Scientific programming patterns

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What is wrong with you?!

- You studied the language
- You learned the libraries
- You coded for months

- And yet the code still feels like a 7-headed apocalyptic monster. Changes are painful, new features break old functionality, reproducing previous results becomes a git-checkout juggling exercise

The good news: you can smell it

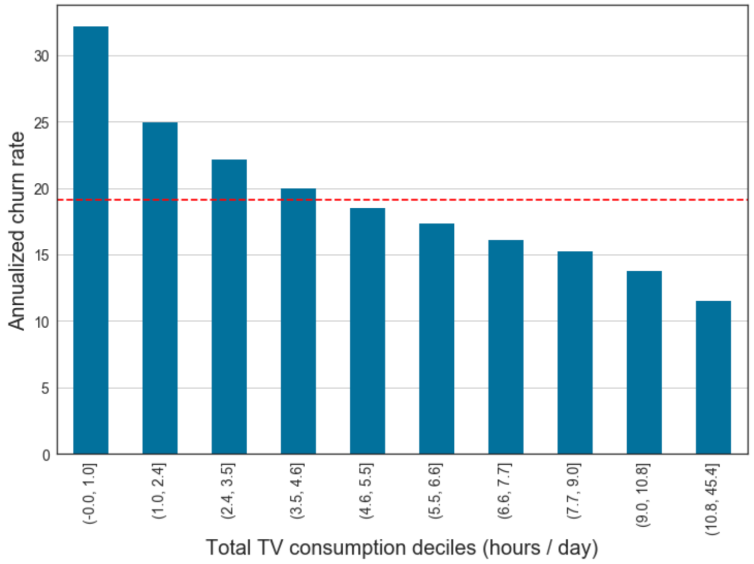
7.1 Total TV

In [118]:

```
ttv_h_deciles = pd.qcut(ttv_h, 10)
ttv_deciles_churn = tv_merged.groupby(ttv_h_deciles).churned_all.mean() * 12 / 10 * 100
```

In [119]:

```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = ttv_deciles_churn.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('Total TV consumption deciles (hours / day)')
    plt.ylabel('Annualized churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')

    t = ['({:.1f}, {:.1f}]'.format(x.left, x.right) for x in ttv_deciles_churn.index]
    plt.xticks(range(len(t)), t)
```

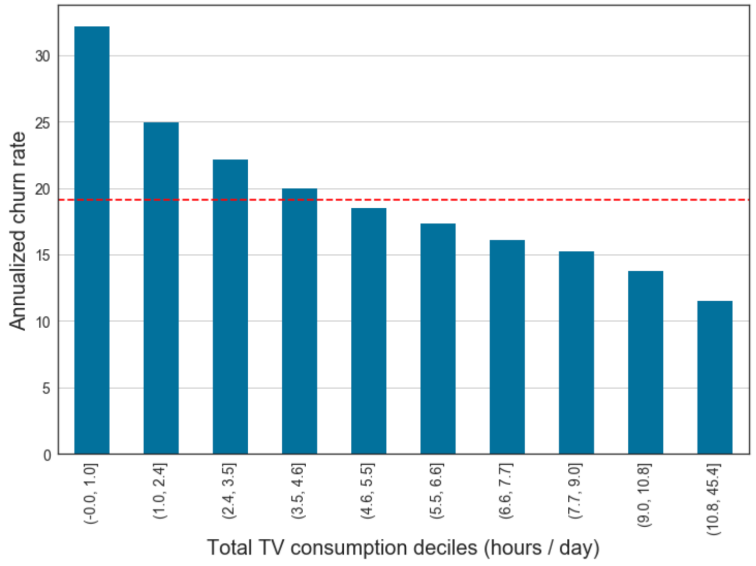


The good news: you can smell it

7.1 Total TV

In [118]:
```
ttv_h_deciles = pd.qcut(ttv_h, 10)
ttv_deciles_churn = tv_merged.groupby(ttv_h_deciles).churned_all.mean() * 12 / 10 * 100
```

