

Practical Computing for Scientists

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Python Basics

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14

32-bit integer
(on most machines)



14	32-bit integer
	(on most machines)
14.0	64-bit float
	(ditto)



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	(on most machines)
14.0	64-bit float
	(ditto)
1+4j	complex number
	(two 64-bit floats)



14	32-bit integer
	(on most machines)
14.0	64-bit float
	(ditto)
1+4j	complex number
	(two 64-bit floats)
x.real, x.imag	real and imaginary parts of complex number







Addition	+	35 + 22	57
		'Py' + 'thon'	'Python'



Addition	+	35 + 22	57
		'Py' + 'thon'	'Python'
Subtraction	_	35 - 22	13



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Multiplication	*	3 * 2	6



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Division	/	3.0 / 2	1.5



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		3 / 2	2.x: 1 3.x: 1.5



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Exponentiation	**	2 ** 0.5	1.41421356



Addition	+	35 + 22	57
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Multiplication	*	3 * 2	6
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Division	/	3.0 / 2	1.5
		3 / 2	2.x: 1 3.x: 1.5
Exponentiation	**	2 ** 0.5	1.41421356
Remainder	010	13 % 5	3





```
>>> years = 500
```

>>>



```
>>> years = 500
>>> years += 1
>>>
```





```
>>> years = 500
>>> years += 1
>>> print(years)
501
>>>
```



```
>>> years = 500
>>> years += 1
>>> print(years)
501
>>> years %= 10
>>>
```



```
>>> years = 500
>>> years += 1
>>> print(years)
501
>>> years %= 10 	— The same as years = years % 10
>>>
```



```
>>> years = 500
>>> years += 1
>>> print(years)
501
>>> years %= 10
>>> print(years)
1
>>>
```





3 < 5

True



3 < 5	True
3 != 5	True



3 < 5	True
3 != 5	True
3 == 5	False



3 < 5	True	
3 != 5	True	Single = is assignment
3 == 5	False	←
	ı	Double == is equality



3 < 5	True
3 != 5	True
3 == 5	False
3 >= 5	False



3 < 5	True
3 != 5	True
3 == 5	False
3 >= 5	False
1 < 3 < 5	True



3 < 5	True	
3 != 5	True	-
3 == 5	False	•
3 >= 5	False	-
1 < 3 < 5	True	But please don't do this
1 < 5 > 3	True	



3 < 5	True
3 != 5	True
3 == 5	False
3 >= 5	False
1 < 3 < 5	True
1 < 5 > 3	True
3+2j < 5	error





Python Control Flow

by Greg Wilson

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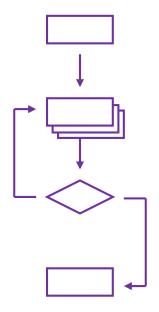
Real power of programs comes from:



repetition

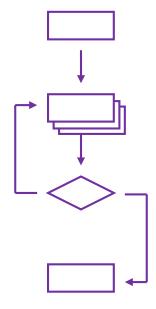


repetition



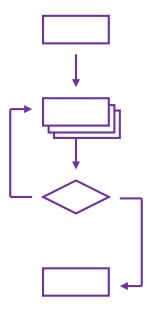


repetition selection

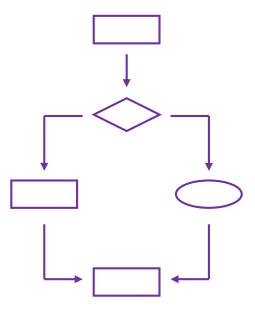




repetition

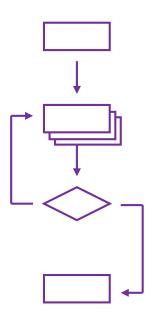


selection





Repetition







```
num_moons = 3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
```



```
num_moons = 3
while num_moons > 0: ← test
    print(num_moons)
    num moons -= 1
```



```
num_moons = 3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
do
```



```
num_moons = 3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
3
```



```
num_moons = 3
while num_moons > 0: ← test again
    print(num_moons)
    num_moons -= 1
3
```



```
num_moons = 3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
3
2
```



```
num_moons = 3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
3
2
1
```





```
print('before')
num_moons = -3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
print('after')
```



```
print('before')
num_moons = -3
while num_moons > 0:  not true when first tested...
    print(num_moons)
    num_moons -= 1
print('after')
```



```
print('before')
num_moons = -3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
print('after')
...so this is never executed
```



```
print('before')
num_moons = -3
while num_moons > 0:
    print(num_moons)
    num_moons -= 1
print('after')
before
after
```



```
print('before')
num moons = -3
while num moons > 0:
    print(num moons)
    num moons -= 1
print('after')
before
after
  Important to consider this case when designing
  and testing code
```





```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
```



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
```



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
```



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
3
```



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
3
3
```



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
3
3
::
```





```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
3
3
:
```

Usually not the desired behavior...



```
print('before')
num_moons = 3
while num_moons > 0:
    print(num_moons)
print('after')
before
3
3
3
::
```

Usually not the desired behavior...

...but there are cases where it's useful





Studies show that's what people actually pay attention to



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Every textbook on C or Java has examples where indentation and braces don't match



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Doesn't matter how much you use, but whole block must be consistent



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Python Style Guide (PEP 8) recommends 4 spaces



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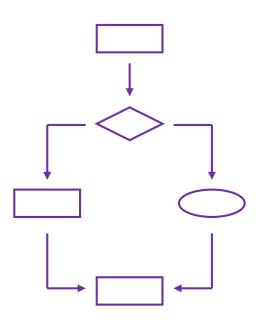
Every textbook on C or Java has examples where indentation and braces don't match

Doesn't matter how much you use, but whole block must be consistent

Python Style Guide (PEP 8) recommends 4 spaces And no tab characters



Selection







```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')</pre>
```













```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater') \leftarrow ...so this is executed</pre>
```



```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')
greater</pre>
```



```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')
greater</pre>
```

Always start with if



```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')
greater</pre>
```

Always start with **if**

Can have any number of **elif** clauses (including none)



```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')
greater</pre>
```

Always start with **if**

Can have any number of **elif** clauses (including none)

And the **else** clause is optional



```
moons = 3
if moons < 0:
    print('less')
elif moons == 0:
    print('equal')
else:
    print('greater')
greater</pre>
```

Always start with **if**

Can have any number of elif clauses (including none)

And the **else** clause is optional

Always tested in order





```
num = 0
while num <= 10:
    if (num % 2) == 1:
        print(num)
    num += 1</pre>
```







```
num = 0
while num <= 10:
    if (num % 2) == 1:
        print(num)
    num += 1

1
3
5
7
9</pre>
```



A better way to do it



A better way to do it

```
num = 1
while num <= 10:
    print(num)
    num += 2</pre>
```



A better way to do it

```
num = 1
while num <= 10:
    print(num)
    num += 2
1
3
5
7
9</pre>
```



Writing a simple program that works,



Writing a simple program that works, then tweaking it to make it more efficient,



Writing a simple program that works, then tweaking it to make it more efficient, is a common pattern in programming.



Writing a simple program that works, then tweaking it to make it more efficient, is a common pattern in programming.

Another is to write programs top-down,



Writing a simple program that works, then tweaking it to make it more efficient, is a common pattern in programming.

Another is to write programs *top-down*, solving one problem at a time.





