

Testing scientific code

Because you're worth it

Introduction to testing project

Excursion: Logistic Map

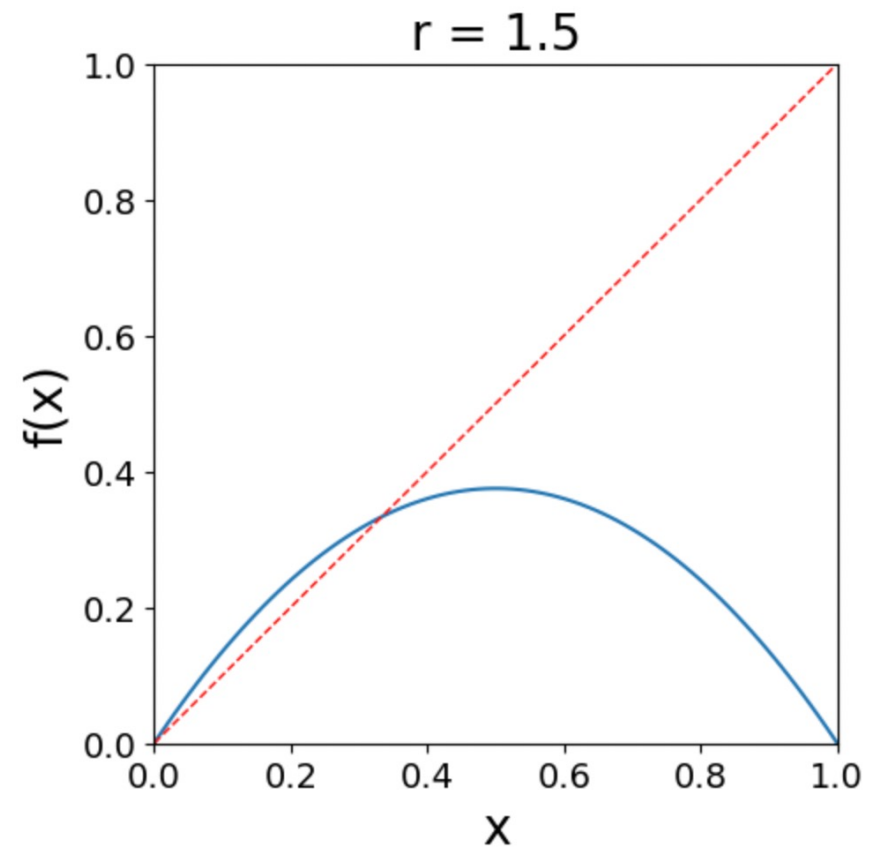
- Simple, discrete model for population growth

$$f(x) = r * x * (1 - x)$$

growth rate, 0...4

reproduction starvation

current population size, as
fraction of maximum
possible size, 0...1



Excursion: Logistic Map

- Simple, discrete model for population growth

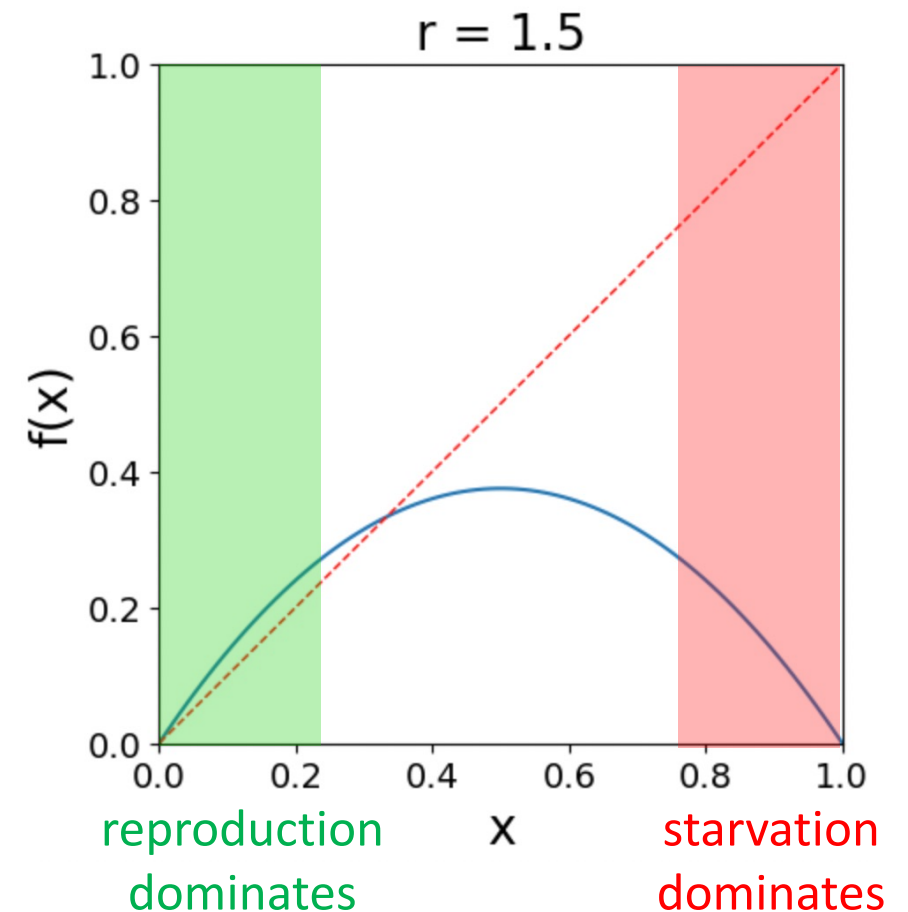
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growth rate, 0...4