In [119]:
```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = ttv_deciles_churn.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('Total TV consumption deciles (hours / day)')
    plt.ylabel('Annualized churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')

    t = ['({:.1f}, {:.1f}]'.format(x.left, x.right) for x in ttv_deciles_churn.index]
    plt.xticks(range(len(t)), t)
```



7.2 Playback

In [120]:
```
replay_deciles = pd.qcut(tv_merged.PLAYBACK / ttv_sec_to_hpd, 10)
replay_deciles_churn = tv_merged.groupby(replay_deciles).churned_all.mean() * 12 / 10 * 100
```

In [121]:
```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = replay_deciles_churn.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('Replay TV consumption deciles (hours / day)')
    plt.ylabel('Annualized churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')

    t = ['({:.1f}, {:.1f}]'.format(x.left, x.right) for x in replay_deciles_churn.index]
    plt.xticks(range(len(t)), t)
```

In [122]:
```
replay_h = pd.cut(tv_merged.PLAYBACK / ttv_sec_to_hpd, np.arange(0, 8), include_lowest=True)
replay_churn = tv_merged.groupby(replay_h).churned_all.mean() * 12 / 10 * 100
```

In [123]:
```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = replay_churn.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('Replay TV consumption (hours / day)')
    plt.ylabel('Annualized churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')
```

7.3 Trends

In [137]:
```
tv_delta = pd.cut(tv_merged.TTV_201703_delta, np.arange(-5.5, 5.6, 1.0))
tv_delta_churn = tv_merged.groupby(tv_delta).churned_all.mean() * 12 / 10 * 100
```

In [138]:
```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = tv_delta_churn.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('TV consumption trend')
    plt.ylabel('Annualized churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')
```

In [1651]:
```
tv_delta = pd.cut(tv_merged.TTV_201703_delta, np.arange(-5.5, 5.6, 1.0))
tv_delta_churn_some = tv_merged[at_least_some_ttv_mask].groupby(tv_delta[at_least_some_ttv_mas
```

In [1652]:
```
with plt.rc_context(rc=get_style(figsize=(12 ,8))):
    ax = tv_delta_churn_some.plot.bar(color=blue)
    plt.grid(axis='y')
    plt.xlabel('TV consumption trend')
    plt.ylabel('Annualized TV+Vodafone churn rate')
    plt.axhline(annual_tv_churn * 100, c='r', ls='--')
```

What is wrong with smelly code?

Smelly code might work right now, but in time it is going to have one or more of these issues:

- **Hard to read and test**: it is difficult to see an overall structure; understanding the code in one place requires checking other code all over
- **Coupled**: an update in one place requires several other changes in other places
- **Not flexible**: adding new functionality and modifying exiting features require extensive rewrites or hacks

