Practical Computing for Scientists

Armin Sobhani
CSCI 2000U
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UNIVERSITY OF ONTARIO INSTITUTE OF TECHNOLOGY

Python

Input and Output

by Greg Wilson

UNIVERSITY OF ONTARIO INSTITUTE OF TECHNOLOGY

Been using print to see what programs are doing

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How to save data to files?

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How to save data to files?

And read data from them?

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Python's solution looks very much like C's

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And read data from them?

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- A file is a sequence of bytes

Been using print to see what programs are doing

How to save data to files?

And read data from them?

Python's solution looks very much like C's

- A file is a sequence of bytes
- But it's often more useful to treat it as a sequence of lines

Sample data file

Three things are certain:
Death, taxes, and lost data.
Guess which has occurred.

Errors have occurred.
We won't tell you where or why.
Lazy programmers.

With searching comes loss
and the presence of absence:
"My Thesis" not found.

A crash reduces
your expensive computer
to a simple stone.

How many characters in a file?

How many ~~characters~~ in a file?

bytes

How many ~~characters~~ in a file?

bytes

Assume each character is one byte for now

How many ~~characters~~ in a file?

bytes

Assume each character is one byte for now

Revisit later

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Create a file object

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

File to connect to

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

To read

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Now holds file object

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Read entire content of file into a string

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Now has a copy of all the bytes that were in the file

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Disconnect from the file

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Disconnect from the file

Not strictly necessary in small programs, but good practice

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Report how many characters were read

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

Report how many ~~characters~~ were read

bytes

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
```

How many characters in a file?

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
print(len(data))
293
```

If the file might be large, better to read in chunks

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
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print(len(data))
reader.close()
```

Read (at most) 64 bytes

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

Read (at most) 64 bytes

Or the empty string

if there is no more data

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

Keep looping as long as the last read returned some data

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

Do something with the data

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

(Try to) reload

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

Should be 0 (or the loop would still be running)

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

```
64
64
64
64
37
0
```

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

```
64
64
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0
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Don't do this unless

If the file might be large, better to read in chunks

```
reader = open('haiku.txt', 'r')
data = reader.read(64)
while data != '':
    print(len(data))
    data = reader.read(64)
print(len(data))
reader.close()
```

```
64
64
64
64
37
0
```

Don't do this unless the file really might be very large (or infinite)

More common to read one line at a time

More common to read one line at a time

```
reader = open('haiku.txt', 'r')
line = reader.readline()
total = 0
count = 0
while line != '':
    count += 1
    total += len(line)
    line = reader.readline()
reader.close()
print('average', total / count)
```

More common to read one line at a time

```
reader = open('haiku.txt', 'r')
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total = 0
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print('average', total / count)
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Read a single line

More common to read one line at a time

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line = reader.readline()
total = 0
count = 0
while line != '':
    count += 1
    total += len(line)
    line = reader.readline()
reader.close()
print('average', total / count)
```

Keep looping until no more lines in file

More common to read one line at a time

```
reader = open('haiku.txt', 'r')
line = reader.readline()
total = 0
count = 0
while line != '':
    count += 1
    total += len(line)
    line = reader.readline()
reader.close()
print('average', total / count)
```

(Try to) reload

More common to read one line at a time

```
reader = open('haiku.txt', 'r')
line = reader.readline()
total = 0
count = 0
while line != '':
    count += 1
    total += len(line)
    line = reader.readline()
reader.close()
print('average', total / count)
average 19.53333333
```

Often more convenient to read all lines at once

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```
reader = open('haiku.txt', 'r')
contents = reader.readlines()
reader.close()
total = 0
count = 0
for line in contents:
    count += 1
    total += len(line)
print('average', total / count)
```

Often more convenient to read all lines at once

```
reader = open('haiku.txt', 'r')
contents = reader.readlines()
reader.close()
total = 0
count = 0
for line in contents:
    count += 1
    total += len(line)
print('average', total / count)
```

All lines in file
as list of strings

Often more convenient to read all lines at once

