672e-01]
[1.82882773e-02 7.50144315e-01]]
```

```
query = np.array([0.5, 0.5])
nn = nearest_neighbour(X, query)
nn
```

8

X[8]

```
array([0.4173048 , 0.55868983])
```

Question: what is the time complexity of $[nearest_neighbour]$ if we have n points in k dimensions?

- A: O(n)
- $\mathsf{B} : O(k)$
- $C: O(n^2k)$
- $\operatorname{D}\!: O(nk)$

Answer: O(nk), because we have to loop over all n points, and computing the distance requires looping over the k dimensions.

- Problem: this may be way too slow!
- For example, if you want to find similar items on Amazon, and they have a billion items, you don't want to have to look through *all* of them every time.

k-d trees (Optional)

- Sometimes we speed things up with faster algorithms.
 - We'll see a lot of that in the future.
- But, as we've seen with trees and hash tables, sometime we speed things up with *better* data structures.
- One of the classic ways to speed up nearest neighbours is a data structure call the k_d tree.
- (Optional) Warning: the use of the letter k here is a bit unfortunate.
 - \circ In future machine learning courses, we'll use d instead of k.
 - \circ This will also help avoid confusion with k-nearest neighbours, which is a totally different k.
 - \circ But I do understand not wanting to call them d-d trees... so we'll use k for today.

```
# You do not need to read/understand this code, but I think
# you shouldn't have any problem understanding it with a bit of time spent.
class KDTree:
    """A k-d tree data structure for fast nearest neighbour searches"""
    def init (self):
        self.location = None
        self.leftSubTree = None # type KDTree
        self.rightSubTree = None # type KDTree
        self.dim = None
        self.data = None
    def build(self, data, depth=0):
        Build the k-d tree from the given data.
        Implementation inspired by https://en.wikipedia.org/wiki/K-d tree
        Parameters
        data : numpy.ndarray
            a 2D array where each row is a point in space
        depth : int
            this can be ignored, for internal bookkeeping (default: 0)
        nrows = data.shape[0]
        self.dim = depth % data.shape[1]
        self.data = data
        self.location = np.median(data[:, self.dim])
        # above, or just data[nrows//2,dim] after sorting
        # although this one will average if there's a tie.
        if nrows == 1:
            return
        data = data[np.argsort(data[:, self.dim])]
        self.leftSubTree = KDTree()
        self.leftSubTree.build(data[:nrows//2], depth+1)
        self.rightSubTree = KDTree()
        self.rightSubTree.build(data[nrows//2:], depth+1)
    def approximateNearestNeighbour(self, query):
        Find the nearest neighbor to the query point.
        However, this is just approximate; it finds a point in
        the same rectangle, not necessarily the actual nearest neighbour.
        This is just for educational purposes; a correct algorithm
        exists but it's too messy to put here.
        Parameters
```

```
query : numpy.ndarray
        a point in space
    Returns
    numpy ndarray
        the coordinates of the point closest to the query
    if self.data.shape[0] == 1:
        return self.data[0]
    if query[self.dim] < self.location:</pre>
        return self.leftSubTree.approximateNearestNeighbour(query)
    else:
        return self.rightSubTree.approximateNearestNeighbour(query)
def plot2d(self, depth=1, minx=0.0, maxx=1.0, miny=0.0, maxy=1.0):
    Plot the k-d tree.
    Parameters
    depth : int
        how deep to go down the tree when plotting (defult: 0)
    minx : int
        the left edge of the plot (default: 0.0)
    maxx : int
        the right edge of the plot (default: 1.0)
    miny : int
        the bottom edge of the plot (default: 0.0)
    maxy : int
        the top edge of the plot (default: 0.0)
    Returns
    _____
    numpy.ndarray
        the coordinates of the point closest to the query
    .....
    data = pd.DataFrame({'x0': self.data[:, 0], "x1": self.data[:, 1]})
    chart1 = alt.Chart(data).mark_circle(size=60).encode(
        x=alt.X('x0',
                axis=alt.Axis(grid=False)),
        y=alt.Y('x1',
                axis=alt.Axis(grid=False)))
    charts_list = [chart1]
    if depth == 0:
        return
    if self.dim == 0:
        data2 = pd.DataFrame(
            {'x0': (self.location, self.location), "x1": (miny, maxy)})
        chart2 = alt.Chart(data2).mark_line().encode(
            x=alt.X('x0',
                    axis=alt.Axis(grid=False)),
```