Code should be as a construction block structure

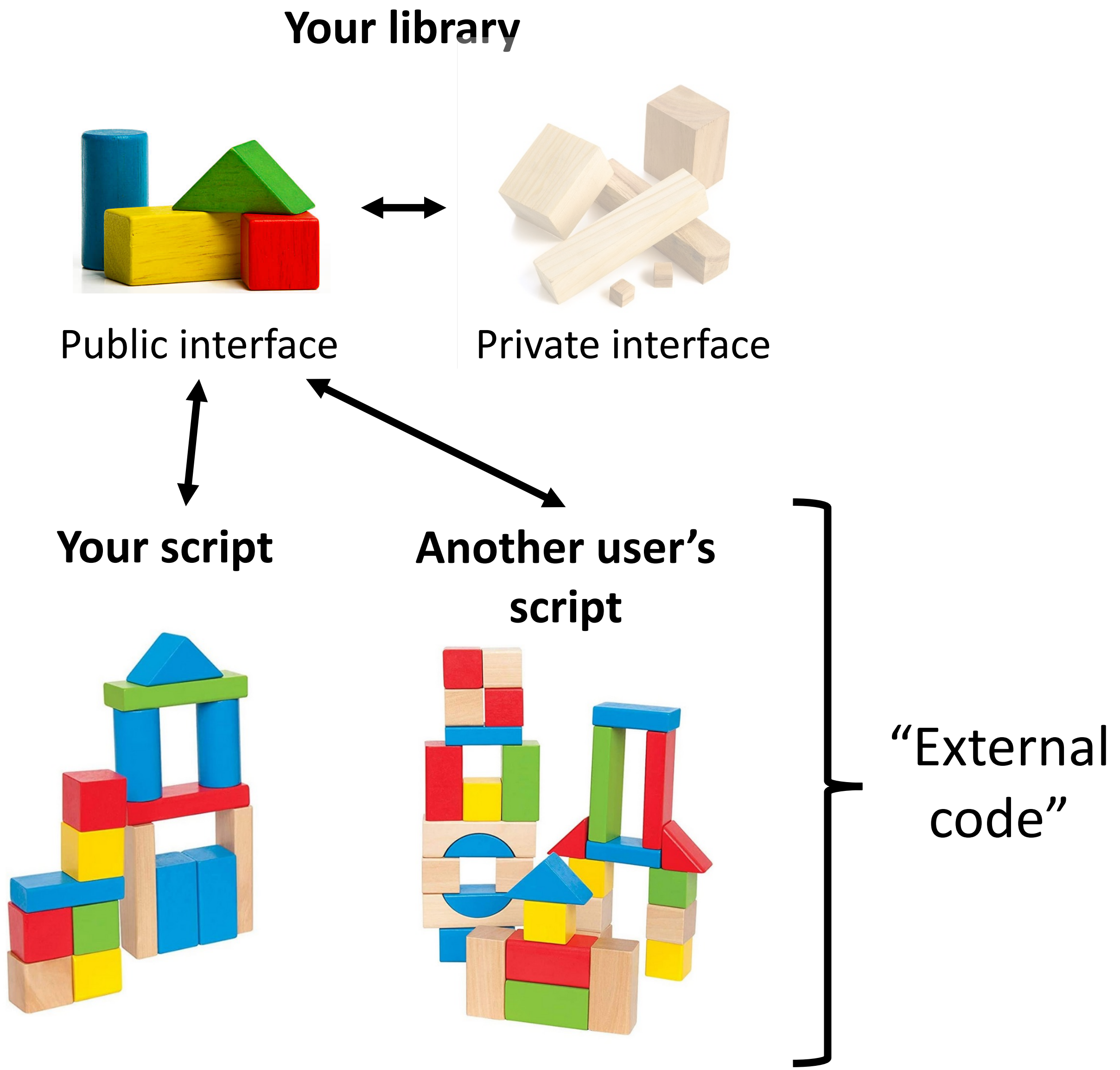
Functions and classes group together things that are coupled together and form the basic blocks.

We can easily and quickly rearrange the blocks to extend a structure or build a new one!

Flexible code is just like a block construction:

- is easy to understand in terms of blocks
- tolerates changes
- is reusable

Words that we'll say a lot



- Library vs external code
  - External code is anything that is not in your library: your script, 3rd party wanting to do other stuff, another library
- Interface, API
  - How you are supposed to call your library. The list of public functions and classes, and how to use them
- Public interface vs private interface
  - Changing the public interface forces all the external code to change

Chapter 1: Introduction to classes
Put together things that belong together

Classes live coding

Live Coding

`notebooks/01a_Classes.ipynb`

Hands-on

Add a new method to the Particle class

Exercise
`exercises/particle_update_position`

- Make the function `update_position` into a method of the class `Particle`.
- Where does the `position` of the particle belong? Modify the class constructor if necessary.
- Submit a PR for Issue #1 on GitHub.