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Excursion: Logistic Map

- Simple, discrete model for population growth

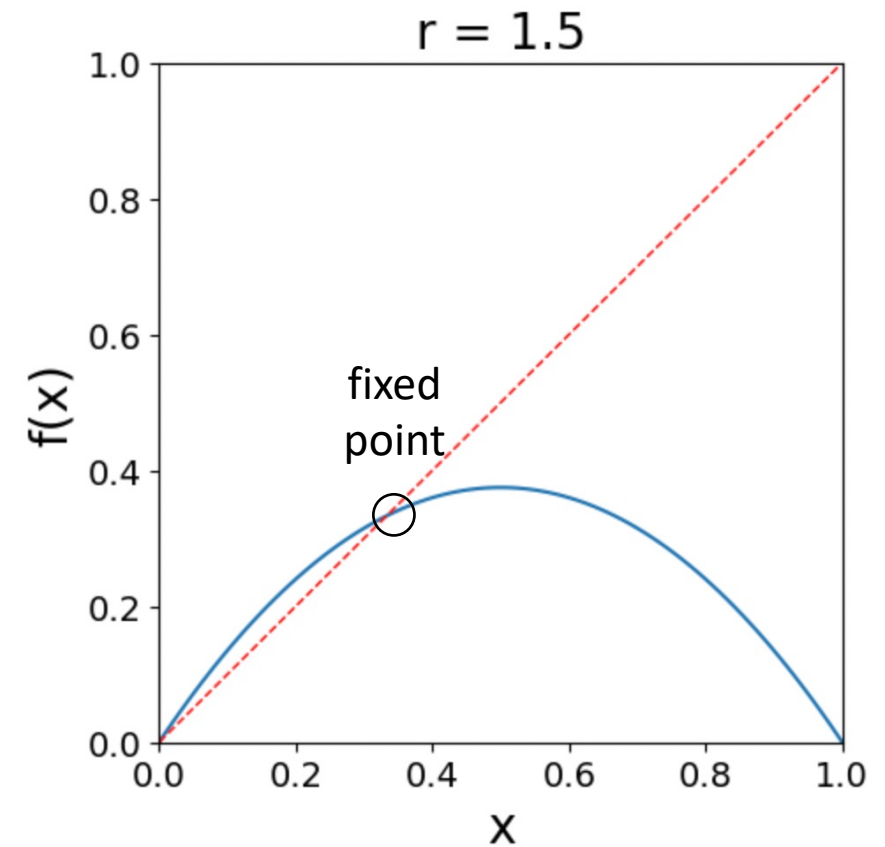
$$f(x) = r * x * (1 - x)$$

growth rate, 0...4

reproduction

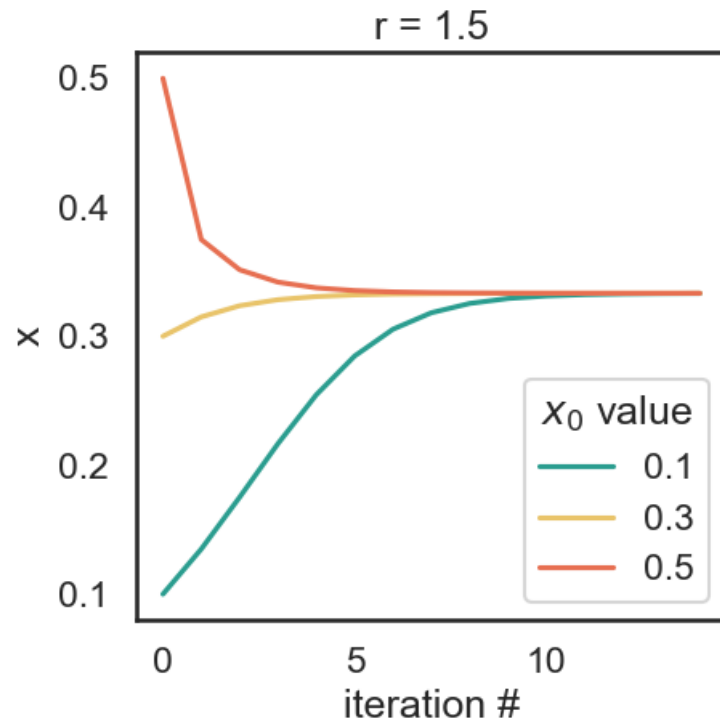
starvation

current population size, as fraction of maximum possible size, 0...1

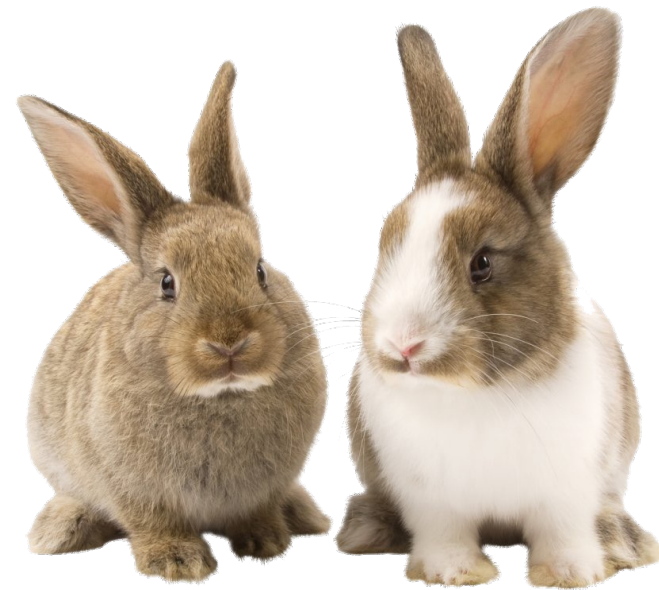


Excursion: Logistic Map

- x_0 : initial population size
- Iterated function: $f(x_0) = x_1 \rightarrow f(x_1) = x_2 \rightarrow f(x_2) = x_3$