```
num = 2
while num <= 1000:
    ...figure out if num is prime...
if is_prime:
    print(num)
num += 1</pre>
```



```
num = 2
while num <= 1000:
    ...figure out if num is prime...
if is_prime:
    print(num)
num += 1</pre>
```

Cannot be evenly divided by any other integer



```
num = 2
while num <= 1000:
    ...figure out if num is prime...
    if is prime:
         print(num)
    num += 1
                      is prime = True
                      trial = 2
                      while trial < num:</pre>
                           if ...num divisible by trial...:
                               is prime = False
                           trial += 1
```



```
num = 2
while num <= 1000:
    ...figure out if num is prime...
    if is prime:
         print(num)
                                   Remainder is zero
    num += 1
                      is prime = True
                      trial = 2
                      while trial < num:</pre>
                           if ...num divisible by trial...:
                               is prime = False
                           trial += 1
```



```
n_{11}m = 2
while num <= 1000:
    ...figure out if num is prime...
    if is prime:
         print(num)
                                    (num % trial) == 0
    num += 1
                      is prime = True
                      trial = 2
                      while trial < num:</pre>
                           if ...num divisible by trial...:
                                is prime = False
                           trial += 1
```



```
num = 2
while num <= 1000:
    is prime = True
    trial = 2
    while trial < num:</pre>
        if (num % trial) == 0:
             is prime = False
        trial += 1
    if is prime:
        print(num)
    num += 1
```



Print primes less than 1000 (more efficient version)



Print primes less than 1000 (more efficient version)

```
num = 2
while num <= 1000:
    is prime = True
    trial = 2
    while trial**2 < num:</pre>
        if (num % trial) == 0:
             is prime = False
        trial += 1
    if is prime:
        print(num)
    num += 1
```



Print primes less than 1000 (more efficient version)

```
num = 2
while num <= 1000:
    is prime = True
    trial = 2
                                  testing whether n is
    while trial**2 < num:←
        if (num % trial) == 0:
                                   multiple of any integer
             is prime = False
        trial += 1
                                   between 2 and \sqrt{n}
    if is prime:
        print(num)
    num += 1
```





```
num = 2
while num <= [10]:
    is prime = True
    trial = 2
    while trial**2 < num:</pre>
         if (num % trial) == 0:
             is prime = False
         trial += 1
    if is prime:
        print(num)
    num += 1
```



```
num = 2
while num <= 10:
    is prime = True
    trial = 2
    while trial**2 < num:</pre>
        if (num % trial) == 0:
             is prime = False
        trial += 1
    if is prime:
        print(num)
    num += 1
```



```
num = 2
while num <= 10:
    is prime = True
    trial = 2
    while trial**2 < num:</pre>
        if (num % trial) == 0:
             is prime = False
        trial += 1
    if is prime:
        print(num)
    num += 1
```



```
num = 2
while num <= 10:
    is prime = True
    trial = 2
    while trial **2 < num:
        if (num % trial) == 0:
            is prime = False
        trial += 1
    if is prime:
        print(num)
    num += 1
```

Where's the bug?







Python Lists

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Loops let us do things many times



Loops let us do things many times

Collections let us store many values together



Loops let us do things many times

Collections let us store many values together

Most popular collection is a list



Create using [value, value, ...]



Create using [value, value, ...]

Get/set values using var[index]



Create using [value, value, ...]
Get/set values using var[index]

gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases)
['He', 'Ne', 'Ar', 'Kr']



```
Create using [value, value, ...]

Get/set values using var[index]

gases = ['He', 'Ne', 'Ar', 'Kr']

print(gases)
['He', 'Ne', 'Ar', 'Kr']

print(gases[1])

Ne
```





Reasons made sense for C in 1970...



Reasons made sense for C in 1970...

It's an error to try to access out of range



Reasons made sense for C in 1970...

It's an error to try to access out of range

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases[4])
```

IndexError: list index out of range



Use len(list) to get length of list



Use len(list) to get length of list

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
4
```



```
Use len(list) to get length of list

gases = ['He', 'Ne', 'Ar', 'Kr']

print(len(gases))

4

Returns 0 for the empty list

etheric = []

print(len(etheric))

0
```



Some negative indices work



Some negative indices work values[-1] is last element, values[-2] next-to-last, ...



Some negative indices work values[-1] is last element, values[-2] next-to-last, ...

