COMP 204: Sequence alignment examples, more dictionaries

Yue Li
based on material from Mathieu Blanchette, Carlos Oliver, Christopher J.F. Cameron

Midterm materials coverage and practice midterms

- Midterm is held on February 22 at 6:30-8:00 pm in LEA 219.
- Our midterm will cover up to Lecture 17 (Feb 13)
- Past midterms in COMP 204 Fall 2018 and COMP 364 Fall 2017 are posted on myCourses for practice

A couple more Needleman-Wunsch examples on blackboard

The most important of Assignment 2 is to understand Needleman-Wunsch global sequence alignment algorithm. Let's do a couple of examples together:

Example 1

Sequence 1: G
Sequnece 2: GCG

Example 2

Sequence 1: TCGA
Sequnece 2: TTCG

A matrix in Python is just a list of lists of the same length

In Assignment #2, we will need to represent two-dimensional tables or matrices, with a fixed number of rows and columns.

Two-dimensional lists can be used to do this in Python.

A 2D list is a list of lists, where each of the lists is of the same length. Example: A tic-tac-toe grid:

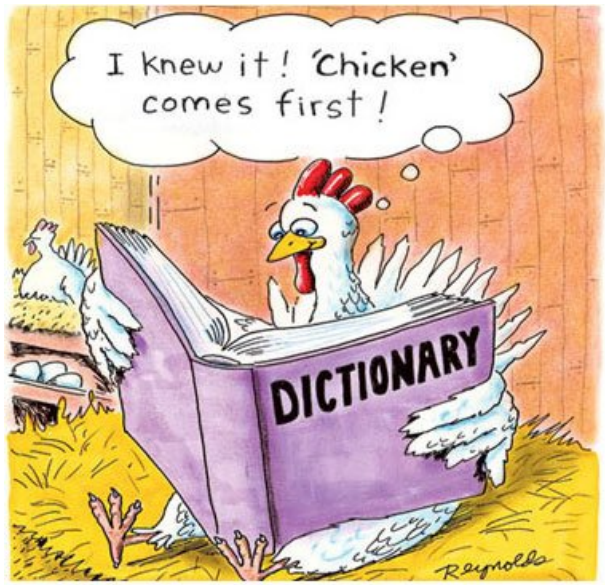
```
tictactoe = [ ["X", "", "O"],
              ["", "X", ""],
              ["O", "", ""] ]

print(tictactoe) # [['X','','O'], ['','X',''], ['O','','']]

# to access an element in a 2D list,
# specify the index of the row and column
tictactoe[1][2] = "X"
print(tictactoe) # [['X','','O'], ['','X','X'], ['O','','']]
```

To create a new matrix with zeros we can use *list comprehension*:

```
# Create an alignment scoring grid for two DNA sequences
seq1="GATTACA"
seq2="GCATGCA"
alignmentScoreGrid=[[0 for j in range(len(seq2)+1)]
                    for i in range(len(seq1)+1)]
print(alignmentScoreGrid) # print out the scoring grid
```