Summary: Classes organize your code

```
def first_function(x, y, z):
    # Something

def second_function(x, y, z):
    # Something else

def third_function(x, y, z):
    # Something more
```

… becomes …

```
class Xyz:
    def __init__(self, x, y, z):
        ...
    def first_function(self):
        # Something
    def second_function(self):
        # Something else
    def third_function(self):
        # Something more
```

- Classes help us group data and functionalities that belong together
- When used judiciously, the code becomes more usable as we get rid of a lot of manual book-keeping; details are hidden away
- Understanding what belongs to the class and what does not is important to keep the code flexible!

Recap: Class structure

```
class MyClass:
    def __init__(self, param1, param2):
        self.param1 = param1
        if param2 is None:
            param2 = 12.3
        self.param2 = param2

    def my_method(self, foo, bar):
        result = self.param2 * foo + self.param2 * bar
        return result

    def to_json(self):
        params = {
            'param1': self.param1,
            'param2': self.param2,
        }
        return json.dumps(params)

    @classmethod
    def from_json(cls, json_str):
        json_dict = json.loads(json_str)
        instance = cls(json_dict['params1'], json_dict['params2'])
        return instance
```

The constructor is used to first populate an instance, called by convention “self”

Classes can define “methods”, i.e. functions that have access to the data stored in an instance

A ”class method” can be used to build an instance in some alternative way, e.g. using data from a file

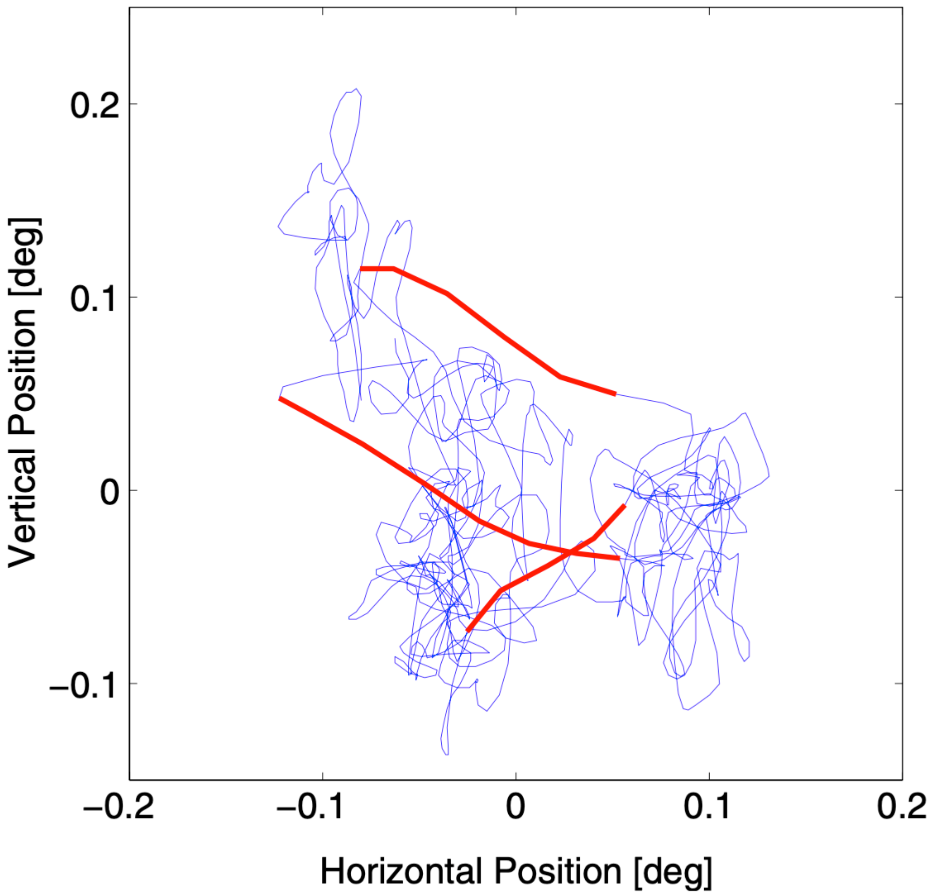
```
instance = MyClass(5, 18)
instance = MyClass.from_json(json_str)
```

