Foundations of Data Science for Biologists

Python programming basics

BIO 724D

22-JAN-2024

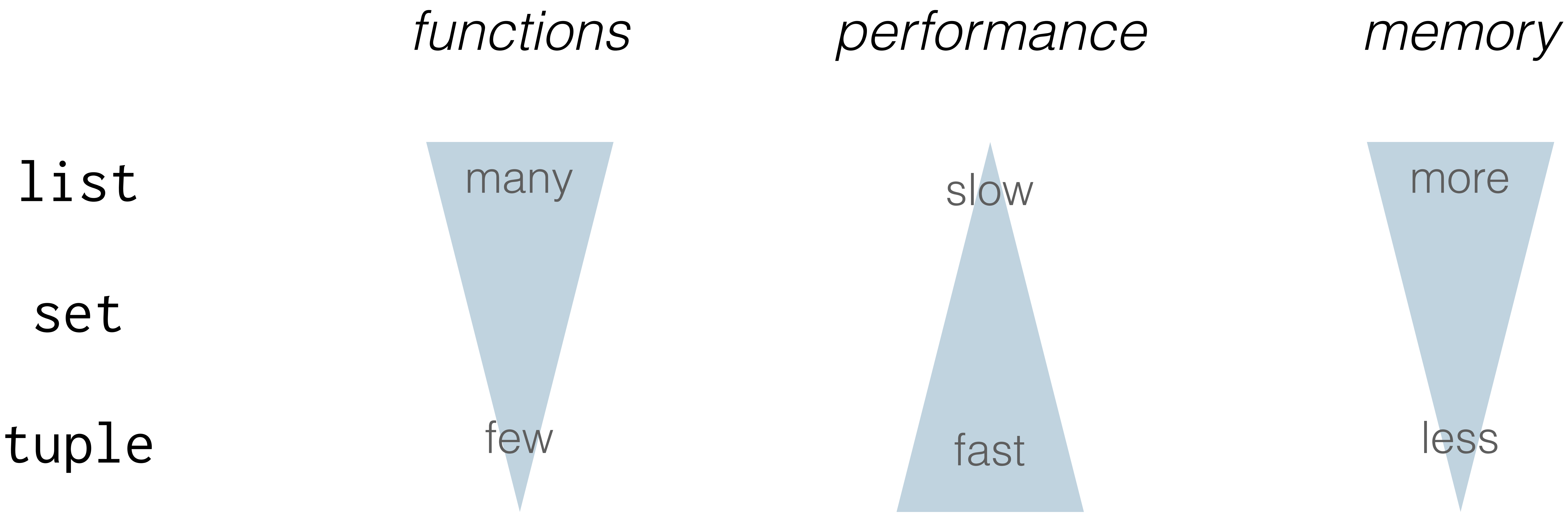
Instructors: Greg Wray and Paul Magwene

Data types and data structures

Why so many different data structures?

Data structures are not passive containers

- Each provides particular functions and prohibits other kinds of functions
- Each uses different organization behind the scenes to optimize its set of tasks