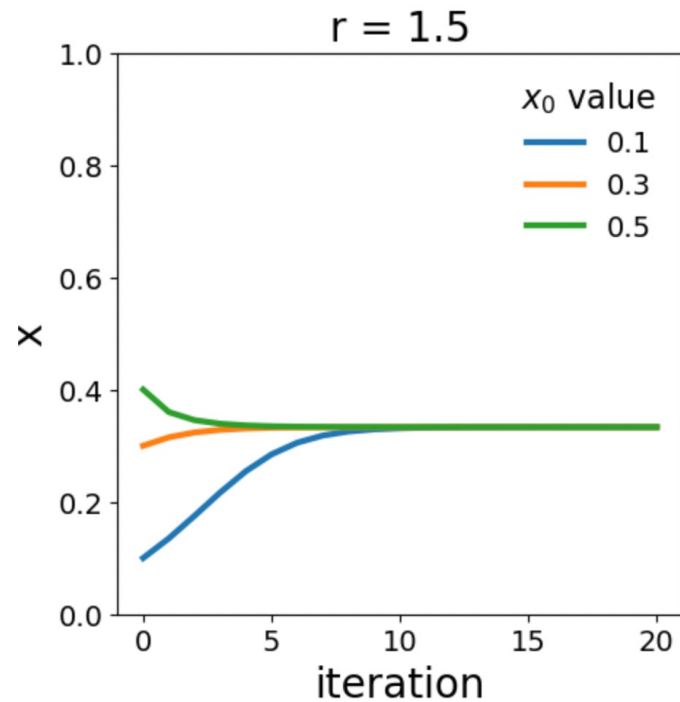
← converges
to fixed
point



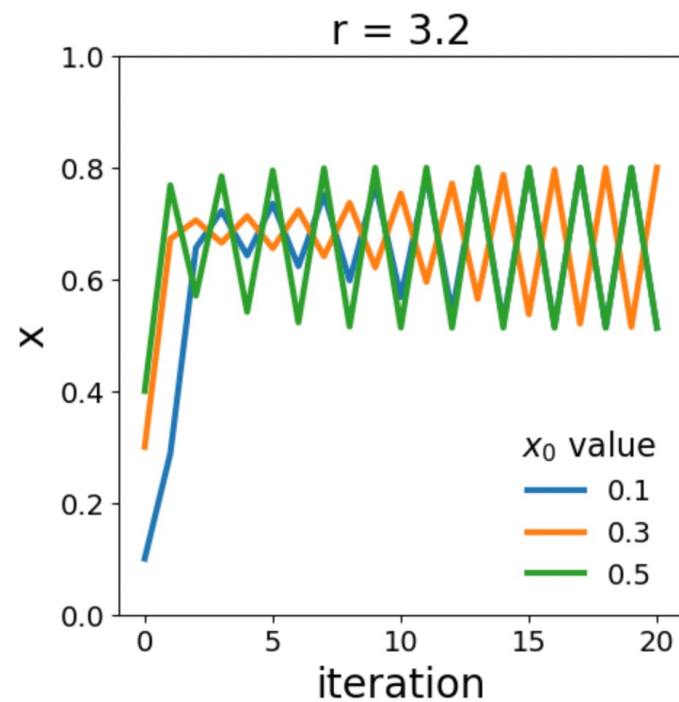
Excursion: Logistic Map

- Different growth rates lead to a variety of population dynamics

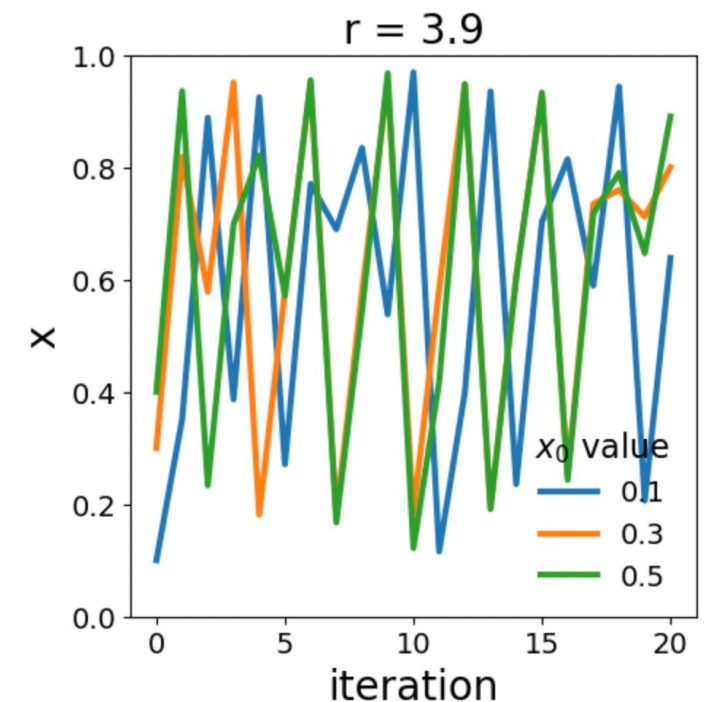
Convergence
to fix point



Convergence
to oscillations



Chaos





Testing patterns

What a good test looks like

- What does a good test look like? What should I test?
- Good:
 - Short and quick to execute
 - Easy to read
 - Tests *one* thing
- Bad:
 - Relies on data files
 - Messes with “real-life” files, servers, databases

Basic structure of test

- **Given:** Put your system in the right state for testing
 - Create data, initialize parameters, define constants...
- **When:** Execute the feature that you are testing
 - Typically, one or two lines of code
- **Then:** Compare outcomes with the expected ones
 - Define the expected result of the test
 - Set of *assertions* that check that the new state of your system matches your expectations

Test simple but general cases

- Start with simple, general case
 - Take a realistic scenario for your code, try to reduce it to the simplest example
- Example: Tests for 'lower' method of strings

```
def test_lower():  
    # Given  
    string = 'HeLlO wOrld'  
    expected = 'hello world'  
  
    # When  
    output = string.lower()  
  
    # Then  
    assert output == expected
```

Test special cases and boundary conditions

- Code often breaks in corner cases: empty lists, None, NaN, 0.0, lists with repeated elements, non-existing file, ...
- This often involves making design decision: handle corner case with special behavior, or raise a meaningful exception?

```
def test_lower_empty_string():  
    # Given  
    string = ''  
    expected = ''  
  
    # When  
    output = string.lower()  
  
    # Then  
    assert output == expected
```

- ▶ Other good corner cases for `string.lower()`:
 - ▶ 'do-nothing case': `string = 'hi'`
 - ▶ symbols: `string = '123 (!'`

Common for-loop pattern for testing multiple cases

- Often these cases are collected in a single test:

```
def test_lower():  
    # Given  
    # Each test case is a tuple of (input, expected_result)  
    test_cases = [('HeLlO wOrld', 'hello world'),  
                  ('hi', 'hi'),  
                  ('123 ([?', '123 ([?'),  
                  ('', '')]  
  
    for string, expected in test_cases:  
        # When  
        output = string.lower()  
        # Then  
        assert output == expected
```

Hands-on!

- Take a look at the logistic map $f(x) = r * x * (1 - x)$
- or, in Python

```
def f(x, r):  
    """ Compute the logistic map for a given value of x and r. """  
    return r * x * (1 - x)
```

- What should we test?
 - Generic cases
 - Corner cases

Hands-on!

- In the `testing_project` folder, open the file `logistic.py` and implement the logistic function, $f(x, r)$
- In `test_logistic.py` we already added a reference test for these corner cases:
 - $x=0, r=1.1 \Rightarrow f(x, r)=0$
 - $x=1, r=3.7 \Rightarrow f(x, r)=0$
- Add a new test for these generic cases using the for-loop pattern:
 - $x=0.1, r=2.2 \Rightarrow f(x, r)=0.198$
 - $x=0.2, r=3.4 \Rightarrow f(x, r)=0.544$
 - $x=0.5, r=2 \Rightarrow f(x, r)=0.5$

The for-loop pattern can be improved

- It is repetitive to write the for-loop pattern
- If one of the cases break, it can be complicated to figure out which one
- pytest has many helpers for simplifying common testing cases!
- One of them is the `parametrize` decorator, that simplifies running the same test with multiple cases

Simple example

```
def test_for_loop_simple():  
    cases = [1, 2, 3]  
    for a in cases:  
        assert a > 0
```

`test_for_loop_simple`
runs once and loops over
3 test cases

Simple example, with the parametrize decorator

Name of the variable that varies

List of values for the variable

```
@pytest.mark.parametrize('a', [1, 2, 3])  
def test_parametrize_simple(a):  
    assert a > 0
```

The test must take an argument with the same name

test_parametrize_simple runs 3 times with a=1, a=2, and a=3

Simple example, with the parametrize decorator

Name of the variable that varies

List of values for the variable

```
@pytest.mark.parametrize('a', [1, 2, 3])  
def test_parametrize_simple(a):  
    assert a > 0
```

The test must take an argument with the same name

```
===== test session starts =====  
platform darwin -- Python 3.11.3, pytest-7.3.1, pluggy-1.0.0 -- /Users/pietro.berkes/miniconda3/envs/aspp/bin/python  
cachedir: .pytest_cache  
rootdir: /Users/pietro.berkes/o/ASPP/testing_project/demos  
plugins: anyio-3.5.0  
collected 3 items  
  
test_parametrize.py::test_parametrize_simple[1] PASSED [ 33%]  
test_parametrize.py::test_parametrize_simple[2] PASSED [ 66%]  
test_parametrize.py::test_parametrize_simple[3] PASSED [100%]  
  
===== 3 passed in 0.00s =====
```

pytest automatically creates one separate test for each test case

Example with multiple values

- This is a more typical case with several input values and the expected result of the test

```
def test_for_loop_multiple():  
    cases = [  
        (1, 'hi', 'hi'),  
        (2, 'no', 'nono')  
    ]  
    for a, b, expected in cases:  
        result = b * a  
        assert result == expected
```

`test_for_loop_multiple`
runs once and loops over
2 test cases

Same example, with the parametrize decorator

Name of all the variables,
separated by commas in
one string

List of tuples with the
values for each variable,
one for each test case

```
@pytest.mark.parametrize('a, b, expected', [(1, 'hi', 'hi'), (2, 'no', 'nono')])  
def test_parametrize_multiple(a, b, expected):  
    result = b * a  
    assert result == expected
```