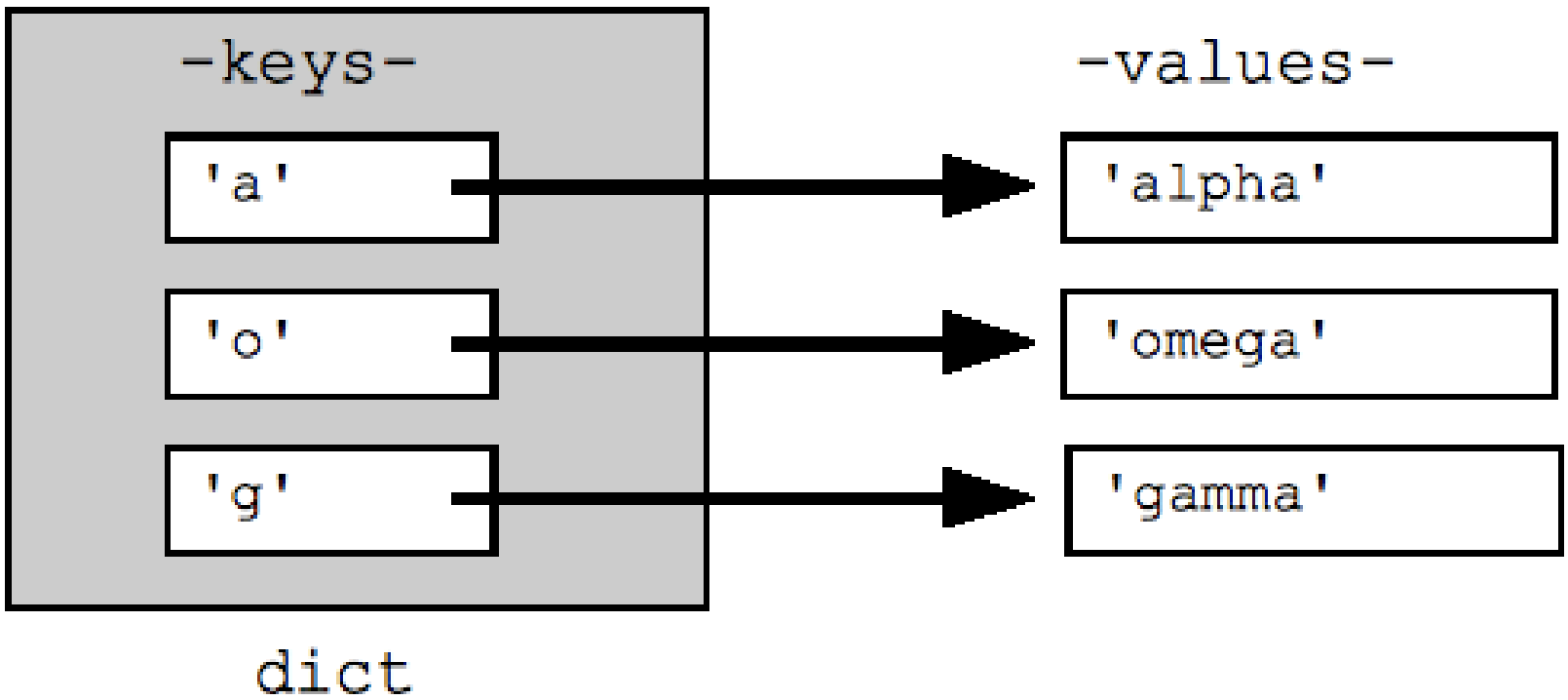
Dictionaries Recap

- 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: `my_dict = {[key]: [value], ...,}`
- The analogy to a real dictionary works. The word you look up is the **key** and the definition is the **value**



Dictionaries: picture

- Keys map to values.
- We use dictionaries when we want to access data using something other than an index (i.e. lists).



Dictionaries: keys and values

- A dictionary's keys can be many different types of **immutable** objects (i.e. int, str, tuple)
- You can access a key's value like a list. Syntax: `my_dict[key]`
- You can mix and match key types
- Values can be any object type. You can also mix and match.

```
record_sales = {
    "Kanye": 2.4,
    "Beyonce": 1.5,
    "Chance": 1.2,
    ("a", 12):  "bob"
    }
print(record_sales["Beyonce"]) # 1.5
print(record_sales[("a", 12)]) # "bob"
```

Adding keys to a dictionary

- Syntax: `my_dict["key"] = value`
- If the key does not yet exist, a new key/value pair is created.
- If the key already exists, its previous value is overwritten

```
>>> d = {"bob": 28}
>>> print(d)
{"bob": 1.2}
>>> d["charlie"] = 33
>>> print(d)
{"bob": 1.2, "charlie": 2.5}
>>> d["bob"] = "woooo"
{"bob": "woooo", "charlie": 33}
>>> del d["bob"] # we can delete keys with the del
 ↪  operator
{"charlie": 33}
```

Important properties of dictionaries

- Dictionaries are **mutable** We can modify the contents of the dictionary as much as we want.

```
>>> d = {"bob": 24, "tina": 11}
>>> d["tameeka"] = 42
>>> d['bob'] = [1, 2, 3, 4]
>>> del d["bob"]
>>> mystring = 'AAAGGG'
>>> mystring[2] = 'T' # this is an error. strings
↪  are immutable
```

Important properties of dictionaries

- Key-value pairs are **NOT** always stored in order. (for the current Python 3.7 they are, but assume it won't be like this forever)
- If you want to iterate over the keys in a dictionary use the `dict.keys()` function.

```
>>> d = {"bob": 24, "tina": 11}
>>> for k in d.keys():
>>> ... print(k)
"tina"
"bob"
```

Useful dictionary methods and operators

- `d.items()` produces an iterator which yields tuples of the form `(key, value)`

```
>>> for k,v in d.items():
>>> ... print("key:", k, "value:", v)
>>>
    key: bob, value 24
    key: tina, value 11
```

