COMP 204

Dictionaries

Mathieu Blanchette, based on material from Carlos Oliver Gonzalez and Christopher Cameron

Note about two-dimensional lists

In your assignment #2, you will need to represent two-dimensional tables, with a fixed number of rows and columns. *Two-dimensional lists* can be used to do this in Python.

A two-dimensional list is a list of lists, where each of the lists is of the same length. Example: A tic-tac-toe grid:

```
1  tictactoe = [ ["X", "", "O"],
2                ["", "X", ""],
3                ["O", "", ""] ]
4
5  print(tictactoe) # [['X','','O'], ['','X',''], ['O','','']]
6
7  # to access an element in a 2D list,
8  # specify the index of the row and column
9  tictactoe[1][2] = "X"
10 print(tictactoe) # [['X','','O'], ['','X','X'], ['O','','']]
```

Note about two-dimensional lists

Example: A position frequency matrix (see assignment #2).

```
# A position frequency matrix of 4 rows and 6 columns
PFM = [ [0, 4, 2, 5, 1, 3],
        [5, 11,4, 10,6, 5],
        [0, 0, 7, 0, 4, 7],
        [10,0, 2, 0, 4, 0] ]

PFM[0][2] = PFM[3][2] + PFM[2][4]
print(PFM[0][2]) # 6
```

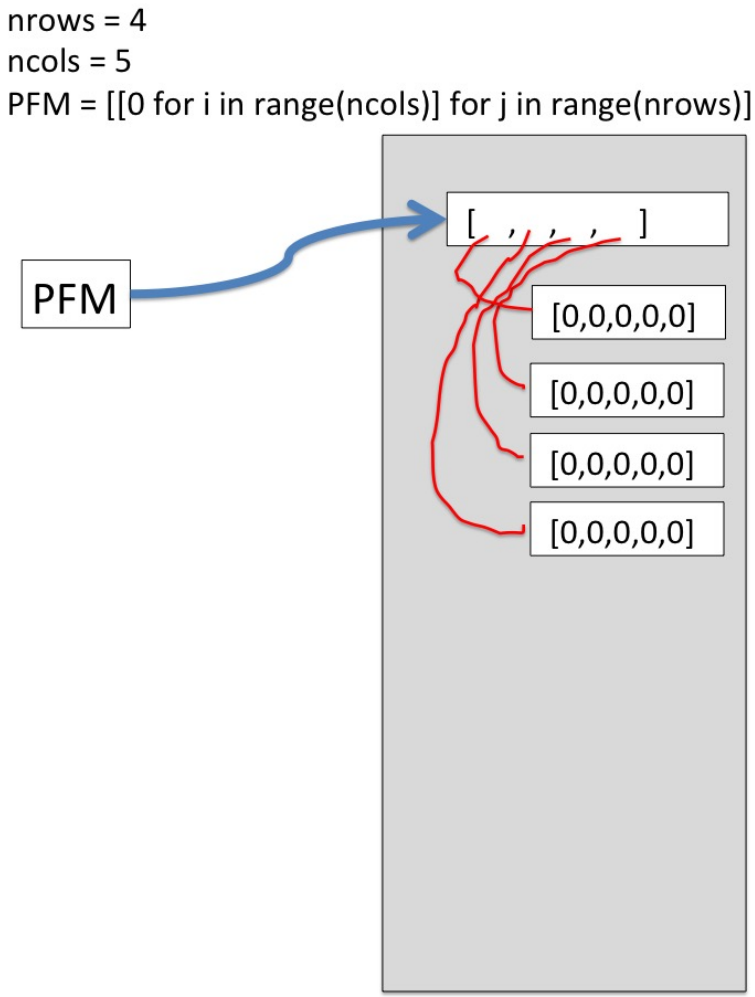
Creating two-dimensional lists

To create a new 2D list filled with zeros:

```
# Creating a two-dimensional list of 4 rows and 5 columns,
# filled with zeros
nrows = 4
ncols = 5
PFM = [[0 for i in range(ncols)] for j in range(nrows)]
print(PFM)
```

Copying 2D lists

Because lists are compound objects, we need to be careful when copying them.



