Python for scientific research

Built-in data types

Bram Kuijper

University of Exeter, Penryn Campus, UK

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  - Python is **case sensitive**; `genename` and `geneName` are different variables
  - First character cannot contain a digit: `1genename` raises an error
  - You cannot use Python's **reserved words/keywords**
  - If you're an R user, **DO NOT** use '.' in your variable names i.e `gene.name` is not a valid variable name

Core data types

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- **Complex numbers:** `complex`

```
1 cnumber = 10 + 2j # 10=real part; 2=complex part
2 type(cnumber) # complex
```

Core data types (continued)

- **Boolean:** `bool` true or false values for logical statements

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1 isTransFactor = True # is protein a transcription
      factor?
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- **Strings:** `str` for any text

```
1 motif = "AATCAGTT" # DNA sequence motif
2 type(motif) # str
```

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- The type of a variable changes dependent on its value:

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- This is also called duck typing *"If it walks like a duck and it quacks like a duck, then it must be a duck"*
  - i.e., we do not have to define from the start what data types we need (compare C or Java).
  - We find out along the way (e.g., by using `type`) what data types we are using

Container data types

- **Lists:** `list` for a collection of variables

```
1 # Interesting genes
2 geneNames = ["Irf1", "Ccl3", "Il12rb1", "Ifng", "Cxcl10
      "]
3 type(geneNames) # list
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- **Tuples:** `tuple` for an *immutable* collection of values

```
1 # Interesting genes
2 geneNames = ("Irf1", "Ccl3", "Il12rb1", "Ifng", "Cxcl10
      ")
3 type(geneNames) # tuple
```

Initializing a single element tuple

- For some (daft) reason one might need a single element tuple. One might try:

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- Parentheses around a single element are having no effect (they are used for grouping). To clarify it is a tuple, one needs a trailing comma:

```
1 singleElementT = ("Irf1",)
2 type(singleElementT) # tuple
```

Container data types (continued)

- **Dictionary:** `dict` for a collection of values and unique labels

```
1 # A phone book
2 phoneBook = {"Bram": "01326 - 259022", "Annette": "
      01326 - 371842", "Angus": "01326 - 255794"}
3 type(phoneBook) # dict
```

Container data types (continued)

- **Sets:** `set`, `frozenset` for a collection of unique values

```
1 # Sets are mutable collections of unique values
2 languages = set(["Python", "R", "MATLAB", "C"])
3 type(languages) # set
```

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# Sets are mutable collections of unique values
languages = set(["Python", "R", "MATLAB", "C"])
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# Frozensets are immutable collections of unique values
languages = frozenset(["Python", "R", "MATLAB", "C"])
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```

- **Range:** `range` for sequences of integers

```
# Create immutable sequence of numbers from 0 to 4
x = range(5)
type(x) # range
```

Mutable vs immutable objects

- **Mutable** objects (`list, dict, set`) can be changed once assigned

```
1 # Lists are mutable
2 geneList = ["Irf1", "Ccl3", "Il12rb1"]
3 geneList[0]="Irf2" # change first gene to Irf2
```

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- **Immutable** objects *cannot* be changed once assigned

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1 geneTuple = ("Irf1", "Ccl3", "Il12rb1") # immutable
2 geneTuple[0]="Irf2"
3 TypeError: 'tuple' object does not support item
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- However you can replace an **immutable** object with a new one