The test must take
arguments with the
same names as in the
string

```
test_parametrize_multiple  
runs 2 times with  
1) a=1 b='hi' expected='hi'  
and  
2) a=2 b='no', expected='nono'
```

Same example, with the parametrize decorator

Name of all the variables,
separated by commas in
one string

List of tuples with the
values for each variable,
one for each test case

```
@pytest.mark.parametrize('a, b, expected', [(1, 'hi', 'hi'), (2, 'no', 'nono')])  
def test_parametrize_multiple(a, b, expected):  
    result = b * a  
    assert result == expected
```

The test must take
arguments with the
same names as in the
string

```
[4] pytest -v test_parametrize.py::test_parametrize_multiple  
===== test session starts =====  
platform darwin -- Python 3.11.3, pytest-7.3.1, pluggy-1.0.0 -- /Users/pietro.berkes/miniconda3/envs/aspp/bin/python  
cachedir: .pytest_cache  
rootdir: /Users/pietro.berkes/o/ASPP/testing_project/demos  
plugins: anyio-3.5.0  
collected 2 items  
  
test_parametrize.py::test_parametrize_multiple[1-hi-hi] PASSED [ 50%]  
test_parametrize.py::test_parametrize_multiple[2-no-nono] PASSED [100%]  
  
===== 2 passed in 0.01s =====
```

pytest automatically
creates one separate
test for each test case

Hands-on!

- Rewrite the test with the generic cases for the logistic map using `parametrize`
- Reference example for the corner cases test:

```
import pytest

@pytest.mark.parametrize('x, r, expected', [
    (0, 1.1, 0),
    (1, 3.7, 0),
])
def test_f_special_x_values(x, r, expected):
    result = f(x, r)
    assert_allclose(result, expected)
```

Hands-on! Simulate a population over time

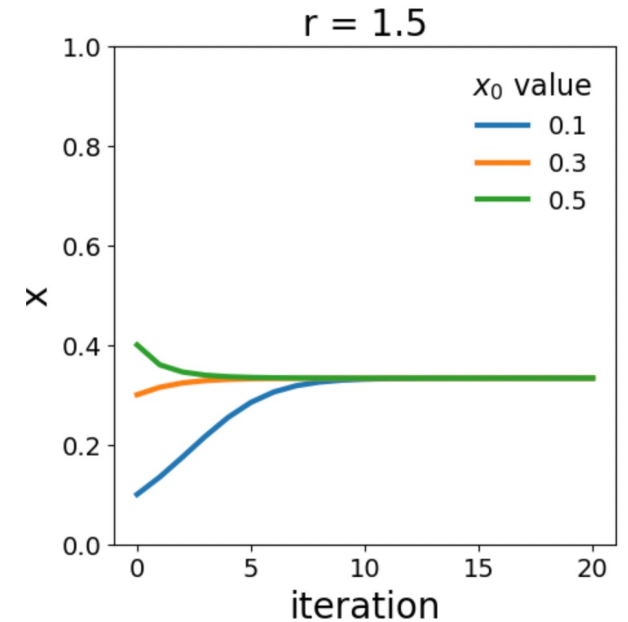
1. Implement a function `iterate_f` that runs `f` for `it` iterations.

Write tests for the following cases:

- `x=0.1, r=2.2, it=1`
=> `iterate_f(it, x, r)=[0.1, 0.198]`
- `x=0.2, r=3.4, it=4`
=> `iterate_f(it, x, r)=[0.2, 0.544, 0.843418, 0.449019, 0.841163]`
- `x=0.5, r=2, it=3`
=> `iterate_f(it, x, r)=[0.5, 0.5, 0.5]`

2. (Bonus) Import the `plot_trajectory` function from the `plot_logistic` module and use it to visualize the trajectories generated by your code.

Try with values $r < 3$, and $3 < r < 4$ to get an intuition for how the function behaves differently with different parameters.

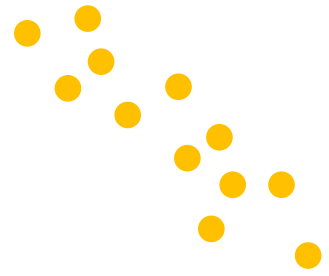


Strategies for testing scientific code

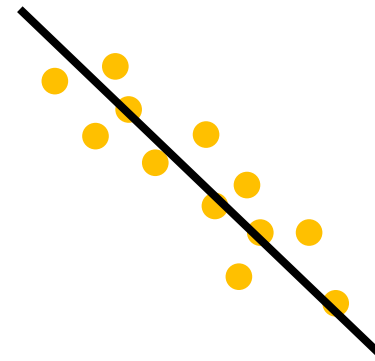
Strategies for testing learning algorithms

- Learning algorithms can get stuck in local maxima, the solution for general cases might not be known (e.g., unsupervised learning)
- Turn your validation cases into tests
- Stability tests:
 - Start from final solution; verify that the algorithm stays there
 - Start from solution and add a small amount of noise to the parameters; verify that the algorithm converges back to the solution
- Parameter Recovery: Generate synthetic data from the model with known parameters, then test that the code can learn the parameters back

Learning algorithms fit the parameters of a model to observed data



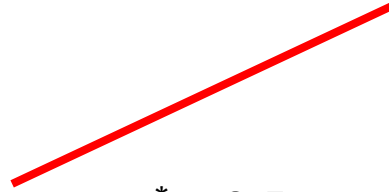
$$y = ax + b + \text{noise}$$



$$a = -1.2$$
$$b = 3$$

Generate synthetic data from the model to test the learning algorithm by recovering the parameters

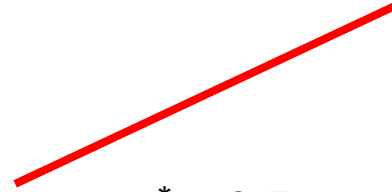
1) Fix initial parameters



$$a^* = 0.5$$
$$b^* = -1.3$$

Generate synthetic data from the model to test the learning algorithm by recovering the parameters

1) Fix initial parameters

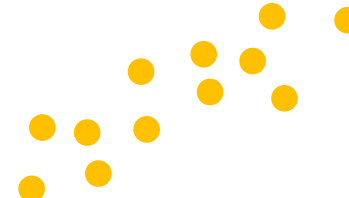


$$a^* = 0.5$$
$$b^* = -1.3$$



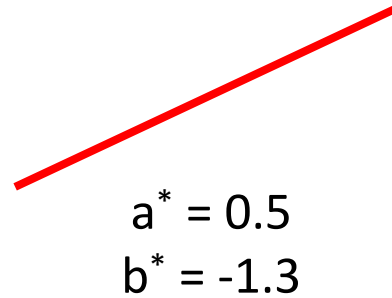
$$y = a^* x + b^*$$
$$+ \text{noise}$$

2) Generate synthetic data



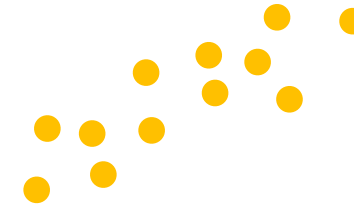
Generate synthetic data from the model to test the learning algorithm by recovering the parameters