functions *performance* *memory*

`list`

`set`

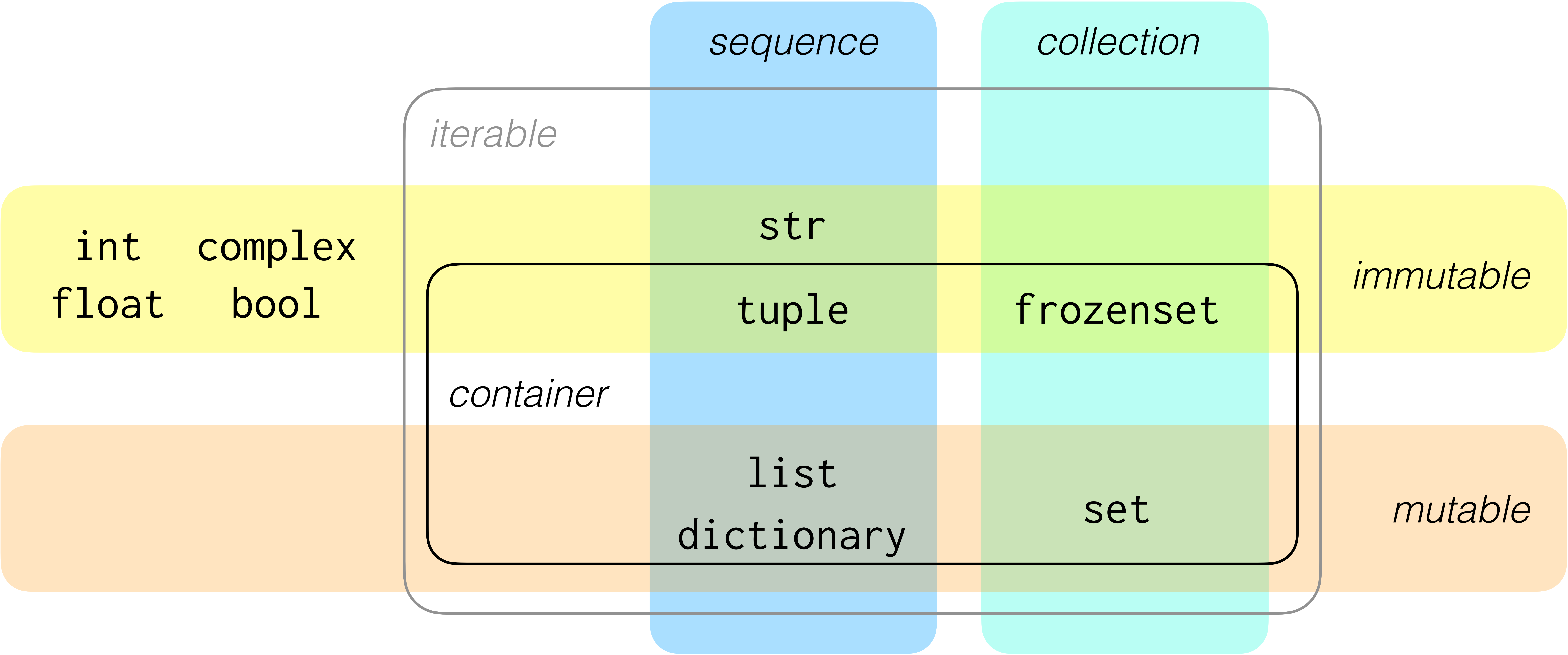
`tuple`

Choosing the right data structure reduces coding errors and speeds performance!

Introducing the four important data structures

	ordered	unique	mutable
`list`: items can be updated Highly versatile but relatively slow	🟢	🔴	🟢
`tuple`: the read-only version of a list Useful for rapid access and protecting data	🟢	🔴	🔴
`set`: the unordered, no duplicates version of a list Provides elegant set operations	🔴	🟢	🔴
`dictionary`: an associative array or hash table Similar to a list but indexed by names	🟢	🔴	🟢

Taxonomy of data structures in Python



Working with the common data structures

Useful and common general-purpose functions

The following can be applied to any data object:

```
type()                          # returns type
isinstance()                    # tests for type
dir()                           # returns valid methods for an object
```

The following can be applied to all iterable data objects:

```
len()
min(), max(), sum()
all(), any()                    # returns bool; tests whether items are True
filter()                        # returns True items
```

The following can be applied to mutable sequence data objects:

```
reversed(), sorted()            # do not alter original object
```

Strings

Some useful string manipulation methods (use assignment to keep the result):

`.upper()`, `.lower()`, `.title()`, `.rjust()`, `.center()`

`.strip()`, `.lstrip()`, `.rstrip()`, `.removeprefix()`, `.removesuffix()`

`.replace()`

`.zfill()`

Concatenating and slicing:

`+`

`[]`, `.split()`, `.splitlines()`

Strings, continued

Testing for properties:

```
.isalpha(), isdigit(), .isupper(), .islower()     # and many others
.isidentifier()                                  # is a variable name valid?
in, not in, startswith(), endswith()
```