```
reader = open('haiku.txt', 'r')
contents = reader.readlines()
reader.close()
total = 0
count = 0
for line in contents:
    count += 1
    total += len(line)
print('average', total / count)
```

Loop over lines with **for**

Often more convenient to read all lines at once

```
reader = open('haiku.txt', 'r')
contents = reader.readlines()
reader.close()
total = 0
count = 0
for line in contents:
    count += 1
    total += len(line)
print('average', total / count)
average 19.53333333
```

"Read lines as list" + "loop over list" is common idiom

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```
reader = open('haiku.txt', 'r')
total = 0
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for line in reader:
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print('average', total / count)
```

"Read lines as list" + "loop over list" is common idiom

So Python provides "loop over lines in file"

```
reader = open('haiku.txt', 'r')
total = 0
count = 0
for line in reader:
    count += 1
    total += len(line)
reader.close()
print('average', total / count)
```

Assign lines of text in file to loop variable one by one

"Read lines as list" + "loop over list" is common idiom

So Python provides "loop over lines in file"

```
reader = open('haiku.txt', 'r')
total = 0
count = 0
for line in reader:
    count += 1
    total += len(line)
reader.close()
print('average', total / count)
average 19.53333333
```

Put data in a file using `write` or `writelines`

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

Same function

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

File to write to

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

File to write to

Created if it doesn't exist

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

For writing instead of reading

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

Write a single string

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

Write each string in a list

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

```
elementsHeNeArKr
```

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements')
writer.writelines(['He', 'Ne', 'Ar', 'Kr'])
writer.close()
```

```
elementsHeNeArKr
```

Python only writes what you tell it to

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements\n')
writer.writelines(['He\n', 'Ne\n', 'Ar\n', 'Kr\n'])
writer.close()
```

Have to provide end-of-line characters yourself

Put data in a file using `write` or `writelines`

```
writer = open('temp.txt', 'w')
writer.write('elements\n')
writer.writelines(['He\n', 'Ne\n', 'Ar\n', 'Kr\n'])
writer.close()
```

```
elements
He
Ne
Ar
Kr
```

Often simpler to use `print(args, file=f1)`

Often simpler to use `print(args, file=f1)`

```
writer = open('temp.txt', 'w')
print('elements', file=writer)
for gas in ['He', 'Ne', 'Ar', 'Kr']:
    print(gas, file=writer)
writer.close()
```

Often simpler to use `print(args, file=f1)`

```
writer = open('temp.txt', 'w')
print('elements', file=writer)
for gas in ['He', 'Ne', 'Ar', 'Kr']:
    print(gas, file=writer)
writer.close()
```

Specify open file after

Often simpler to use `print(args, file=f1)`

```
writer = open('temp.txt', 'w')
print('elements', file=writer)
for gas in ['He', 'Ne', 'Ar', 'Kr']:
    print(gas, file=writer)
writer.close()
```

`print` automatically adds the newline

For python 2.x use `print >> f1, args .`

In Python 3.0+, `print(args, file=f1)`

print is a function, which you'd call with `print(...)`

Copy a file

Copy a file

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
writer = open('temp.txt', 'w')
write.write(data)
writer.close()
```

Copy a file

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
writer = open('temp.txt', 'w')
write.write(data)
writer.close()
```

Read all

Copy a file

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
writer = open('temp.txt', 'w')
write.write(data)
writer.close()
```

Write all

Copy a file

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
writer = open('temp.txt', 'w')
write.write(data)
writer.close()
```

Probably won't work with a terabyte…

Copy a file

```
reader = open('haiku.txt', 'r')
data = reader.read()
reader.close()
writer = open('temp.txt', 'w')
write.write(data)
writer.close()
```

Probably won't work with a terabyte...