```
gases = ['He', 'Ne', 'Ar', 'Kr']
```



Some negative indices work values[-1] is last element, values[-2] next-to-last, ...

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases[-1], gases[-4])
Kr He
```



Some negative indices work

values[-1] is last element, values[-2] next-to-last, ...

gases = ['He', 'Ne', 'Ar', 'Kr']

print(gases[-1], gases[-4])

Kr He

values[-1] is much nicer than values[len(values)-1]



```
Some negative indices work
  values[-1] is last element, values[-2] next-to-last, ...
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases[-1], gases[-4])
Kr He
  values[-1] is much niser than values[len(values)-1]
                  less error prone
```





```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
```



```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
gases[3] = 'Kr'
```



```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
gases[3] = 'Kr'
print(gases)
['He', 'Ne', 'Ar', 'Kr']
```



```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
gases[3] = 'Kr'
print(gases)
['He', 'Ne', 'Ar', 'Kr']
```

Location must exist before assignment



```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
gases[3] = 'Kr'
print(gases)
['He', 'Ne', 'Ar', 'Kr']
```

Location must exist before assignment

```
gases = ['He', 'Ne', 'Ar', 'Kr']
```



```
gases = ['He', 'Ne', 'Ar', 'K'] # last entry misspelled
gases[3] = 'Kr'
print(gases)
['He', 'Ne', 'Ar', 'Kr']
```

Location must exist before assignment

```
gases = ['He', 'Ne', 'Ar', 'Kr']
gases[4] = 'Xe'
```

IndexError: list assignment index out of range



Heterogeneous: can store values of many kinds



Heterogeneous: can store values of many kinds

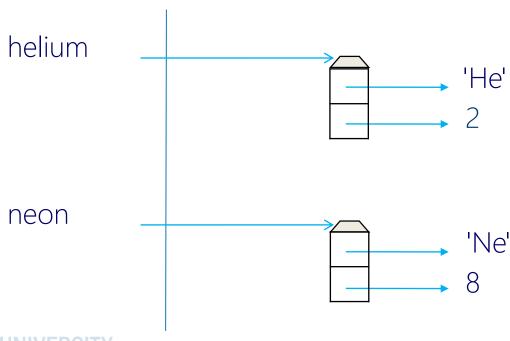
```
helium = ['He', 2]
neon = ['Ne', 8]
```



Heterogeneous: can store values of many kinds

```
helium = ['He', 2]
neon = ['Ne', 8] [string, int]
```



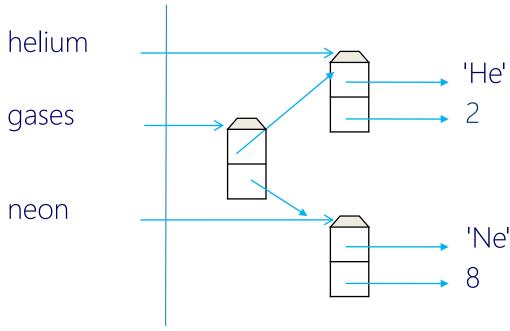




```
helium = ['He', 2]
neon = ['Ne', 8]
gases = [helium, neon]
```

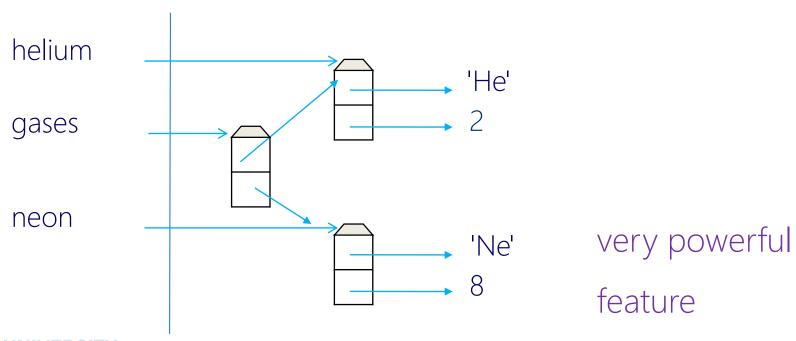


```
helium = ['He', 2]
neon = ['Ne', 8]
gases = [helium, neon]
```





```
helium = ['He', 2]
neon = ['Ne', 8]
gases = [helium, neon]
```