```
y=alt.Y('x1',
                axis=alt.Axis(grid=False)))
   charts_list.append(chart2)
    if self.leftSubTree is not None:
        chart0l = self.leftSubTree.plot2d(
            depth-1, minx=minx, maxx=self.location, miny=miny, maxy=ma
        charts list.append(chart0l)
    if self.rightSubTree is not None:
        chart0r = self.rightSubTree.plot2d(
            depth-1, minx=self.location, maxx=maxx, miny=miny, maxy=ma
        charts list.append(chart0r)
elif self.dim == 1:
   data3 = pd.DataFrame(
        {'x0': (minx, maxx), "x1": (self.location, self.location)})
    chart3 = alt.Chart(data3).mark_line().encode(
        x=alt.X('x0',
                axis=alt.Axis(grid=False)),
        y=alt.Y('x1',
                axis=alt.Axis(grid=False)))
    charts_list.append(chart3)
    if self.leftSubTree is not None:
        chart1l = self.leftSubTree.plot2d(
            depth-1, minx=minx, maxx=maxx, miny=miny, maxy=self.locati
        charts_list.append(chart1l)
    if self.rightSubTree is not None:
        chart1r = self.rightSubTree.plot2d(
            depth-1, minx=minx, maxx=maxx, miny=self.location, maxy=ma
        charts_list.append(chart1r)
params = list(filter(None, charts_list))
return alt.layer(*params).encode()
# alt.layer(*params).display()
#alt.layer(whisker low, box, whisker high, midline, data=data)
```

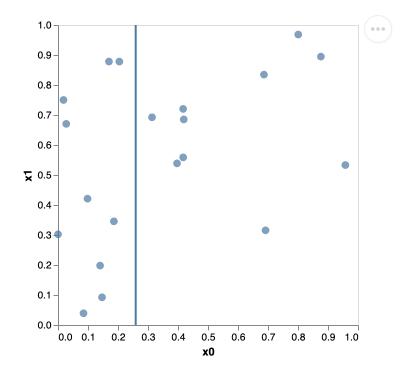
Basic idea:

- In each recursive step, there is a certain number of datapoints. If there's only one, we're done.
- Otherwise, for one of the two dimensions (we alternate back and forth), find the median value along the dimension.
- Split the data into two subsets based on being above or below that median, and build a (sub)tree for each of those subsets.
- Starting from the full dataset, you will create a tree where each leaf is a datapoint.
- You can find an approximate nearest neighbour by traversing the down the tree using the same decision points as were used to original split the data; the final leaf is the desired neighbour.

```
np.median(X[:,0])
```

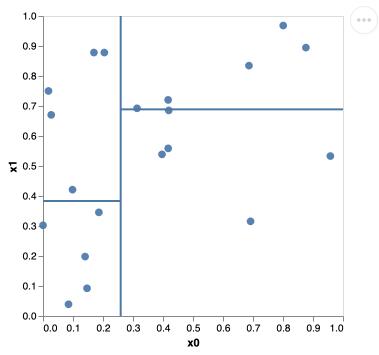
0.25893821394538014

```
kdt = KDTree()
kdt.build(X)
kdt.plot2d(depth=1)
```

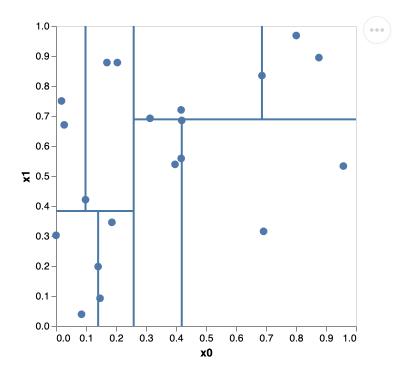