```
1 geneTuple = ("Irf1", "Ccl3", "Il12rb1")
2 # Replace with a new object
3 geneTuple = ("Irf2", "Ccl3", "Il12rb1")
```

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Immutable objects such as a `tuple` cannot be changed once assigned. Why use them?

- It is faster: ideal if one only needs to iterate through a constant list of values
- Assures that data is "write-protected" (i.e., elements cannot be changed after initialization)
  - Handy when one wants to ensure certain values are not changed during the course of a simulation

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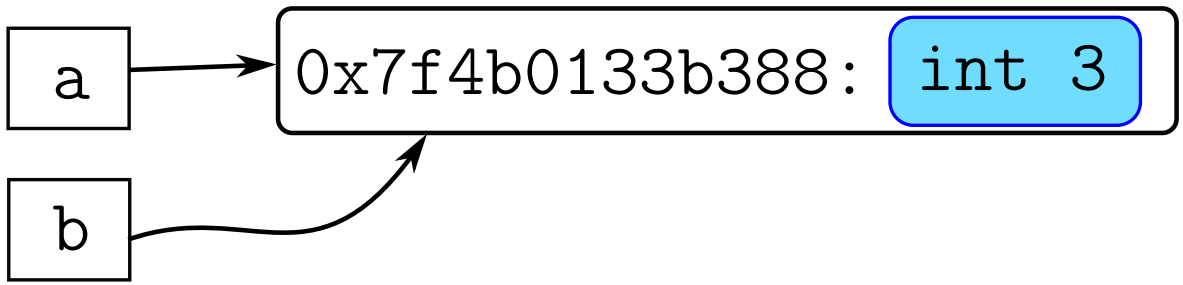
2 b = a # copy of a
```

- Both `a` and `b` then point to the same address in memory (say, `0x7f4b0133b388`), which holds `3`:



Making copies of objects

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1 a = 5
2 print(a) # 5
3 print(b) # 3
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- What happens is that `a` is assigned a reference to a new position (0x8a8960) containing `5`
- While `b` keeps its reference to the old position (containing 3)

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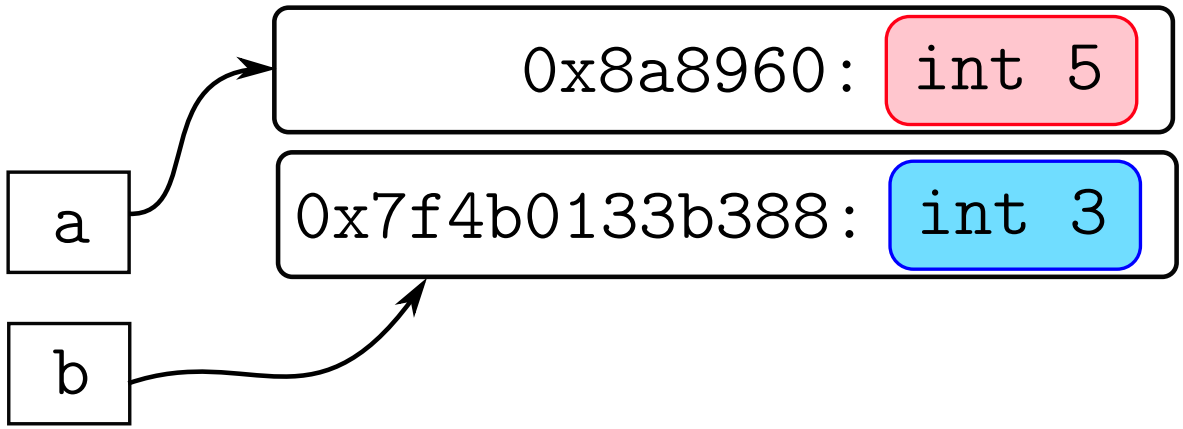

Making copies of objects: lists

- What happens when making copies of objects which themselves contain objects (as happens in `list`, `dict`)?