Here is how you create instances from the constructor or a class method

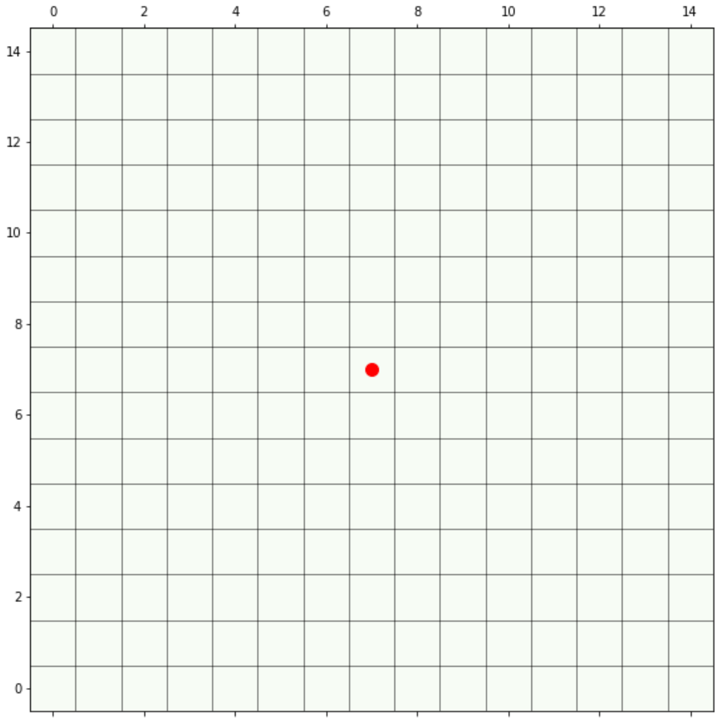
Chapter 2: Break out things that vary independently

Excursion: let’s walk!

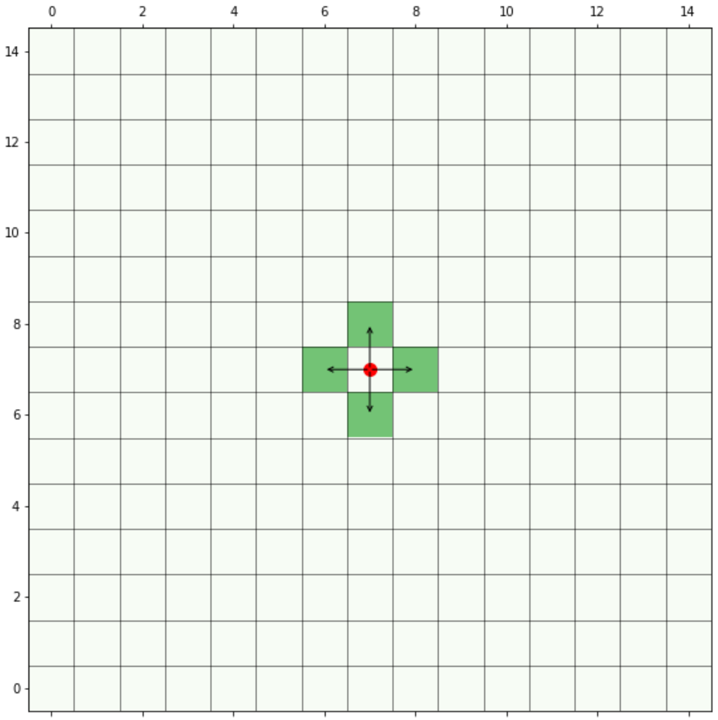
- Even when people think they are holding their eyes still, they still move around:
  - Drift, microsaccades, jitter
- The movement has statistical properties such as self avoidance, directional persistence…
- The upcoming exercise is a simplified version of a model Lisa is working on