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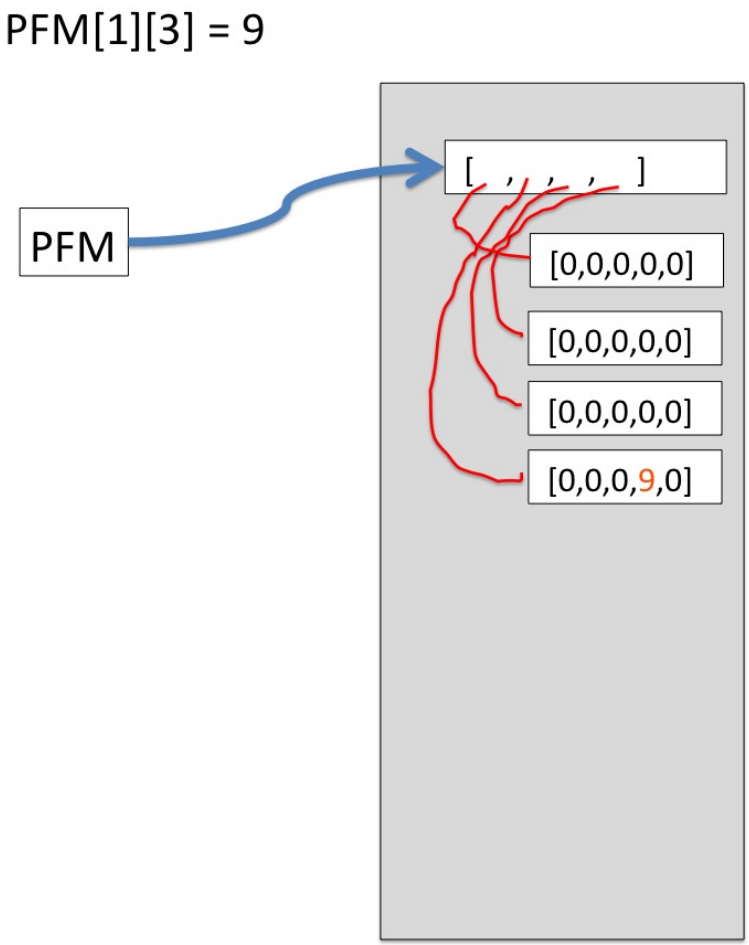

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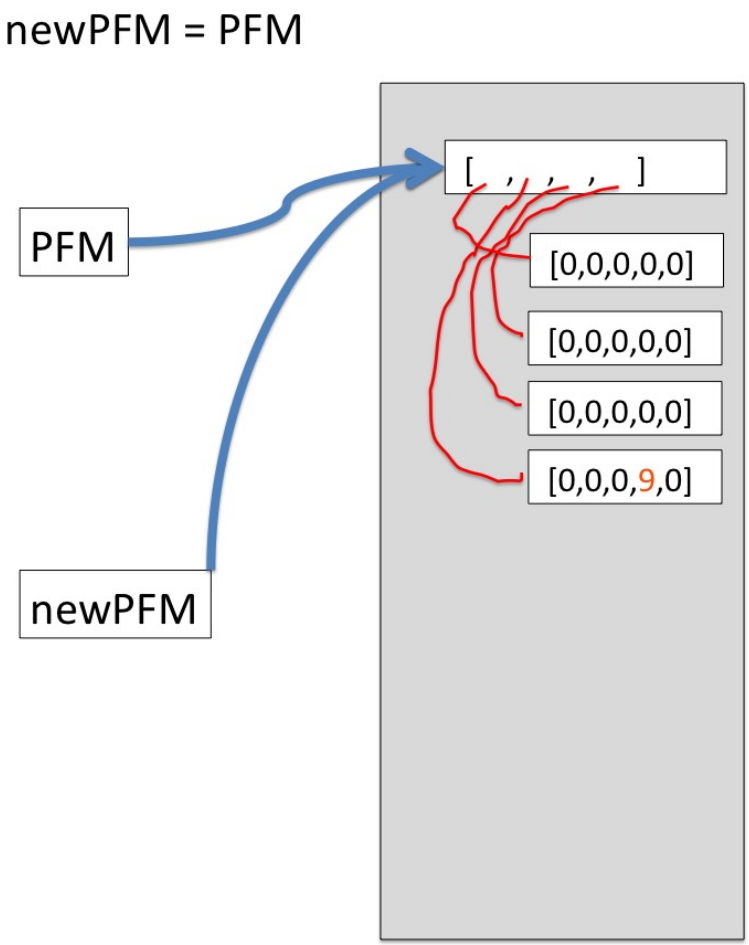