1) Fix initial parameters



2) Generate synthetic data

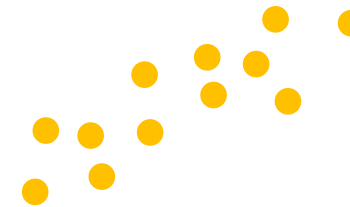
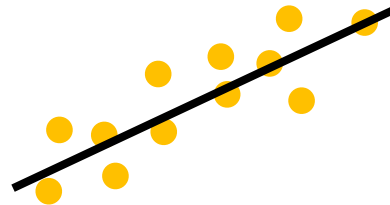
$y = a^* x + b^*$
+ noise



3) Run the algorithm

$a = 0.5098$
 $b = -1.287$

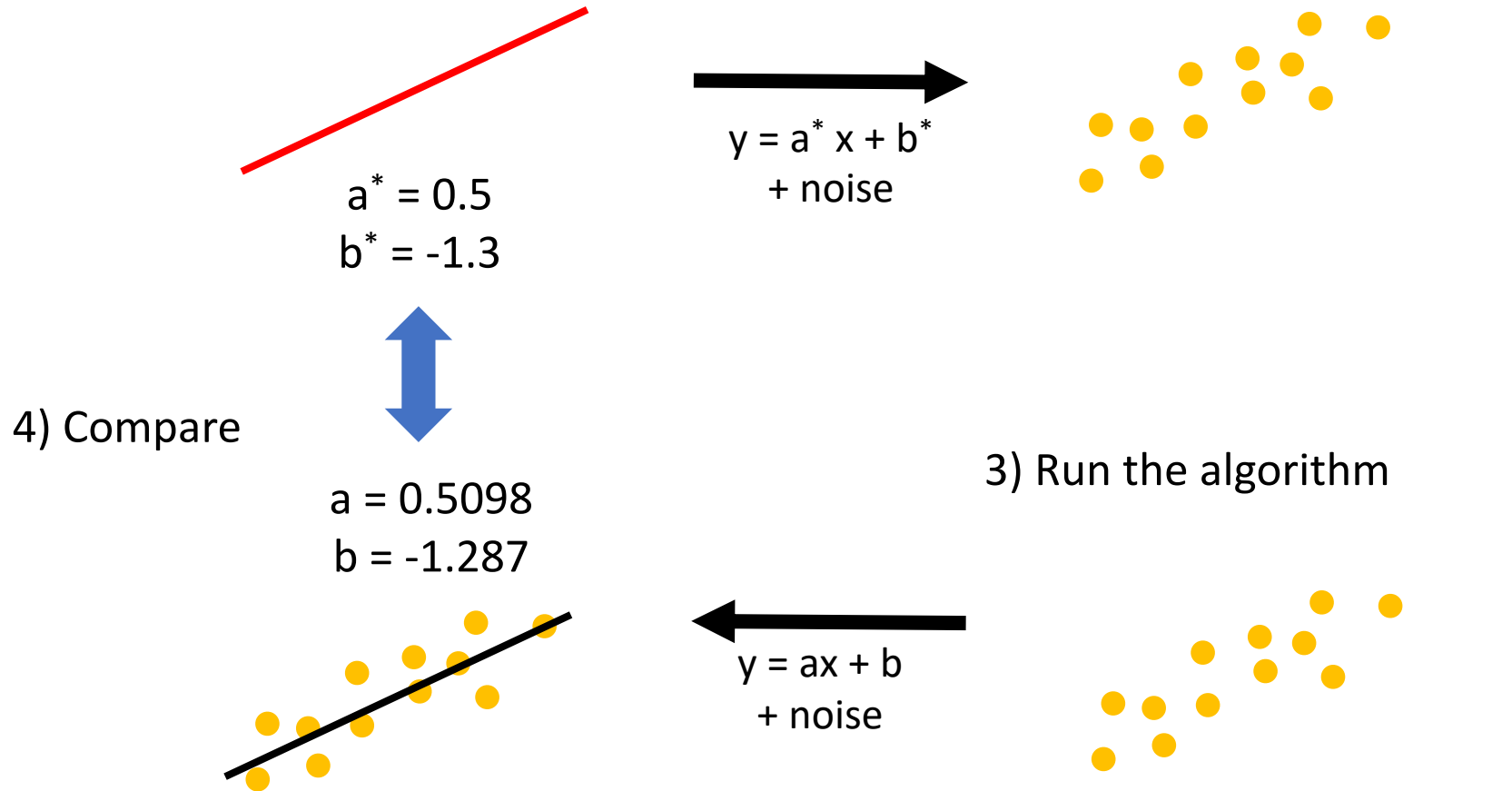
$y = ax + b$
+ noise



Generate synthetic data from the model to test the learning algorithm by recovering the parameters

1) Fix initial parameters

2) Generate synthetic data



Hands-on! Recover the population growth, r

- In the module `logistic_fit`, we implemented a function `fit_r` that, given a population trajectory, finds the value of r that generated it
- For example:

```
In [1]: from logistic import iterate_f
In [2]: from logistic_fit import fit_r
In [3]: xs = iterate_f(it=23, x0=0.3, r=3.421)

In [4]: fit_r(xs)
Out[4]: 3.4210000000000003
```

Hands-on!

- Write a test for the function `fit_r` using the parameters recovery method
- The test should
 1. Set a initial value for `x0` and `r`
 2. Use `iterate_f` to generate a population trajectory
 3. Pass the population trajectory to `fit_r` and collect the result parameters
 4. Check that the fitted `r` is close enough to the original `r`

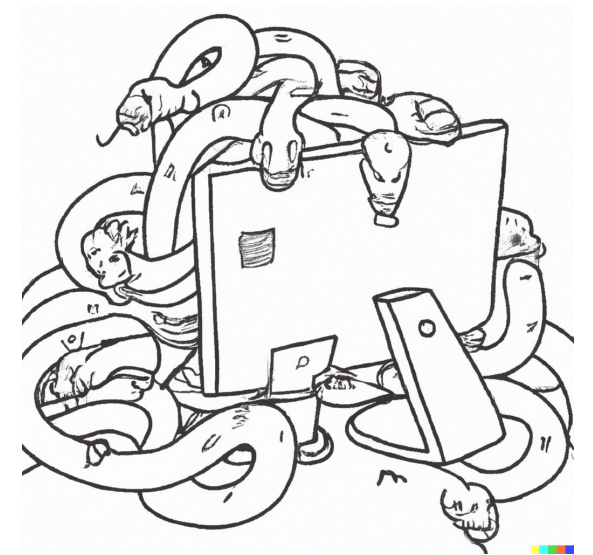
```
In [1]: from logistic import iterate_f
In [2]: from logistic_fit import fit_r
In [3]: xs = iterate_f(it=23, x0=0.3, r=3.421)

In [4]: fit_r(xs)
Out[4]: 3.4210000000000003
```

Randomness in Testing

- Using randomness in testing can be useful
 - To check that the code is stable and works correctly in many different cases
 - To find corner cases or numerical problems

```
def test_logistic_fit_randomized():  
    random_state = np.random.RandomState(SEED)  
    for _ in range(100):  
        x0 = random_state.uniform(0.0001, 0.9999)  
        r = round(random_state.uniform(0.001, 3.999), 3)  
  
        xs = iterate_f(it=17, x0=x0, r=r)  
        recovered_r = fit_r(xs)  
  
        assert_allclose(r, recovered_r, atol=1e-3)
```



Random Seeds and Reproducibility

- When running tests that involve randomness and some test doesn't pass it is vital to be able to reproduce that test exactly!
- Computers produce pseudo-random numbers: setting a seed resets the basis for the random number generator
- This is essential for reproducibility
- At a minimum, you should manually set the seed for each of your random tests

```
SEED = 42  
random_state = np.random.RandomState(SEED)  
random_state.rand()
```

Hands On!