...but we probably don't care

Copy a file (version 2)

Copy a file (version 2)

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    writer.write(line)
reader.close()
writer.close()
```

Copy a file (version 2)

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    writer.write(line)
reader.close()
writer.close()
```

Assumes the file is text

Copy a file (version 2)

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    writer.write(line)
reader.close()
writer.close()
```

Assumes the file is text

Or at least that the end-of-line character appears frequently

This version doesn't make an exact copy

This version doesn't make an exact copy

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    print(line, file=writer)
reader.close()
writer.close()
```

This version doesn't make an exact copy

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    print(line, file=writer)
reader.close()
writer.close()
```

Python keeps the newline when reading

This version doesn't make an exact copy

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    print(line, file=writer)
reader.close()
writer.close()
```

Python keeps the newline when reading

print automatically adds a newline

This version doesn't make an exact copy

```
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
for line in reader:
    print(line, file=writer)
reader.close()
writer.close()
```

Python keeps the newline when reading

print automatically adds a newline

Result is double-spaced output

Copy a file (version 3)

Copy a file (version 3)

```
BLOCKSIZE = 1024
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
data = reader.read(BLOCKSIZE)
while len(data) > 0:
    writer.write(data)
    data = reader.read(BLOCKSIZE)
reader.close()
writer.close()
```

Copy a file (version 3)

```
BLOCKSIZE = 1024
reader = open('haiku.txt', 'r')
writer = open('temp.txt', 'w')
data = reader.read(BLOCKSIZE)
while len(data) > 0:
    writer.write(data)
    data = reader.read(BLOCKSIZE)
reader.close()
writer.close()
```

(Needlessly?) harder to understand

Python

Strings

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Strings are sequences of characters

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No separate character type: just a string of length 1

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No separate character type: just a string of length 1

Indexed exactly like lists

Strings are sequences of characters

No separate character type: just a string of length 1

Indexed exactly like lists

```
name = 'Darwin'
print(name[0], name[-1])
D n
```

`for` iterates through characters

for iterates through characters

```
name = 'Darwin'
for c in name:
    print(c)
```

```
D
a
r
w
i
n
```

Use either ' or " (as long as they match)

Use either ' or " (as long as they match)

```
print('Alan', "Turing“)
Alan Turing
```

Use either ' or " (as long as they match)

```
print('Alan', "Turing“)
Alan Turing
```

Strings are the same no matter how they're created

Use either ' or " (as long as they match)

```
print('Alan', "Turing“)
Alan Turing
```

Strings are the same no matter how they're created

```
print 'Alan' == "Alan"
True
```

Strings are compared character by character from left to right

Strings are compared character by character from left to right

```
print('a' < 'b')
True
```

Strings are compared character by character from left to right

```
print('a' < 'b')
True
print('ab' < 'abc')
True
```

Strings are compared character by character from left to right

```
print('a' < 'b')
True
print('ab' < 'abc')
True
print('1' < '9')
True
```

Strings are compared character by character from left to right

```
print('a' < 'b')
True
print('ab' < 'abc')
True
print('1' < '9')
True
print('100' < '9')
True
```

Strings are compared character by character from left to right

```
print('a' < 'b')
True
print('ab' < 'abc')
True
print('1' < '9')
True
print('100' < '9')
True
print('A' < 'a')
True
```

Strings are immutable : cannot be changed in place

Strings are immutable : cannot be changed in place

```
name = 'Darwin'
name[0] = 'C'
TypeError: 'str' object does not support item assignment
```

Strings are immutable : cannot be changed in place

```
name = 'Darwin'
name[0] = 'C'
TypeError: 'str' object does not support item assignment
```

Immutability improves performance

Strings are immutable : cannot be changed in place

```
name = 'Darwin'
name[0] = 'C'
TypeError: 'str' object does not support item assignment
```

Immutability improves performance

See later how immutability improves programmers' performance

Use + to concatenate strings

Use + to concatenate strings

```
name = 'Charles' + ' ' + 'Darwin'
print(name)
Charles Darwin
```

Use + to concatenate strings

```
name = 'Charles' + ' ' + 'Darwin'
print(name)
Charles Darwin
```