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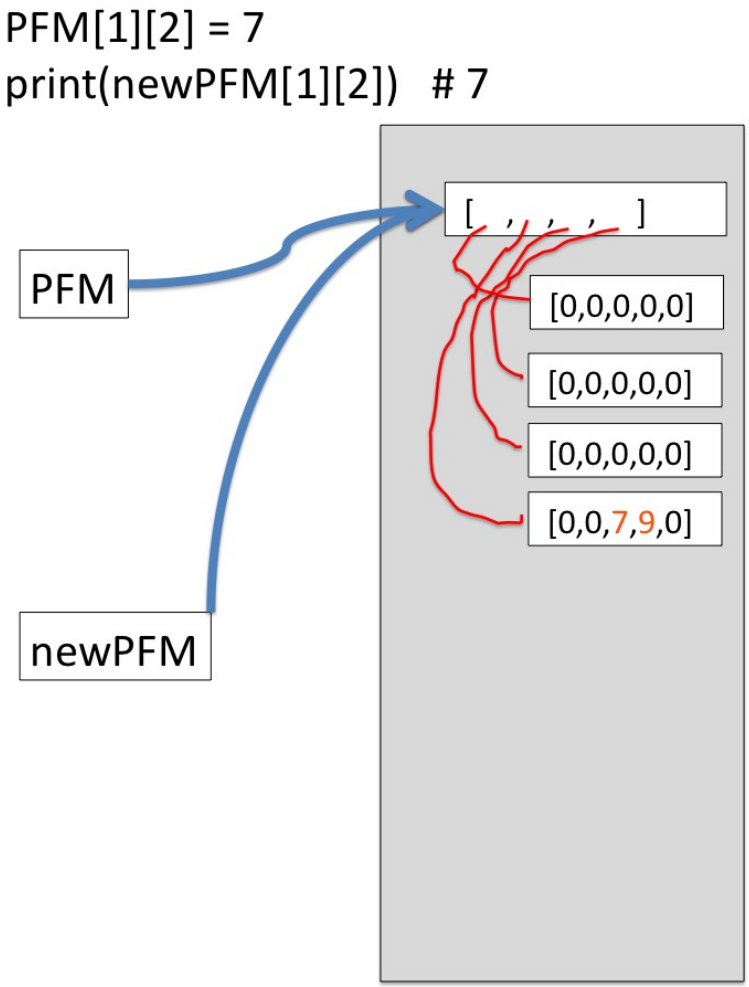
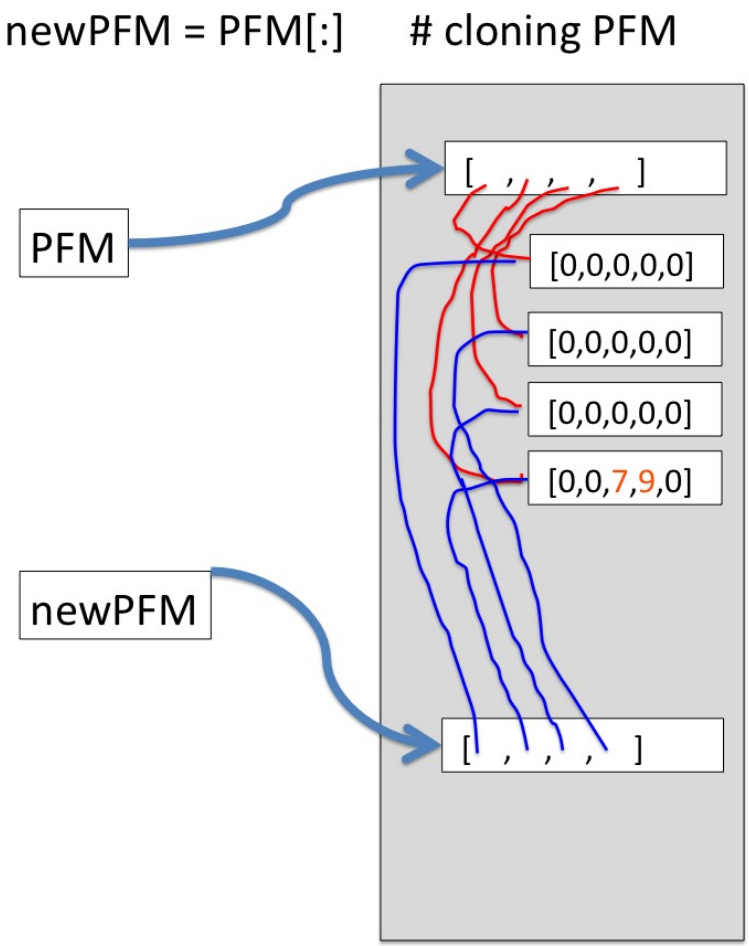