- a) Write a randomized test that checks that for $r=1.5$, for any random starting point x_0 , the logistic equation converges to $1/3$
- Write a for loop of 100 iterations, in each iteration create a random x_0
 - For each value of x_0 , test that after many iterations in `iterate_f` the value of x is equal to $1/3$

A Pytest Solution

- Non-scientific coding uses random testing more rarely, so there is no helper tools for that in pytest
- However, in scientific coding it is quite common
- What do we want?
 - For each (random) test there should be a seed
 - For each run of the test, the seed should be different
 - That seed should be printed with the test result
 - It needs to be possible to explicitly run the test again with that seed!

Fixtures (minimal solution)

- Fixtures are functions that are run before the tests are executed

```
import numpy as np
import pytest

# set the random seed for once here
SEED = np.random.randint(0, 2**31)

@pytest.fixture
def random_state():
    print(f'Using seed {SEED}')
    random_state = np.random.RandomState(SEED)
    return random_state

def test_something(random_state):
    random_state.rand()
```

If an input argument of a test matches the name of a fixture, then the fixture is called and the return value assigned to the argument.

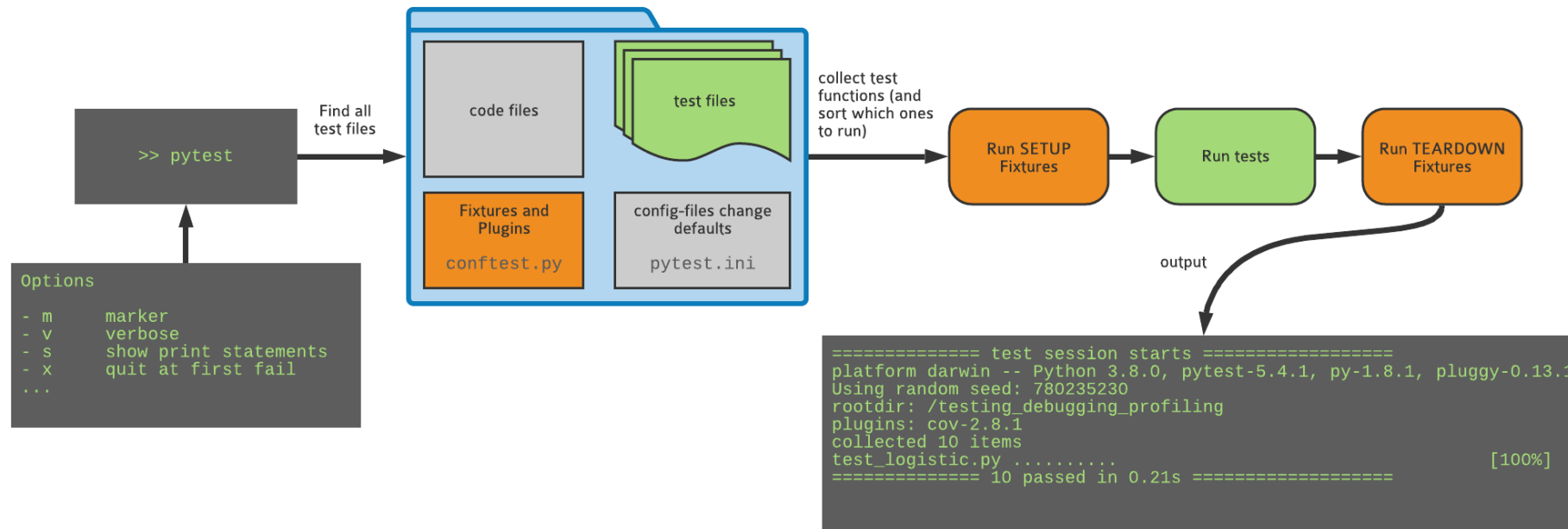
pytest handles that automatically as part of running the test suite

Hands On!

- a) Write a randomized test that checks that `fit_r` can recover `r` for any random value of `x0` and `r`
- b) Add a fixture at the top of your test file, that lets you print the seed to the console.

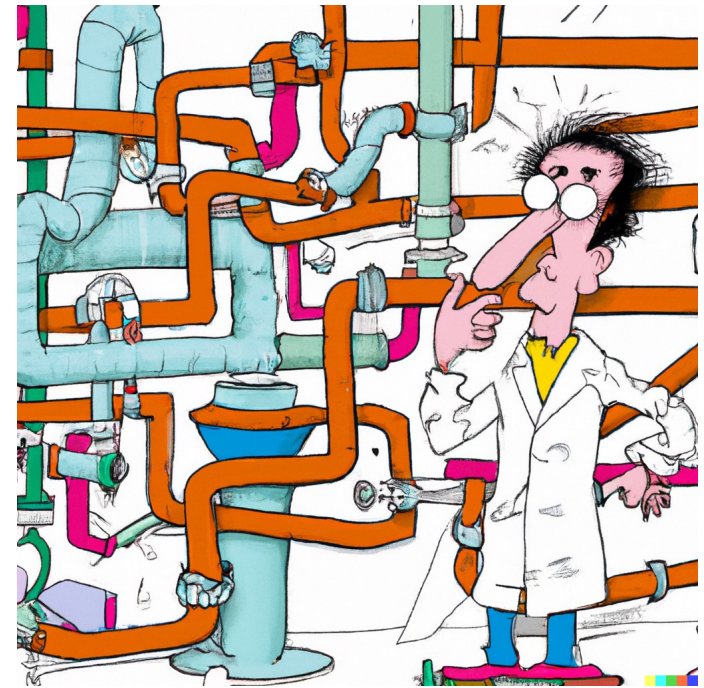
```
[L]$ pytest
===== test session starts =====
platform darwin -- Python 3.8.0, pytest-5.4.1, py-1.8.1, pluggy-0.13.1
Using random seed: 892358865
```

What happens when you run pytest



Fixtures (real solution)

- `conftest.py` is a special pytest config file (don't import it!)
- `conftest.py` can be used to define custom behavior or plugins. Fixtures can also be defined here, so that they can be used by all tests.
- See the file `demos/conftest_example.py` in the repo you forked. If you move it to the main folder and rename it, the functions defined there select a seed for each test and allow you to pass a seed on the command line using `--seed 123`



Hands On!