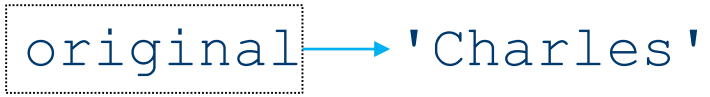
Concatenation always produces a new string

Use + to concatenate strings

```
name = 'Charles' + ' ' + 'Darwin'
print(name)
Charles Darwin
```

Concatenation always produces a new string

```
original = 'Charles'
```

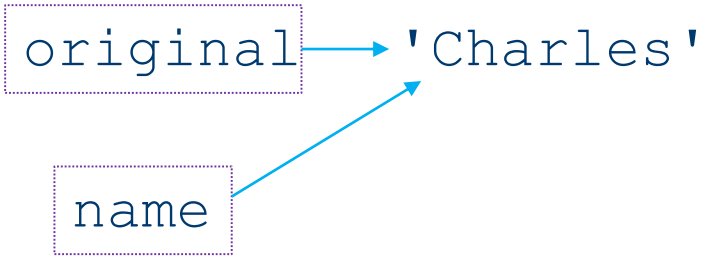


Use + to concatenate strings

```
name = 'Charles' + ' ' + 'Darwin'
print(name)
Charles Darwin
```

Concatenation always produces a new string

```
original = 'Charles'
name = original
```

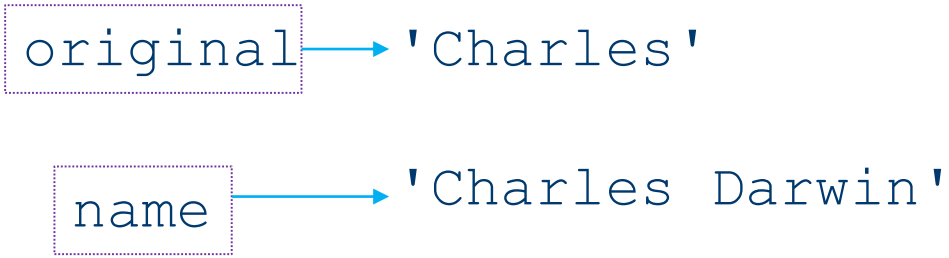


Use + to concatenate strings

```
name = 'Charles' + ' ' + 'Darwin'
print(name)
Charles Darwin
```

Concatenation always produces a new string

```
original = 'Charles'
name = original
name += ' Darwin'
```



Often used to format output

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```
print('reagant: ' + str(reagant_id) + ' produced ' +
      str(percentage_yield) + '% yield')
```

Often used to format output

```
print('reagant: ' + str(reagant_id) + ' produced ' +
      str(percentage_yield) + '% yield')
```

There's a better way…

Use string % value to format output

Use string % value to format output

```
output = 'reagant: %d' % 123
print(output)
reagant: 123
```

Use string % value to format output

```
output = 'reagant: %d' % 123
print(output)
reagant: 123
```

```
percentage_yield = 12.3
print('yield: %6.2f' % percentage_yield)
yield:  12.30
```

And string `% (v1, v2, ...)` for multiple values

And string `% (v1, v2, ...)` for multiple values

```
reagant_id = 123
percentage_yield = 12.3
print('reagant: %d produced %6.2f%% yield' %
      (reagant_id, percentage_yield))
reagant: 123 produced  12.30% yield
```

And string `% (v1, v2, ...)` for multiple values

```
reagant_id = 123
percentage_yield = 12.3
print('reagant: %d produced %6.2f%% yield' %
      (reagant_id, percentage_yield))
reagant: 123 produced  12.30% yield
```

`%` operator turns double '`%%`' into single '`%`'

Use `\n` to represent a newline character

Use `\n` to represent a newline character

Use `\'` for single quote, `\"` for double quote

Use `\n` to represent a newline character

Use `\'` for single quote, `\"` for double quote

```
print('There isn\'t time\nto do it right.')
There isn't time
to do it right.
```

Use `\n` to represent a newline character

Use `\'` for single quote, `\"` for double quote