Searching:

```
.find(), .count()
```

Printing: f-string formatting

```
my_string = f'The planet {var_1} has a radius of {var_2} km'
```

Lists

Basic list content manipulation methods (most operate in-place, “mutating”):

```
.append(), .insert(), .remove(), .pop(), .extend()
.sort(), .reverse()          # non-mutating alternatives mentioned earlier
.copy(), .clear()
```

Retrieve information about the contents of a list:

```
in,  not in, .count(), .index()
```

Two useful things to know:

```
my_list = list(set(my_list))     # removes duplicates from a list
zip()                            # conjoins two equal-length lists
```

Tuples

Only 2 methods because — immutable!

Retrieve information about the contents of a tuple:

`in`, `not in`, `.count()`, `.index()`

Extract the contents of a tuple so they can be manipulated (leaving the original intact):

```
my_list = list(my_tuple)
```

Sets

Basic set content manipulation methods (most are mutating):

`.add()`, `.update()`, `.remove()`, `.discard()`, `.pop()`

`.copy()`, `.clear()`

Set operations:

`|`, `.union()`, `&`, `.intersection()`, `-`, `.difference()`, `^`, `.symmetric_difference()`

`in`, `not in`

`.isdisjoint()`, `.issubset()`, `.issuperset()`

Dictionaries

Two common ways to create a dictionary:

```
my_dict = {'A':, 'B':2, 'C':3}
my_dict = dict(zip(['A', 'B', 'C'], [1, 2, 3]))
```

Basic dictionary content manipulation methods (most are mutating):

```
[], .add(), .update(), .remove(), .discard(), .pop()
.sort(), .reverse()              # non-mutating alternatives mentioned earlier
.copy(), .clear()
```

Extract information from a dictionary:

```
[], .values(), .keys(), .items()
.get()                           # no run-time error if key does not exist
```

Useful information for Python programming

Assignment

Plain assignment: create, modify, and access all of the standard data objects

Augmented assignment

```
i += 1                                # i = i + 1; works with many operators
```

Simultaneous assignment

```
i, j = 'spam', 42
i, j = j, i                           # swaps values
```

Unpacking

```
i, j = my_tuple                       # assigns without need for indexing
i, _ = my_tuple                       # _ means ignore other items
i, j*  = my_tuple                     # * means remaining items are a list
i, _*, j  = my_tuple                  # assigns first and last items
```

Representing numbers

Plain numbers

Decimal point indicates float; no decimal indicates integer; `j` indicates complex

Scientific notation

```
35e3, 12E-4                  # valid floats (not integers)
e3,  E-4                     # not valid; significand (mantissa) required
```

Long numbers

```
10_039_001                   # interpreted as integer 10039001
10,039,001                   # interpreted as list [1, 39, 1]
```

Integers in other bases

```
0b1, 0b110010                 # binary integers
0o23, 0h2A                    # octal and hexadecimal integers, respectively
```

Data types and casting

Data type for iterables:

```
my_list = [1, 2, 3]                 # implicit based on formatting
my_list = list(42)                  # explicit; class creator takes 1 argument
```