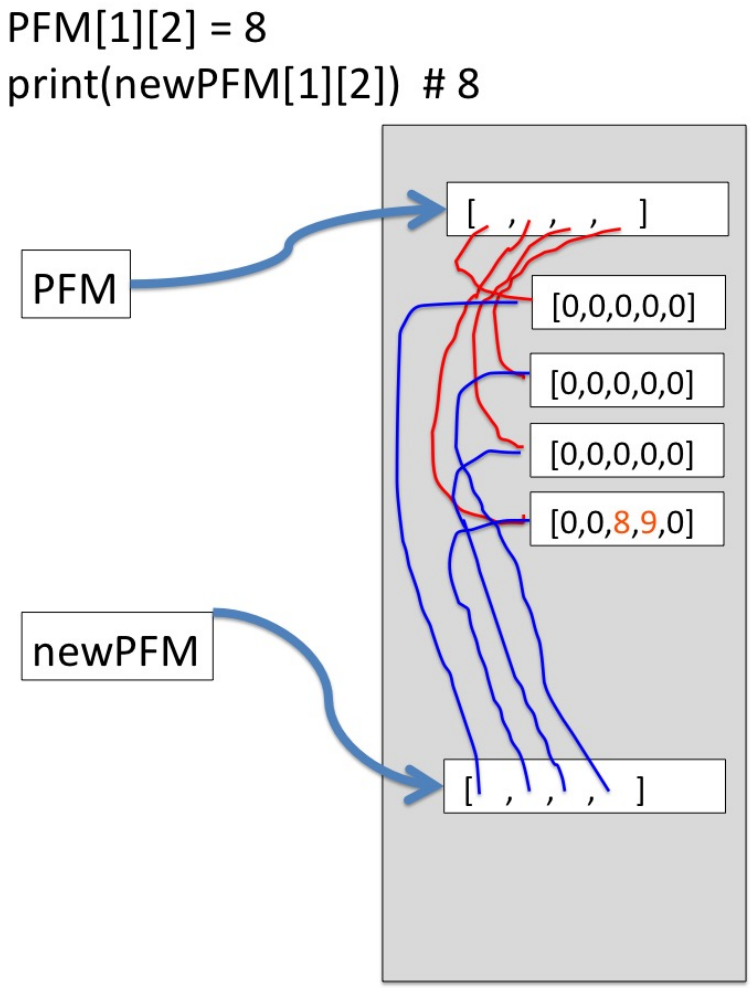
Copying 2D lists

Cloning PFM results in newPFM being a different list object than PFM. *However, the elements of newPFM are the same 1D lists as the elements of PFM.*