```
print('There isn\'t time\nto do it right.')
There isn't time
to do it right.
```

```
print("But you said,\n\"There is time to do it over.\"")
But you said,
"There is time to do it over."
```

Use \\ for a literal \ character

Use \\ for a literal \ character

```
print('Most mathematicians write a\\b instead of a%b.')
```

Most mathematicians write a\b instead of a%b.

Use \\ for a literal \ character

```
print('Most mathematicians write a\\b instead of a%b.')
Most mathematicians write a\b instead of a%b.
```

Common pattern with escape sequences

Use \\ for a literal \ character

```
print('Most mathematicians write a\\b instead of a%b.')
Most mathematicians write a\b instead of a%b.
```

Common pattern with escape sequences

- Use a character to mean "what follows is special"

Use \\ for a literal \ character

```
print('Most mathematicians write a\\b instead of a%b.')
Most mathematicians write a\b instead of a%b.
```

Common pattern with escape sequences

- Use a character to mean "what follows is special"
- Double it up to mean "that character itself"

Use triple quotes (either kind) for multi-line strings

Use triple quotes (either kind) for multi-line strings

```
quote = '''We can only see
a short distance ahead,
but we can see plenty there
that needs to be done.'''
```

Use triple quotes (either kind) for multi-line strings

```
quote = '''We can only see
a short distance ahead,
but we can see plenty there
that needs to be done.'''
```

Use triple quotes (either kind) for multi-line strings

```
quote = '''We can only see
a short distance ahead,
but we can see plenty there
that needs to be done.'''


quote = 'We can only see\na short distance ahead,\n'
        + 'but we can see plenty there\nthat needs
        to be done.'
```

Strings have methods

Strings have methods

```
name = 'newTON'
print(name.capitalize(), name.upper(), name.lower(), name)
Newton NEWTON newton newTON
```

Strings have methods

```
name = 'newTON'
print(name.capitalize(), name.upper(), name.lower(), name)
Newton NEWTON newton newTON
dna = 'acggtggtcac'
print(dna.count('g'), dna.count('x'))
4 0
```

Strings have methods

```
name = 'newTON'
print(name.capitalize(), name.upper(), name.lower(), name)
Newton NEWTON newton newTON
dna = 'acggtggtcac'
print(dna.count('g'), dna.count('x'))
4 0
print(dna.find('t'), dna.find('t', 5), dna.find('x'))
4 7 -1
```

Strings have methods

```
name = 'newTON'
print(name.capitalize(), name.upper(), name.lower(), name)
Newton NEWTON newton newTON
dna = 'acggtggtcac'
print(dna.count('g'), dna.count('x'))
4 0
print(dna.find('t'), dna.find('t', 5), dna.find('x'))
4 7 -1
print(dna.replace('t', 'x'), dna)
acggxggxcac acggtggtcac
```

Strings have methods

```
name = 'newTON'
print(name.capitalize(), name.upper(), name.lower(), name)
Newton NEWTON newton newTON
dna = 'acggtggtcac'
print(dna.count('g'), dna.count('x'))
4 0
print(dna.find('t'), dna.find('t', 5), dna.find('x'))
4 7 -1
print(dna.replace('t', 'x'), dna)
acggxggxcac acggtggtcac
print(dna.replace('gt', ''))
acggcac
```

Can chain method calls together

Can chain method calls together

```
element = 'cesium'
print(element.upper().center(10, '.'))
```

Can chain method calls together

```
element = 'cesium'
print(element.upper().center(10, '.'))
```

convert to upper case

Can chain method calls together