Loop over elements to "do all"

Use while to step through all possible indices



```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
while i < len(gases):
    print(gases[i])
    i += 1</pre>
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
First legal index
while i < len(gases):
    print(gases[i])
    i += 1</pre>
```





```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
while i < len(gases) Defines set of legal indices
    print(gases[i])
i += 1</pre>
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
while i < len(gases):
    print(gases[i])
    i += 1
He
Ne
Ar
Kr</pre>
```



Use while to step through all possible indices

```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
while i < len(gases):
    print(gases[i])
    i += 1
He
Ne
Ar
Kr</pre>
```

Tedious to type in over and over again



Use while to step through all possible indices

```
gases = ['He', 'Ne', 'Ar', 'Kr']
i = 0
while i < len(gases):
    print(gases[i])
    i += 1
He
Ne
Ar
Kr</pre>
```

Tedious to type in over and over again

And it's easy to forget the "+= 1" at the end

Use a for loop to access each value in turn



Use a for loop to access each value in turn

```
gases = ['He', 'Ne', 'Ar', 'Kr']
for gas in gases:
    print(gas)
He
Ne
Ar
Kr
```



Use a for loop to access each value in turn

```
gases = ['He', 'Ne', 'Ar', 'Kr']
for gas in gases:
    print(gas)
He
Ne
Ar
Kr
```

Loop variable assigned each value in turn



```
Use a for loop to access each value in turn
```

```
gases = ['He', 'Ne', 'Ar', 'Kr']
for gas in gases:
    print(gas)
He
Ne
Ar
Kr
```

Loop variable assigned each value in turn

Not each index



```
Use a for loop to access each value in turn
gases = ['He', 'Ne', 'Ar', 'Kr']
for gas in gases:
    print(gas)
He
Ne
Ar
```

Loop variable assigned each value in turn

Not each index

Because that's the most common case



Kr



```
gases = ['He', 'Ne', 'Ar', 'Kr']
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
del gases[0]
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
del gases[0]
print(gases)
['Ne', 'Ar', 'Kr']
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
del gases[0]
print(gases)
['Ne', 'Ar', 'Kr']
del gases[2]
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
del gases[0]
print(gases)
['Ne', 'Ar', 'Kr']
del gases[2]
print(gases)
['Ne', 'Ar']
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
del gases[0]
print(gases)
['Ne', 'Ar', 'Kr']
del gases[2]
print(gases)
['Ne', 'Ar']
```

Yes, deleting an index that doesn't exist is an error





```
gases = []
```



```
gases = []
gases.append('He')
```



```
gases = []
gases.append('He')
gases.append('Ne')
```



```
gases = []
gases.append('He')
gases.append('Ne')
gases.append('Ar')
```



```
gases = []
gases.append('He')
gases.append('Ne')
gases.append('Ar')
print(gases)
['He', 'Ne', 'Ar']
```



```
gases = []
gases.append('He')
gases.append('Ne')
gases.append('Ar')
print(gases)
['He', 'Ne', 'Ar']
```

Most operations on lists are methods



```
gases = []
gases.append('He')
gases.append('Ne')
gases.append('Ar')
print(gases)
['He', 'Ne', 'Ar']
```

Most operations on lists are methods

A function that belongs to (and usually operates on) specific data



```
gases = []
gases.append('He')
gases.append('Ne')
gases.append('Ar')
print(gases)
['He', 'Ne', 'Ar']
```