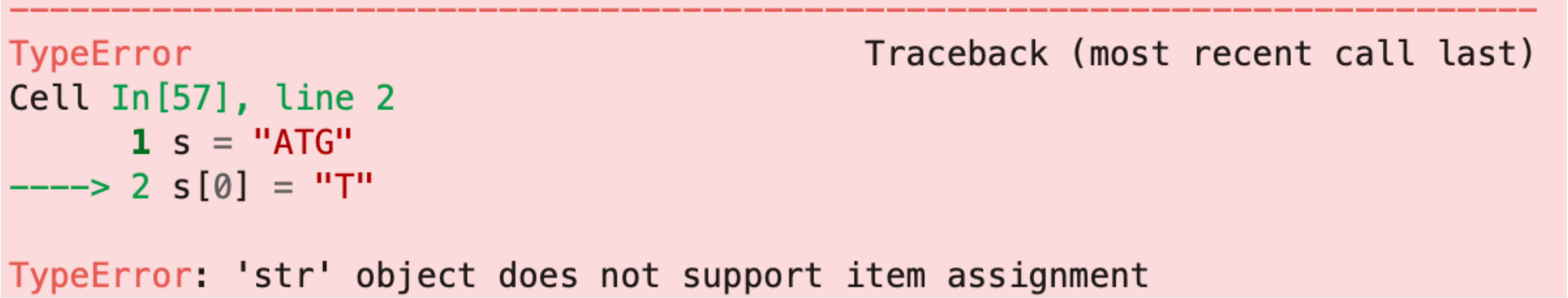
Data types can be converted when sensible:

```
my_list = list(my_tuple)            # tuple to list
my_integer = int(42.0)              # float to integer
my_str = str(42)                    # integer to string
```

Errors and exceptions

Syntax errors: code that does not conform to Python syntax

E.g.: missing comma, no closing bracket, = instead of ==

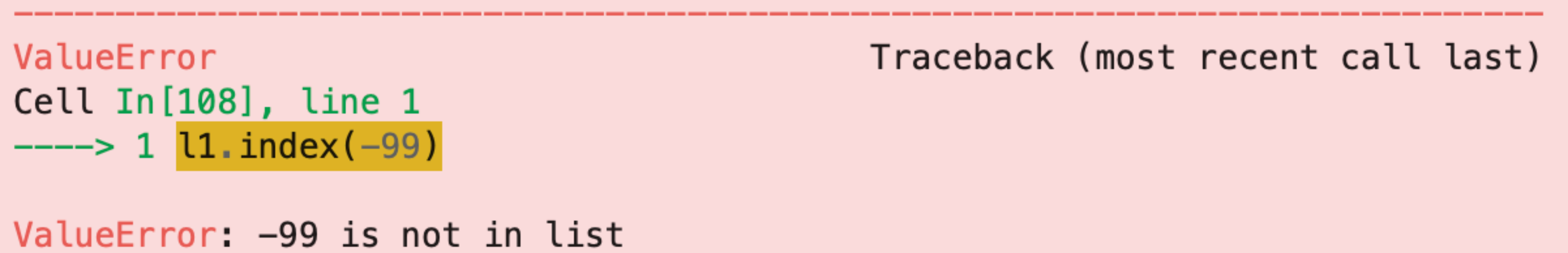


```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[57], line 2
      1 s = "ATG"
----> 2 s[0] = "T"

TypeError: 'str' object does not support item assignment
```

Exceptions: errors detected during runtime

E.g.: divide by zero, import module does not exist, input file in wrong format



```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
Cell In[108], line 1
----> 1 l1.index(-99)

ValueError: -99 is not in list
```

Naming rules and conventions

Valid names:

- Must begin with a letter (or underscore, but reserve for special objects)
- May contain letters, digits, underscore, some additional Unicode
- Case matters (but avoid relying on case alone!)
- Can be arbitrarily long
- Cannot be keywords (but *can* be names of built-in functions: beware!)

Conventions:

- Use all-lowercase names for variables, functions, methods, modules, packages
- Use all-caps for constants
- Use nouns for variables and verbs for functions
- There are other common conventions, but these are the basic ones

Operators (for reference)

Arithmetic: `+`, `-`, `*`, `/`, `%`, `//`; but use `**` for exponentiation

String: `+` (concatenate), `*` (repeat)

Comparison: `==`, `!=`, `>`, `<`, `>=`, `<=`

Logical: `and`, `or`, `not`

Membership: `in`, `not in`, `<=` (subset), `>=` (superset)

Sets: `|` (union), `&` (intersection), `-` (difference), `^` (symmetric difference)

Bitwise: `|` (or), `^` (exclusive or), `&` (and), `<<` (shift left n bits), `>>` (shift right n bits)