```
element = 'cesium'
print(element.upper().center(10, '.'))
```

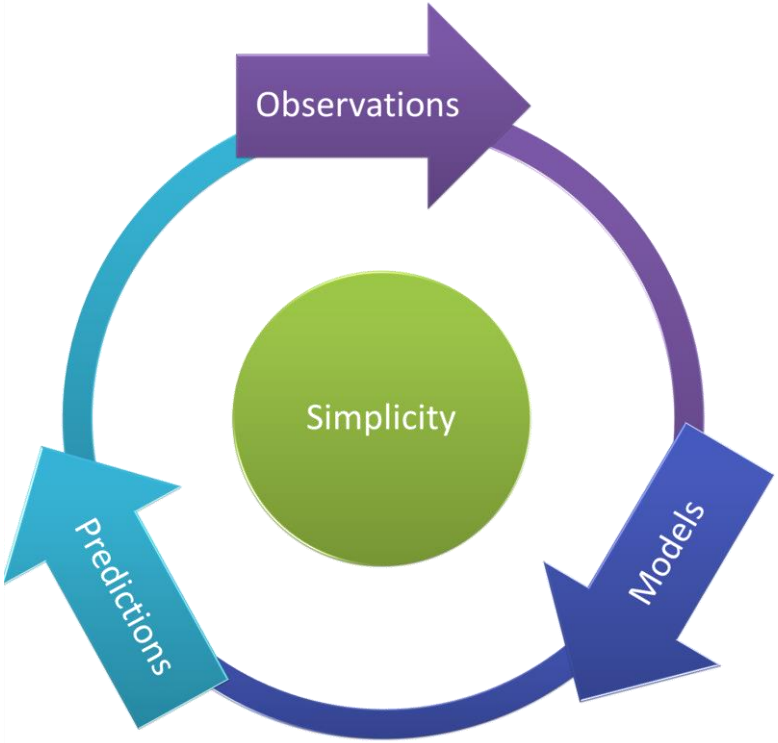
center in a field 10 characters wide

Can chain method calls together