```
kdt = KDTree()
kdt.build(X)
```

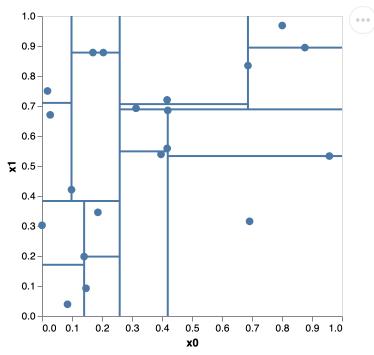
kdt.plot2d(depth=2)



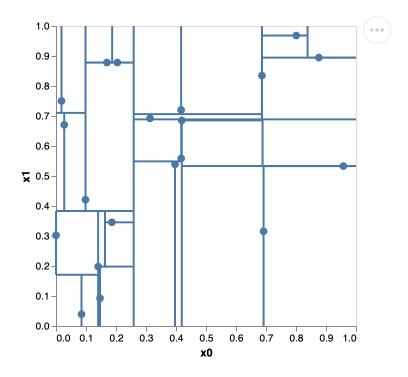
kdt.plot2d(depth=3)



kdt.plot2d(depth=4)



kdt.plot2d(depth=6)



kdt.approximateNearestNeighbour(np.array([1, 1]))

```
array([0.87638915, 0.89460666])
```

```
X[nearest_neighbour(X, np.array([1,1]))]
```

```
array([0.87638915, 0.89460666])
```

```
kdt.approximateNearestNeighbour(np.array([0.5, 0.5]))
```

```
array([0.69187711, 0.31551563])
```

```
X[nearest_neighbour(X, np.array([0.5,0.5]))]
```

```
array([0.4173048 , 0.55868983])
```

- Doesn't work perfectly here, but there is a fast correct algorithm, which is beyond the scope of the course.
 - See sklearn.neighbors.KDTree.
- However, k-d trees get slow when the number of dimensions is large.
- Some alternative methods are discussed below.

```
# ??sklearn.neighbors.KNeighborsClassifier
```

```
# ??sklearn.neighbors.KDTree
```

Timing experiments

We'll time scikit-learn's KDTree and compare it to brute force.

```
n sizes = [100, 1000, 10 000, 100 000]
results = defaultdict(list)
results["n"] = n_sizes
d = 10
for n in n sizes:
   print('n: ', n)
   X = np.random.rand(n, d)
    query = np.random.rand(1, d)
    print(" KDTree")
    time = %timeit -q -o -r 3 sklearn.neighbors.KDTree(X)
    results["KDTree init"].append(time.average)
   KDT = sklearn.neighbors.KDTree(X)
    time = %timeit -q -o -r 3 KDT.query(query)
    results["KDTree query"].append(time.average)
    print(" Brute force")
   time = %timeit -q -o -r 3 nearest_neighbour(X, query)
    results["Brute force"].append(time.average)
```

```
n: 100
KDTree
Brute force
n: 1000
KDTree
Brute force
n: 10000
KDTree
Brute force
n: 100000
KDTree
Brute force
n: 100000
KDTree
Brute force
```

```
df = pd.DataFrame(results, columns=list(results.keys()))
df
```

	n	KDTree init	KDTree query	Brute force
0	100	0.000030	0.000020	0.000004
1	1000	0.000073	0.000025	0.000028
2	10000	0.001106	0.000037	0.000128
3	100000	0.023279	0.000096	0.001414

Question: What does the time complexity look like for the 3 columns?

Answer: Brute force looks linear, the query looks logarithmic(?), the initialization grows *faster* than linear, perhaps $O(n \log n)$ or perhaps something else, we won't worry about that here.

Question: Which is better, the k-d tree or brute force?

A: KD Tree

B: Brute Force

C: It depends

Answer: It depends how many queries you do.

Amortization (Optional)

Let's focus on n=10000, and k=10. Then,

- k-d tree initialization takes pprox 4 ms
- k-d tree query takes pprox 0.1 ms
- brute force search takes $\approx 1 \, \mathrm{ms}$

Question: How many queries do we need to do such that the k-d tree is better?

Answer: around 5.

- So if we're doing 100 queries, the *k*-d tree is much better.
- This reflects a general phenomenon in algorithms: **doing a lot of work up front to save time later**.
 - We saw this earlier with sorting a list and then doing binary search multiple times.
- We say the up-front effort is amortized (or spread out) over the many queries.
- In some cases, we can make more precise calculations.
 - \circ For example, we say hash table operations are O(1).
 - In fact, once in a while a slower operation must be done.
 - \circ However, we can show that an O(n) operation only needs to be done every 1/n steps.
 - \circ In which case we say the cost is amortized and the overall cost is still O(1).
 - This is an important idea.
 - You will see this in DSCI 513 with the idea of indexing a database.

Other nearest neighbour approaches

- Note: there are other nearest neighbour approaches besides k-d trees, including some very fast approximate algorithms.
- In general, you can often do something faster if the result can be slightly wrong.
- There are approaches based on hashing instead of trees.
- Here are some resources:
 - **sklearn.neighbours** documentation
 - Approximate nearest neighbours, e.g. <u>locality-sensitive hashing</u> (LSH), <u>this package</u>.

Related: amortization of hash table growth

• Growth is slow, but only occurs rarely, and so the cost "averages out" because after adding n elements you've spent O(n) time on growth, for an average of O(1) per insertion.

defaultdict & Counter (optional)

Meta-comment: As with parts of our labs, this could be considered DSCI 511 content. But 1 course isn't enough for all the Python we need!

- Python dictionaries are super useful
- It's often the case that we want to add something to the value of a dictionary.
- Example: listing multiples