Most operations on lists are methods

A function that belongs to (and usually operates on) specific data

thing . method (args)



Some useful list methods



Some useful list methods

```
gases = ['He', 'He', 'Ar', 'Kr'] # 'He' is duplicated
```



```
gases = ['He', 'He', 'Ar', 'Kr'] # 'He' is duplicated
print(gases.count('He'))
2
```



```
gases = ['He', 'He', 'Ar', 'Kr'] # 'He' is duplicated
print(gases.count('He'))
2
print(gases.index('Ar'))
2
```



```
gases = ['He', 'He', 'Ar', 'Kr'] # 'He' is duplicated
print(gases.count('He'))
2
print(gases.index('Ar'))
2
gases.insert(1, 'Ne')
```



```
gases = ['He', 'He', 'Ar', 'Kr'] # 'He' is duplicated
print(gases.count('He'))
2
print(gases.index('Ar'))
2
gases.insert(1, 'Ne')
print(gases)
['He', 'Ne', 'He', 'Ar', 'Kr']
```





Two that are often used incorrectly gases = ['He', 'Ne', 'Ar', 'Kr']



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
print(gases)
['Ar', 'He', 'Kr', 'Ne']
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
print(gases)
['Ar', 'He', 'Kr', 'Ne']
print(gases.reverse())
None
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
print(gases)
['Ar', 'He', 'Kr', 'Ne']
print(gases.reverse())
None
print(gases)
['Ne', 'Kr', 'He', 'Ar']
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
print(gases)
['Ar', 'He', 'Kr', 'Ne']
print(gases.reverse())
None
print(gases)
['Ne', 'Kr', 'He', 'Ar']
  A common bug
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(gases.sort())
None
print(gases)
['Ar', 'He', 'Kr', 'Ne']
print(gases.reverse())
None
print(gases)
['Ne', 'Kr', 'He', 'Ar']
  A common bug
  gases = gases.sort() assigns None to gases
```



Use **in** to test for membership



```
Use in to test for membership

gases = ['He', 'Ne', 'Ar', 'Kr']
```



Use in to test for membership

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print('He' in gases)
True
```



```
Use in to test for membership
```

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print('He' in gases)
True
if 'Pu' in gases:
    print('But plutonium is not a gas!')
else:
    print('The universe is well ordered.')
```



```
Use in to test for membership
```

```
gases = ['He', 'Ne', 'Ar', 'Kr']
print('He' in gases)
True
if 'Pu' in gases:
    print('But plutonium is not a gas!')
else:
    print('The universe is well ordered.')
The universe is well ordered.
```





```
print(range(5))
[0, 1, 2, 3, 4]
```



```
print(range(5))
[0, 1, 2, 3, 4]
print(range(2, 6))
[2, 3, 4, 5]
```



```
print(range(5))
[0, 1, 2, 3, 4]
print(range(2, 6))
[2, 3, 4, 5]
print(range(0, 10, 3))
[0, 3, 6, 9]
```



```
print(range(5))
[0, 1, 2, 3, 4]
print(range(2, 6))
[2, 3, 4, 5]
print(range(0, 10, 3))
[0, 3, 6, 9]
print(range(10, 0))
[]
```





gases = ['He', 'Ne', 'Ar', 'Kr']



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
4
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
4
print(range(len(gases)))
[0, 1, 2, 3]
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
4
print(range(len(gases)))
[0, 1, 2, 3]
for i in range(len(gases)):
    print(i, gases[i])
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
print(range(len(gases)))
[0, 1, 2, 3]
for i in range(len(gases)):
    print(i, gases[i])
0 He
1 Ne.
2 Ar
3 Kr
```



```
gases = ['He', 'Ne', 'Ar', 'Kr']
print(len(gases))
print(range(len(gases)))
[0, 1, 2, 3]
for i in range(len(gases)):
    print(i, gases[i])
0 He
1 Ne.
2 Ar
3 Kr
```

A very common idiom in Python