```
element = 'cesium'
print(element.upper().center(10, '.'))
..CESIUM..
```

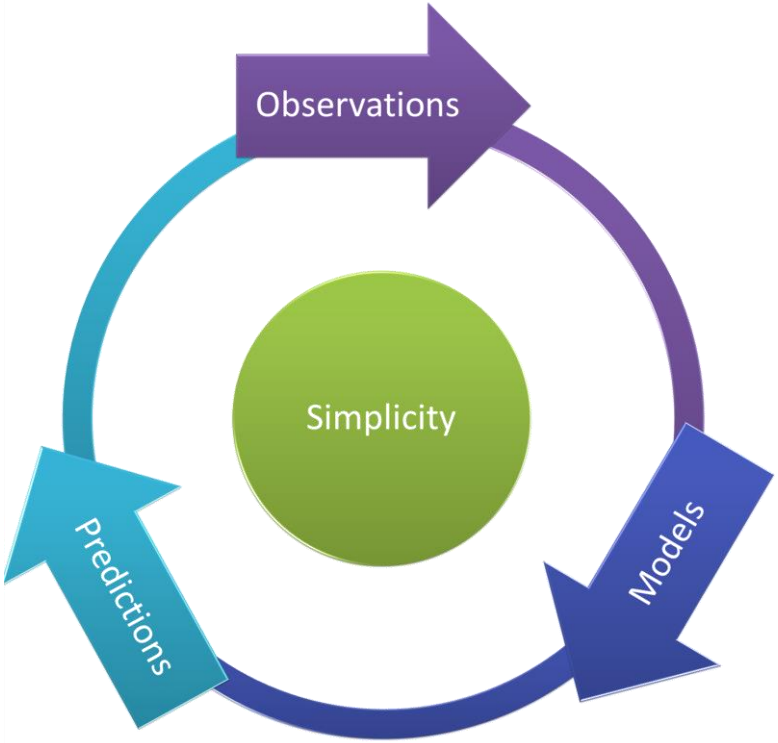
Scientific Method

- Begin with a set of observations



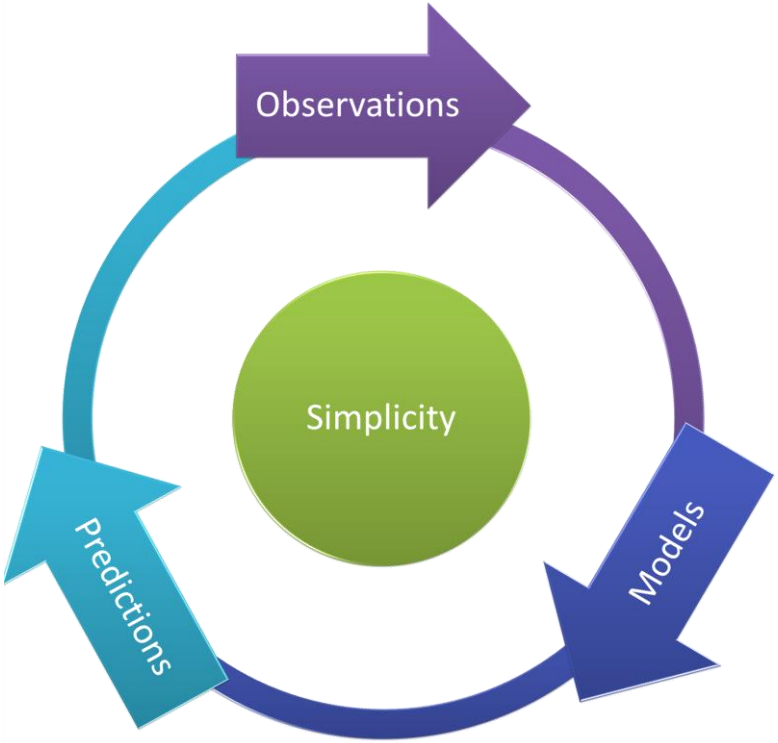
Scientific Method

- Begin with a set of observations
- Create a model to explain the observations



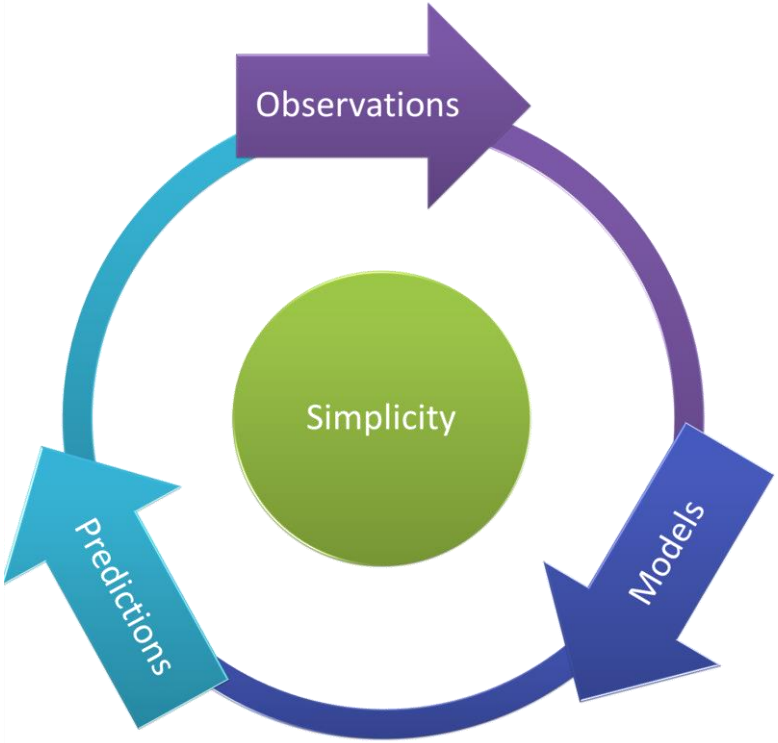
Scientific Method

- Begin with a set of observations
- Create a model to explain the observations
- Make testable predictions using the model



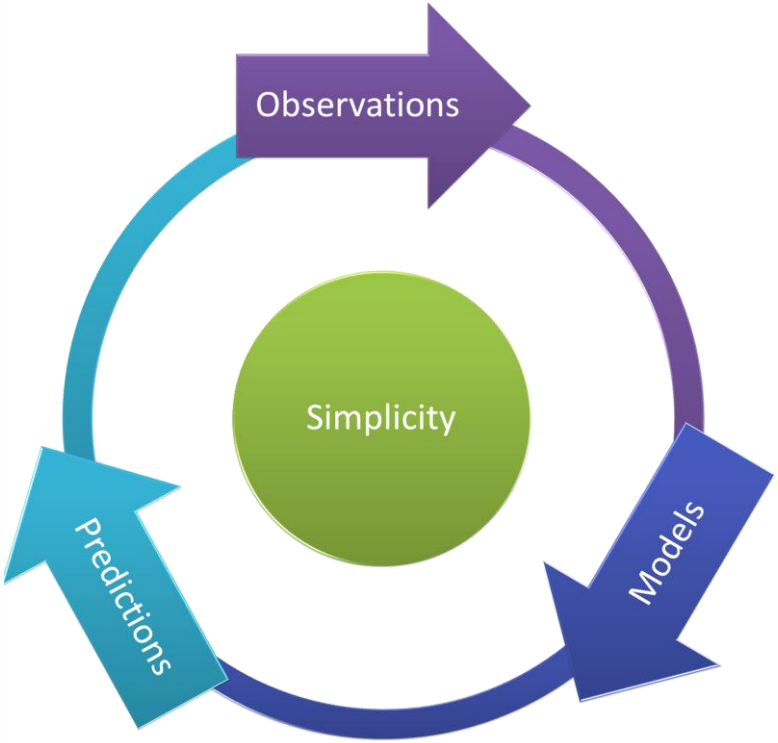
Scientific Method

- Begin with a set of observations