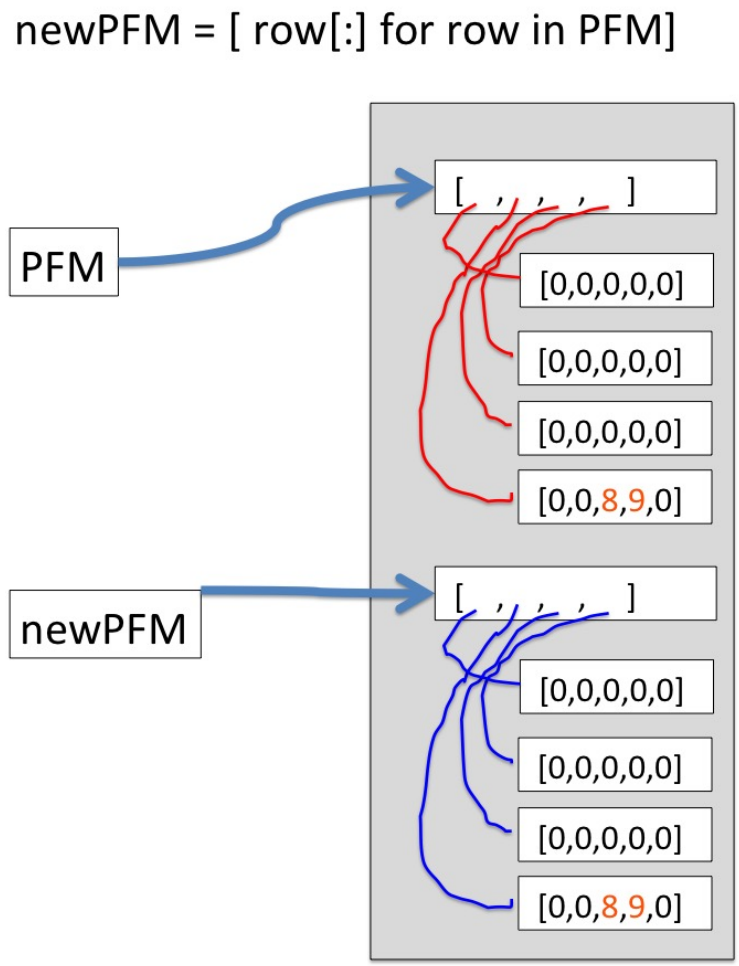
Copying 2D lists

So changing a value in PFM still changes the value in newPFM!



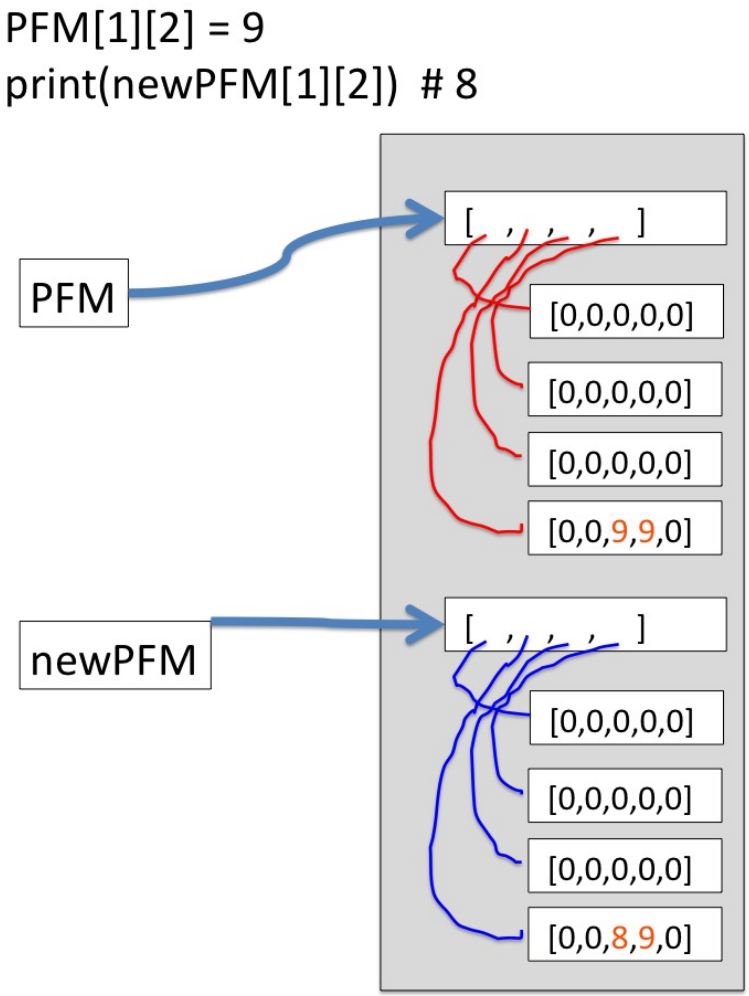
Copying 2D lists

The correct way to clone a 2D list is:



Copying 2D lists

Now the two 2D lists share no elements, and change values in one does not change the values in the other.