- a) Write a randomized test that checks that `fit_r` can recover `r` for any random value of `x0` and `r`
- b) Add a fixture at the top of your test file, that lets you print the seed to the console.
- c) Add the `confptest.py` file to the root directory of the project (hint: it is hiding in the `demos` folder!). It sets a random seed before each run and makes it possible to reproduce failures in random tests
- d) `confptest.py` defines a new `random_state` fixture, modify your test accordingly
- e) Check that the console output of `pytest` now includes the seed!

```
[L]$ pytest
===== test session starts =====
platform darwin -- Python 3.8.0, pytest-5.4.1, py-1.8.1, pluggy-0.13.1
Using random seed: 892358865
```


Other commonly used helpers in pytest

Decorating “special” tests

- `@xfail`: Expected failure, outputs an “x” (or “X”) in the report

```
@pytest.mark.xfail
def test_something():
    ...
```

- `@skip`: Skip test, useful e.g. when the feature doesn’t exist yet

```
@pytest.mark.skip(reason="functionality not yet
implemented")
def test_something():
    ...
```

- `@skipif`: Skip the test if a condition is met, useful for tests that only works on a specific platform, or for a specific version of Python

```
@pytest.mark.skipif(sys.version_info < (3, 10),
                    reason="requires python3.10 or higher")
def test_something():
    ...
```

Marking tests with custom markers

- If you have lots of tests, you can categorize them with your own markers
 - although for custom mark names you need to register the marks “pytest.ini”
 - <https://docs.pytest.org/en/7.1.x/example/markers.html#registering-markers>
- Example:
 - Smoke tests check for really basic features: run these frequently
 - Other tests may be many or too slow to run every time and test for more edge cases

```
@pytest.mark.smoke
def test_something_basic():
    ...
```


```
> pytest -m smoke
> pytest -m "smoke and not slow"
```

Writing temporary files: `tmp_path`

- To test functions that write to disk without leaving around the files when the test is finished, use the `tmp_path` fixture
- The value of `tmp_path` is a `pathlib.Path` object
- The directory is created at the start of the test, and removed at the end

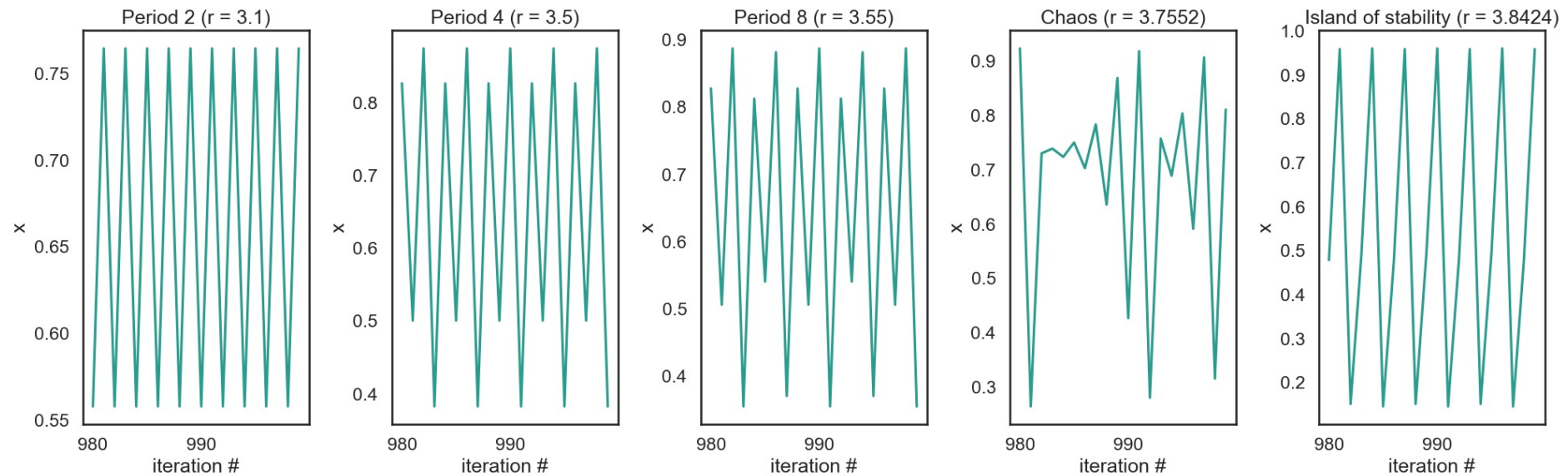
```
def test_create_file(tmp_path):  
    d = tmp_path / "sub"  
    d.mkdir()  
    p = d / "hello.txt"  
    content = "some random text"  
    p.write_text(content)  
    assert p.read_text() == content  
    assert len(list(tmp_path.iterdir())) == 1
```

