

# Python for scientific research

## Built-in data types

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  - Be **consistent** in your naming convention (see [PEP 8](#))
  - 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

- **Integers:** `int`

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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
```

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

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1 sequence = "AATCAGTT" # DNA sequence
2 type(sequence) # str
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4 sequence = 123456 # a numerical sequence
5 type(sequence) # int
```

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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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```

# Container data types

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

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1 # Interesting genes
2 geneNames = ["Irf1", "Ccl3", "Il12rb1", "Ifng", "Cxc110"]
3 type(geneNames) # list
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5 # Get elements of list
6 geneNames[0] # "Irf1"
7 geneNames[-1] # "Cxc110"
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```

- **Tuples:** tuple for an *immutable* collection of values

```
1 # Interesting genes
2 geneNames = ("Irf1", "Ccl3", "Il12rb1", "Ifng", "Cxc110")
3 type(geneNames) # tuple
```

# Initializing a single element tuple

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

```
1 singleElementT = ("Irf1")  
2 type(singleElementT) # str, not a tuple!
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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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1 # Sets are mutable collections of unique values
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5 # Frozensets are immutable collections of unique values
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```

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

```
1 # Create immutable sequence of numbers from 0 to 4
2 x = range(5)
3 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
  assignment
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1 geneTuple = ("Irf1", "Ccl3", "Il12rb1") # immutable
2 geneTuple[0]="Irf2"
3 TypeError: 'tuple' object does not support item
  assignment
```

- 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")
```



# Why ever use immutable objects?

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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

# Making copies of objects

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- Let us copy an `int`:

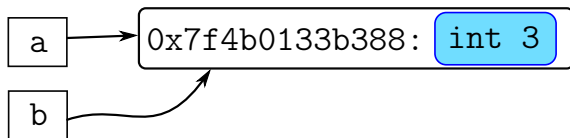
```
1 a = 3
2 b = a # copy of a
```

# Making copies of objects

- In Python, copies are made by *reference*, not by *value*
- Let us copy an `int`:

```
1 a = 3  
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

- So if we assign a new value to `a`, will `b` change too? No:

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

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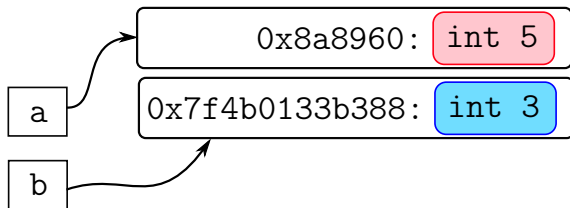
- What happens is that `a` is assigned a reference to a new position (0x8a8960) containing 5
- While `b` keeps its reference to the old position (containing 3)

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- What happens is that `a` is assigned a reference to a new position (0x8a8960) containing 5
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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)?

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

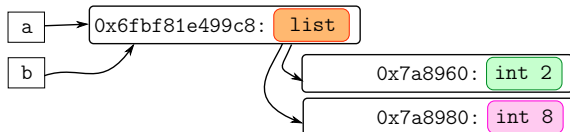


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1 a = [2,8] # list with two ints
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```

- 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!

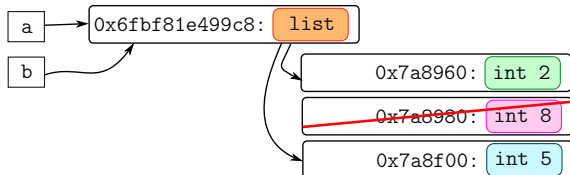
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1 a[1] = 5
2 print(a) # [ 2, 5]
3 print(b) # [ 2, 5]
```

# 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]
```

- 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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```
1 a = [1,2]
2 b = a[:] # go through all elements of a and assign to b
3 a[0] = 5
4 print(a) # [5,2]
5 print(b) # [1,2]: deep copy unaffected
```

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- If you want to change elements only of the copied variable or not the original (but not both), make a *deep* copy:

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

3 a[0] = 5
4 print(a) # [5,2]
5 print(b) # [1,2]: deep copy unaffected
6
7 # alternatively, use the copy module
8 import copy
9
10 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"
```

- 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
```