A very useful type: Dictionary

- A dictionary is said to be a *mapping* type because it maps *key* objects to *value* objects.
- Dictionaries are immensely useful and are the magic behind a lot of Python functionality
- Syntax:

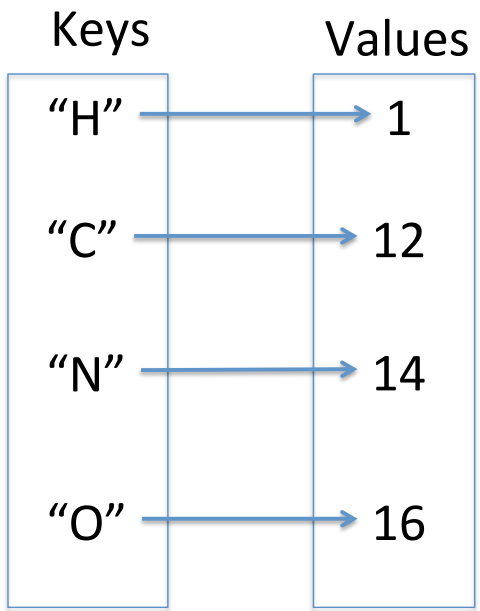
```
1 my_dict = { [key1]: [value1], [key2]: [value2],...}
```

- The analogy to a real dictionary works. The word you look up is the **key** and the definition is the **value**

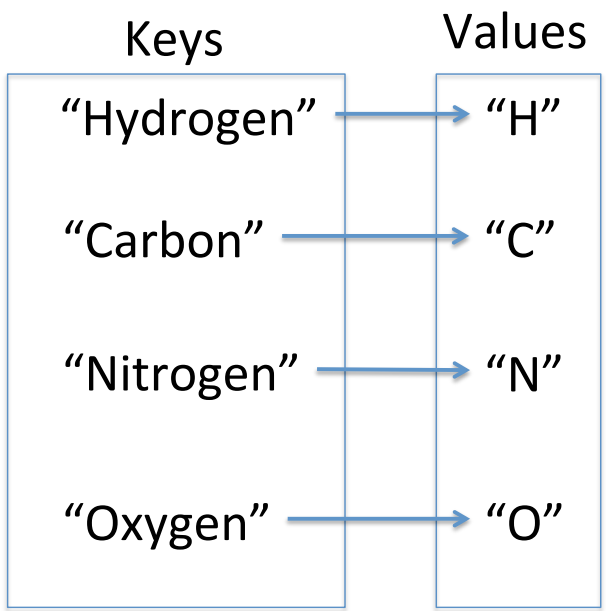
```
# this dictionary maps strings to integers
periodicTable = {"H":1, "C":12, "N":14, "O": 16}

elementsCodes = {"Hydrogen":"H", "Carbon":"C",
                 "Nitrogen":"N", "Oxygen":"O"}
```

periodicTable dictionary:



elementCodes dictionary:



Accessing elements in a dictionary

```
# this dictionary maps strings to integers
periodicTable = {"H":1, "C":12, "N":14, "O": 16}

elementsCodes = {"Hydrogen":"H", "Carbon":"C",
                 "Nitrogen":"N", "Oxygen":"O"}

mass = periodicTable["K"]


periodicTable["He"] = 4  # adds key "He" with value 4
periodicTable["Na"]= 23  # adds key "Na" with value 23

#periodicTable now contains 6 keys,value pairs

periodicTable["C"] = 12.01  # overwrites value for key "C"

del periodicTable["N"]  # deletes key "N" and its value 14
```

Adding and deleting key/value pairs to a dictionary

Adding new key/value pairs:

- Syntax: myDict[key] = value
- If key does not already exist in the dictionary, the new key/value pair is added
- If the key already exists, its previous value is overwritten

Deleting key/values: del myDict[key]

```
# this dictionary maps strings to integers
periodicTable = {"H":1, "C":12, "N":14, "O": 16}

elementsCodes = {"Hydrogen":"H", "Carbon":"C",
                 "Nitrogen":"N", "Oxygen":"O"}

mass = periodicTable["K"]


periodicTable["He"] = 4  # adds key "He" with value 4
periodicTable["Na"]= 23  # adds key "Na" with value 23

#periodicTable now contains 6 keys,value pairs

periodicTable["C"] = 12.01  # overwrites value for key "C"

del periodicTable["N"]  # deletes key "N" and its value 14
```

About keys and values

Keys:

- Have to be immutable objects: int, float, str, tuple.
- Have to be unique in the dictionary: A dictionary cannot contain two elements with the same key.