All you need to do is
add an argument
with this exact name



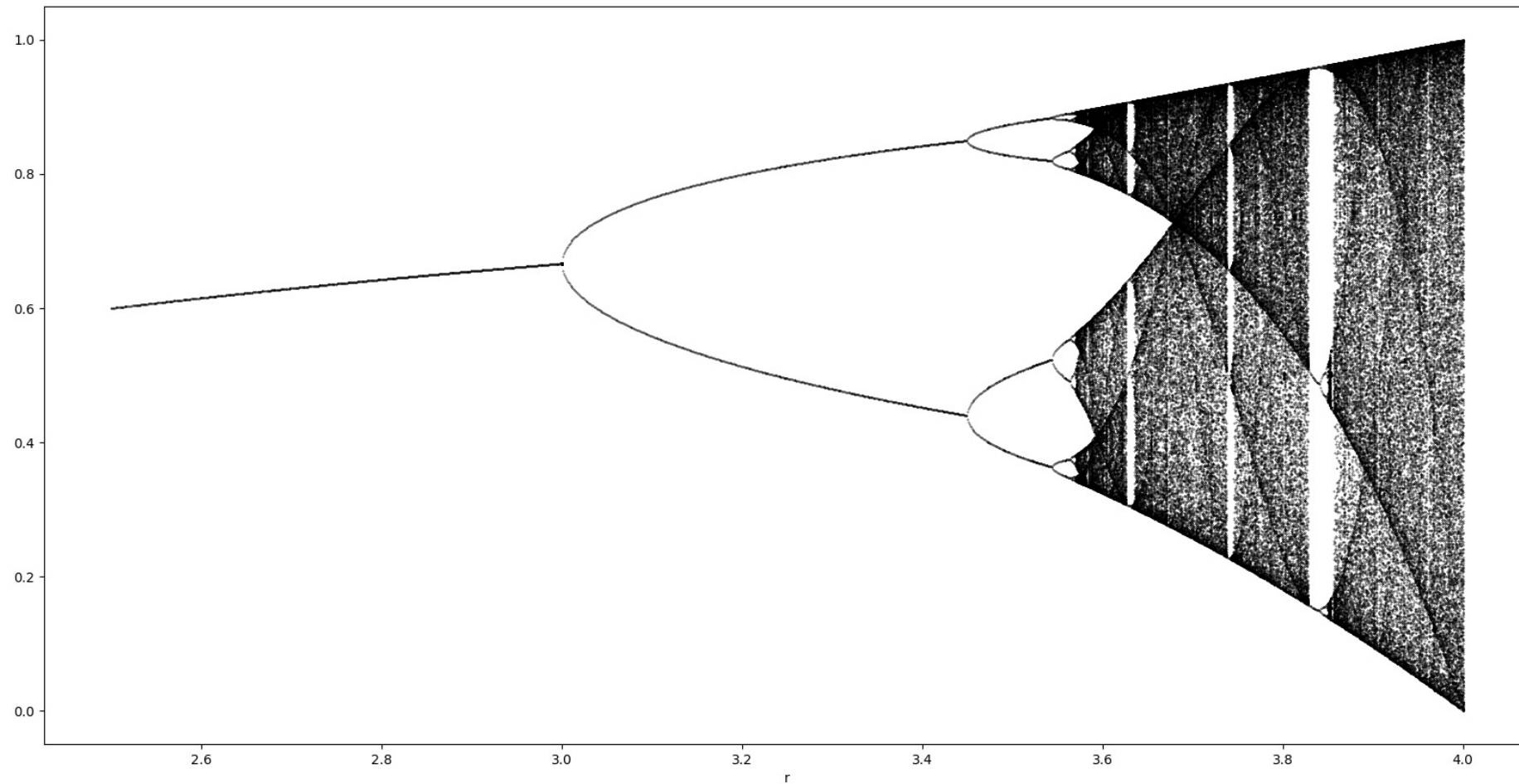
Final exercise

Excursion: Logistic map

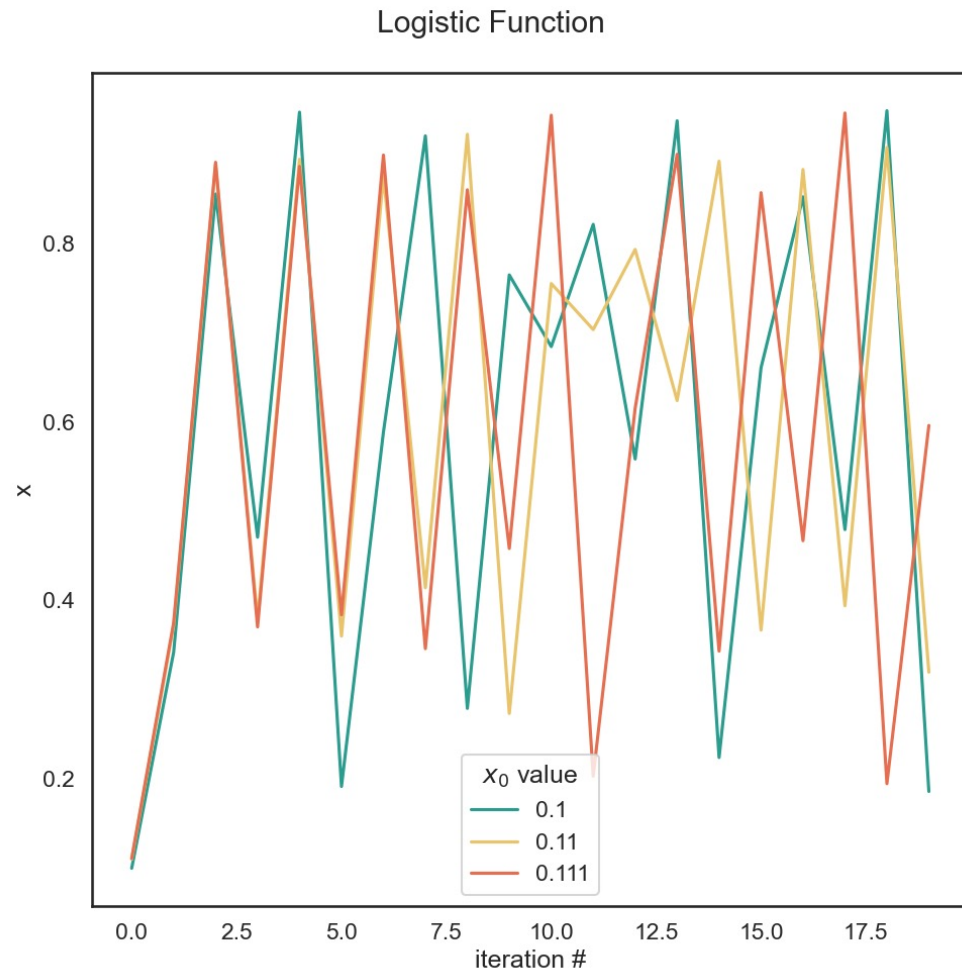


- Between $r=3$ and $r=4$ the logistic map has a range of behaviors
- Periodic vs. chaotic

Excursion: Logistic map



Excursion: Logistic map and chaos



- Sensitive Dependence on Initial Conditions (SDIC)
- Even starting points that are very close quickly diverge to completely different itineraries
- This is called the “Butterfly effect”



Hands on!

Some r values for $3 < r < 4$ have some interesting properties: a chaotic trajectory neither diverges nor converges.

a) Use the `plot_bifurcation` function from the `plot_logfun` module using your implementation of `f` and `iterate` to look at the bifurcation diagram. The function generates an output image, `bifurcation_diagram.png`

b) Write a test that checks for chaotic behavior when $r=3.8$. Run the logistic map for 100'000 iterations and verify the conditions for chaotic behavior:

- 1) The function is deterministic: *this does not need to be tested in this case*
- 2) Orbits must be bounded: check that all values are between 0 and 1
- 3) Orbits must be aperiodic: check that the last 1000 values are all different
- 4) Sensitive dependence on initial conditions: *this is the bonus exercise (in readme)*

The test should check conditions 2) and 3)!

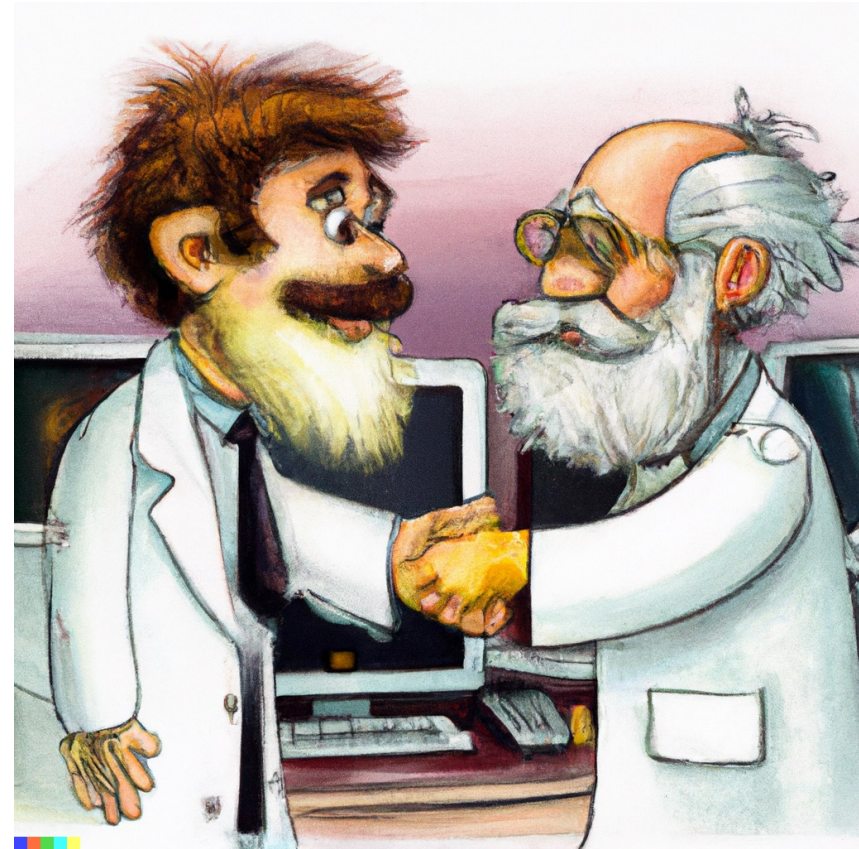
Testing is good for your self-esteem

- Immediately: Always be confident that your results are correct, whether your approach works or not
- In the future: **save your future self some trouble!**
- If you are left thinking “it’s cool but I cannot test *my* code because XYZ”, talk to us during the week and we’ll show you how to do it ;-)

You, in 2023



You, in 2024



Up next:



Debugging