- `k in d` evaluates to `True` if the key exists in the dictionary and `False` otherwise.
- `d.update(d2)` "merges" two dictionaries into one.

```
>>> d = {"a": 3, "b": 4}
>>> d.update({"c": 5})
{"a": 3, "c": 5, "b": 4}
```

Quick dictionary example: mini BLAST

- BLAST is a very popular bioinformatics tool used to compare DNA sequences. One of the main innovations is to index a genome by 'words'.
- *words* are short sequences. `AT, CG, CC, GG, AA`
- Goal: Given a genome and a list of words return a dictionary with a list of positions where each given word occurs.
- **Example:** for words `AAG, AAT` in genome `GAAGAAGGGAATGGAAGAAT` we should return `'AAG': [1,4, 14], 'AAT': [9,17]`.

Note BLAST is a *heuristic approach* to do fast sequence search but Needleman-Wunsch global alignment algorithm (or Smith-Waterman local alignment) is a more principled way to find optimal match(es) at the cost of speed.

Building genomic dictionary

```
#Args: genome_seq: a DNA sequence as a string
#      words: an iterable of sequences
#Returns:
#   genomeDict: a dict with a key for each word mapping to
    list of indices.
def buildGenomeDict(genome_seq, words):
    genomeDict = {}
    for w in words:
        for i in range(len(genome_seq)-len(w)+1):
            if genome_seq[i:i+len(w)] == w:
                if w not in genomeDict:
                    genomeDict[w] = []
                genomeDict[w].append(i)
    return genomeDict

genome_seq = "AGCGACGTATAATCGACTA"
words=["CG", "TATA"]
genomeDict = buildGenomeDict(genome_seq, words)
print(genomeDict)
# {'CG': [2, 13], 'TATA': [7]}
```

Searching genomic dictionary

```
#Args: genomeDict: build from genome_index
#      genome_seq: DNA sequence corresponding to genomeDict
#      queries: a list of query sequences
#Returns: blasthits: a dict with a key for each query and
    their genomic location(s)
def searchGenomeDict(genomeDict, genome_seq, queries):
    blasthits={}
    for q in queries:
        blasthits[q]=[] # initialize query hit list
        for genomeDictKey in genomeDict.keys():
            for i in range(len(q)-len(genomeDictKey)+1):
                wordlen = len(genomeDictKey)
                querySubstr = q[i:i+wordlen]
                if querySubstr == genomeDictKey:
                    genomePosList = genomeDict[querySubstr]
                    for pos in genomePosList:
                        if genome_seq[pos-i:pos+len(q)-i] ==
     q: # mistake: genome_seq[pos:pos+len(q)] == q:
                            blasthits[q].append(pos-i)
        if len(blasthits[q])>0:
            blasthits[q] = set(blasthits[q]) # set returns
    unique values (more info on set in the next lecture)
    return blasthits
queries = ["ACGT", "CGACGT", "TATAAT", "CGACT", "XYZ"]
myhits = searchGenomeDict(genomeDict, genome_seq, queries)
print(myhits) # {'ACGT': {4}, 'CGACGT': {2}, 'TATAAT': {7}
```

A convenient method: setdefault

- Let's look at line 15 in the previous example:

```
1  if w not in word_index:
2          word_index[w] = []
3  word_index[w].append(i)
```

- You will find yourself writing this statement many times.
- `mydict.setdefault(key, [default])` If key is in the dictionary, return its value. If not, insert key with a value of `default` and return `default`.
- We can replace it with one line using `setdeafult`

```
1  word_index.setdefault(w, []).append(i)
```

Dictionaries Pop Quiz

- True or False: dictionaries are immutable.
- Error? `myd = {[1,2]: "hello"}`
- True or False: dictionary keys must be unique.
- Error? `d2 = {'bob': 2, 'susan': 3, 'bob':4}`
- Error? `d = {}; d['bob'].append(3)`
- True/False: once a key-value is stored we can't update it.

Dictionaries Pop Quiz Answers

- True or False: dictionaries are immutable.
- Error? `myd = {[1,2]}: "hello"` – **Yes. Keys must be immutable.**
- True or False: dictionary keys must be unique.
- Error? `d2 = {'bob': 2, 'susan': 3, 'bob':4}` – **No. Duplicate keys are overwritten**
- Error? `d = {}; d['bob'].append(3)` – **Yes. Key 'bob' has not been created.**
- True/False: once a key-value is stored we can't update it. `d['bob'] = 3; d['bob']='hi'` is valid.