Values:

- Values can be any type of object: int, float, str, tuple, list, dictionary, etc.
- Many keys can map to the same value

A dictionary can contain keys of many different types, and values of many different types:

```
# a dictionary with keys and values of different types
mixedDict = {"H":"Hydrogen", 17:"prime",
             30:[1,2, 3, 5], (4,5):20}


product = mixedDict[(4,5)]  # 20
primeFactors = mixedDict[30]     # [1,2, 3, 5]

fac = mixedDict[20]   # KeyError: 20 not in mixedDict
```

Dictionaries of dictionaries

The values stored in a dictionary can themselves be dictionaries!

```
# a dictionary where each value is itself a dictionary
periodicTable = {"H": {"name":"Hydrogen", "mass":1},
                 "C": {"name":"Carbon", "mass":12},
                 "N": {"name":"Nitrogen", "mass":14},
                 "O": {"name":"Oxygen", "mass":16} }

carbonDic = periodicTable["C"]  # {"name":"Carbon", "mass":12}
m = carbonDic["mass"]  # 12

#or more directly
m = periodicTable["C"]["mass"]  #12
```

Iterating through dictionaries

The function keys() returns all the keys present in the dictionary.

```
per = {"H":1, "C":12, "N":14, "O": 16}

keyList = list( per.keys() ) # ["H", "C", "N", "O"]
# Note: the keys() function returns an object of
#       type dict_keys. This object is converted to a
#       list using the list() function

for k in keyList:
    print("Key",k,"has value",per[k])
```

The function items() returns the key/value tuples in the dictionary

```
per = {"H":1, "C":12, "N":14, "O": 16}

itemList = list( per.items() )
# Note: the items() function returns an object of
#       type dict_items. This object is converted to a
#       list using the list() function

# itemList is now a list of tuples:
# [('H', 1), ('C', 12), ('N', 14), ('O', 16)]

for k,v in itemList:
    print("Key",k,"has value",v)
```

More functions on dictionaries

To test if a key is present in a dictionary, use the in operator: key in myDict , which evaluates to True if key is in myDict.

```
periodic = {"H":1, "C":12, "N":14, "O": 16}

newElement = "Na"
if newElement in periodic:
    print("Na is already in the dictionary")
else:
    print("Na is not in the dictionary")
```

To add the content of one dictionary, use the update() function.

```
per = {"H":1, "C":12, "N":14, "O": 16}
newTable = {"Na":23, "K":39}

# Add the content of newTable to per
per.update(newTable) # per now has 6 elements
                     # newTable still has 2
```

For more functions on dictionaries:

`https://docs.python.org/3/library/stdtypes.html#mapping-types-dict`

Example

Goal: Count the number of occurrences of all characters in a string.

```
1  sequence = "Hello my name is MAThieu"
2  nucleotides = "acgt"
3  counts = {}  # an empty dictionary
4  for nuc in sequence:
5      if nuc in nucleotides:
6          if (nuc in counts)==False:
7              counts[nuc] = 1
8          else:
9              counts[nuc] += 1
10
11 print(counts)
```

Example

Goal: Compute the mass of a molecule based on its chemical composition. Assume that you have access to a dictionary of atomic masses.

```
periodicTable = {"H":1, "C":12, "N":14, "O": 16}

aceticAcid = "CHHHCOOH"

mass = 0
for element in aceticAcid:
    mass += periodicTable[element]

print("Mass of acetic acid is",mass)
```

Example

Goal: Create a dictionary using as keys the english name of molecules and as values their molar mass. Assume that you have access to a dictionary of atomic masses and a dictionary of chemical compositions:

```
periodicTable = {"H":1, "C":12, "N":14, "O": 16}

molecules = {"Carbon dioxyde":"COO",
             "Nitric oxyde":"NO",
             "Acetic acid":"CHHHCOOH"}

moleculeMass = {}  # the new dictionary we are about
                   # to populate with name/mass pairs
for name, composition in molecules.items():
    mass = 0
    for atom in composition:
        mass += periodicTable[atom]
    moleculeMass[name] = mass

print(moleculeMass)
```