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1 a = [2,8] # list with two ints
2 b = a # copy to the reference of that list
```

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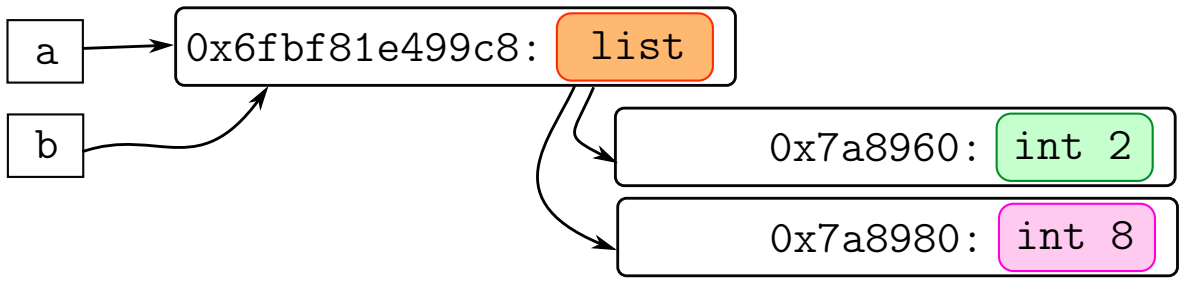
- Now our reference layout looks like this:



Making copies of objects: lists

- If we reassign a different variable to a list element, both `a` and `b` are affected!

```
1 a[1] = 5
2 print(a) # [ 2, 5]
3 print(b) # [ 2, 5]
```

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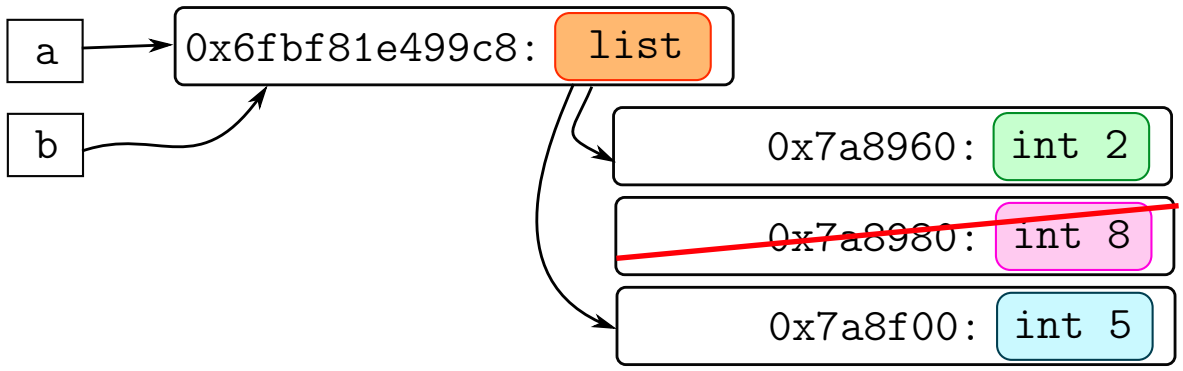
- If we reassign a different variable to a list element, both `a` and `b` are affected!

```
1 a[1] = 5
2 print(a) # [ 2, 5]
3 print(b) # [ 2, 5]
```

- Both `b` and `a` still point to the same `list` object
- Within the list, however, references have now changed:



Making copies of objects: lists

- **Bottom line**: be careful when using copies of mutable objects like `list` or `dict`
- If you want to change elements only of the copied variable or not the original (but not both), make a *deep* copy:

```
1 a = [1,2]
2 b = a[:] # go through all elements of a and assign to b
```

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4 a[0] = 5
5 print(a) # [5,2]
6 print(b) # [1,2]: deep copy unaffected
```

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2  b = a[:] # go through all elements of a and assign to b
3
4  a[0] = 5
5  print(a) # [5,2]
6  print(b) # [1,2]: deep copy unaffected
7
8  # alternatively, use the copy module
9  import copy
10
11 b = copy.deepcopy(a)
```

Methods of objects

- A Python variable is called an **object**
- Every object has **methods** (functions) associated with it
- These methods are called using the dot notation (‘ . ’)

```
1 # DNA sequence motif
2 motif = "AATCAGTT"
3
4 # Use the count method to count occurrence of nucleotide "T"
5 motif.count("T") # 3
6
7 # Use the lower method to convert to lower case
8 motif.lower() # "aatcagtt"
```

Methods of objects

- A complete list of an object's methods can be found using the `__dir__()` function:

```
1 motif.__dir__()
2 # long list of methods associated to
```