```
multiples_of_5 = list()
for i in range(100):
    if i % 5 == 0:
        multiples_of_5.append(i)

print(multiples_of_5)
```

```
[0, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, 95]
```

```
multiples_of_2 = list()
for i in range(100):
    if i % 2 == 0:
        multiples_of_2.append(i)

print(multiples_of_2)
```

```
[0,\ 2,\ 4,\ 6,\ 8,\ 10,\ 12,\ 14,\ 16,\ 18,\ 20,\ 22,\ 24,\ 26,\ 28,\ 30,\ 32,\ 34,\ 36,\ 38,\ 40]
```

```
multiples_of_3 = list()
for i in range(100):
    if i % 3 == 0:
        multiples_of_3.append(i)

print(multiples_of_3)
```

```
[0, 3, 6, 9, 12, 15, 18, 21, 24, 27, 30, 33, 36, 39, 42, 45, 48, 51, 54, 57, 60
```

- But now let's say we want multiples of 2, 3, 4, 5, 6, 7, 8, 9 all in one place.
- Well, we don't want to violate DRY and copy-paste the above code.

A dictionary would be ideal for this!

```
multiples_of = dict()

for base_number in range(2, 10):
    print("Finding the multiples of", base_number)

for i in range(100):
    if i % base_number == 0:
        multiples_of[base_number].append(i)

print(multiples_of)
```

Finding the multiples of 2

- What happened here?
- I tried [multiples_of[base_number]] but that key was not present in the dictionary.
- I need to initialize all those lists!
- Another attempt:

```
multiples_of = dict()

for base_number in range(2, 10):
    print("Finding the multiples of", base_number)

for i in range(100):
    if i % base_number == 0:
        if base_number not in multiples_of: # added
            multiples_of[base_number] = list() # added

            multiples_of[base_number].append(i)

print(multiples_of)
```

```
Finding the multiples of 2
Finding the multiples of 3
Finding the multiples of 4
Finding the multiples of 5
Finding the multiples of 6
Finding the multiples of 7
Finding the multiples of 8
Finding the multiples of 9
{2: [0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38]
```

- This works but we Python users are a bit lazy.
- Enter the defaultdict.
- A dictionary with a **default value** for cases when the key does not exist.
- Use case here: the default is an empty list!

```
d = dict()
d["hello"]
```

```
KeyError
Cell In[152], line 2
        1 d = dict()
----> 2 d["hello"]
KeyError: 'hello'
Traceback (most recent call last)

KeyError: of the lock (most recent call last)

Traceback (most recent call last)

Traceback
```

```
# equivalent to d["hello"] but returns 5 if "hello" is not in d
d.get("hello", 5)
```

5

```
d[4] = 100000 # since d[4] DOES exist, we get the stored value rather than the default d.get(4, 5)
```

100000

```
from collections import defaultdict
```

```
dd = defaultdict(list)
dd["hello"]
```

```
dd["new key"].append(5)
```

dd

```
defaultdict(list, {'hello': [], 'new key': [5]})
```

- The beauty here is that we can call append on a key that doesn't exist.
- It defaults to a new empty list and then immediately appends.
- Side effect: reading from the dictionary can modify the dictionary (eg. reading dd["hello"])
- So... our original (broken) code works again, if we change multiples_of to a defaultdict:

```
multiples_of = defaultdict(list)

for base_number in range(2, 10):
    print("Finding the multiples of", base_number)

    for i in range(100):
        if i % base_number == 0:
            multiples_of[base_number].append(i)

print(multiples_of)
```

```
Finding the multiples of 2
Finding the multiples of 3
Finding the multiples of 4
Finding the multiples of 5
Finding the multiples of 6
Finding the multiples of 7
Finding the multiples of 8
Finding the multiples of 9
defaultdict(<class 'list'>, {2: [0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24]
```

Type of defaultdict

- In DSCI 511 you saw classes and inheritance.
- Just for fun, we can look at the implementation of defaultdict in PyPy, which is an implementation of Python in Python (the OG Python is written in C): https://github.com/reingart/pypy/blob/master/lib_pypy/_collections.py#L387
- We can see here that defaultdict inherits from dict. Indeed:

type(d)
dict
type(dd)
collections.defaultdict
<pre>type(d) == type(dd)</pre>
False
<pre>isinstance(d, dict)</pre>
True
<pre>isinstance(dd, dict)</pre>
True
<pre>type(dd) == dict</pre>

```
False
```

So in general people prefer the use of <code>isinstance(obj, class)</code> over <code>type(obj) == class</code>.

Aside: list vs list()

- Question: why was it [defaultdict(list)] instead of [defaultdict(list())]?
- What happens when I run this code:

```
my_list = list()
my_list
```

[]

```
bad = defaultdict([])
```

```
TypeError
Cell In[167], line 1
----> 1 bad = defaultdict([])

TypeError: first argument must be callable or None
```

```
bad = defaultdict(list())
```

```
TypeError Traceback (most recent call last)
Cell In[168], line 1
----> 1 bad = defaultdict(list())

TypeError: first argument must be callable or None
```

- But why?
- The code that executes first is list().
- So we pass in a particular list.
- But we don't want one particular list, we want to create new lists all the time.

- So we need to pass in the ability to create lists
 - in other words, a function that creates lists
- That function is list

```
list # This is a function
```

list

```
list() # This is one list
```

[]

```
x = defaultdict(lambda : "hello I am your friendly neighbourhood default value"
```

x[5]

```
'hello I am your friendly neighbourhood default value'
```

In lab you need to count occurrences. So, in that case, what is my default value?

```
text = "Blah blah is he still talking about dictionaries??"
```

This can be done with a Python function:

```
text.count('a')
```

5

If we're doing something more sophisticated, we might want to ignore this for now, and implement the counting ourselves:

```
number_of_a = 0
for t in text:
    if t == "a":
        number_of_a += 1
number_of_a
```

```
5
```

- Ok, but now we want to count "a" and "b".
- Same as before, let's use a dict.
- We already know this won't work it's the same problem as before:

```
number_of_times = dict()

for char in ('a', 'b'):
    for t in text:
        if t == char:
            number_of_times[char] = number_of_times[char] + 1

number_of_times
```

So, we use a defaultdict.

Question: What do we want the default value to be?

Answer: 0

```
defaultdict(0)
                                              Traceback (most recent call last)
  TypeError
  Cell In[177], line 1
  ----> 1 defaultdict(0)
  TypeError: first argument must be callable or None
Oops! Right, it needs to be a function, not a specific value.
  defaultdict(lambda: 0)
  defaultdict(<function __main__.<lambda>()>, {})
  # The `int` function will return zero, so we can use that too
  defaultdict(int)
  defaultdict(int, {})
  int()
  0
Back to the code:
```

```
number_of_times = defaultdict(int)

for char in ('a', 'b', 'c'):
    for t in text:
        if t == char:
            number_of_times[char] += 1

number_of_times
```

```
defaultdict(int, {'a': 5, 'b': 2, 'c': 1})
```

Counter

And finally, for the supremely ~~lazy~~ awesome, we can use Counter:

```
from collections import Counter
```

This is basically a defaultdict(int) but with some fancy methods added:

```
number_of_times = Counter()

for char in ('a', 'b'):
    for t in text:
        if t == char:
            number_of_times[char] += 1

number_of_times
```

```
Counter({'a': 5, 'b': 2})
```

```
number_of_times.most_common(1)
```

```
[('a', 5)]
```