- Create a model to explain the observations
- Make testable predictions using the model
- Compare the predictions with new observations



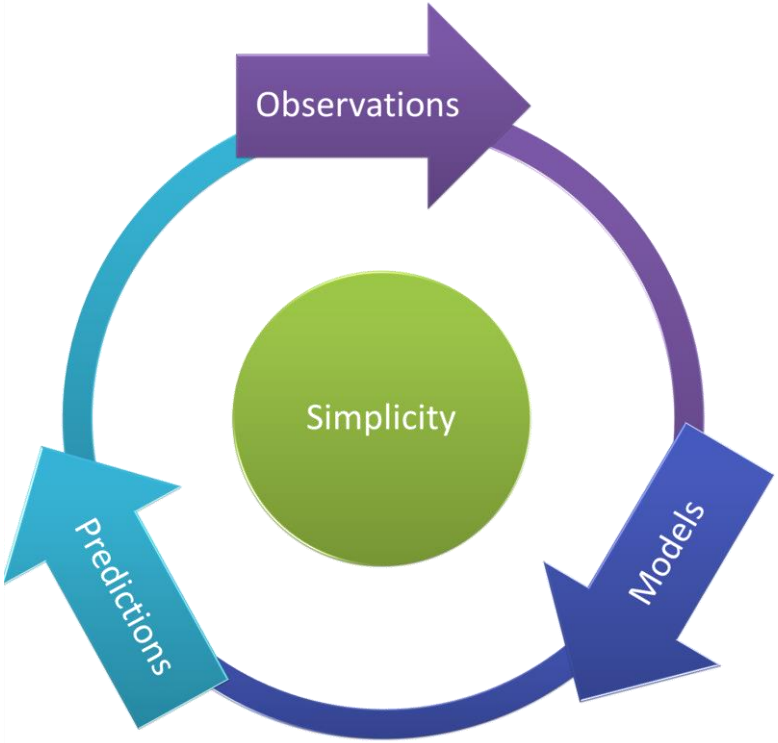
Scientific Method

- Begin with a set of observations
- Create a model to explain the observations
- Make testable predictions using the model
- Compare the predictions with new observations
- Use comparison to asses and modify the model



Scientific Method

- Repeat as required



Scientific Method

- Repeat as required
- Simplicity selects one preferred model from the many possible models that describe any set of observations