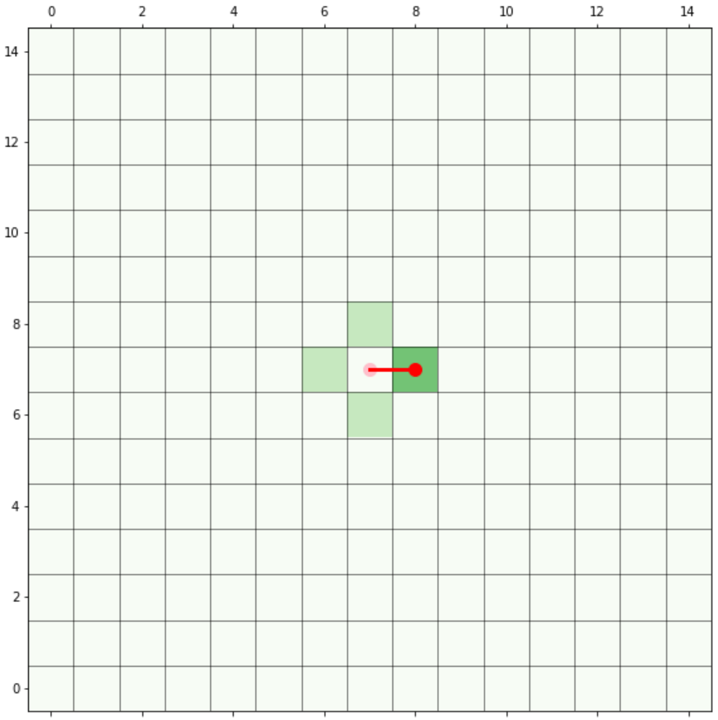
Excursion: let’s walk!



Walker starts somewhere

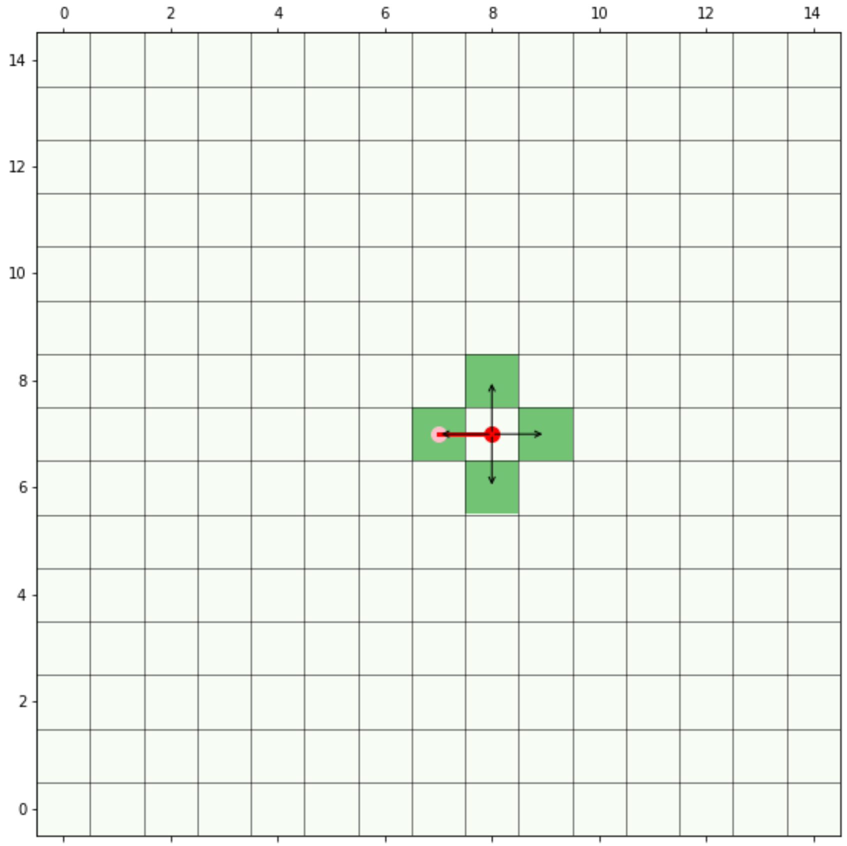


It could walk one step in any direction

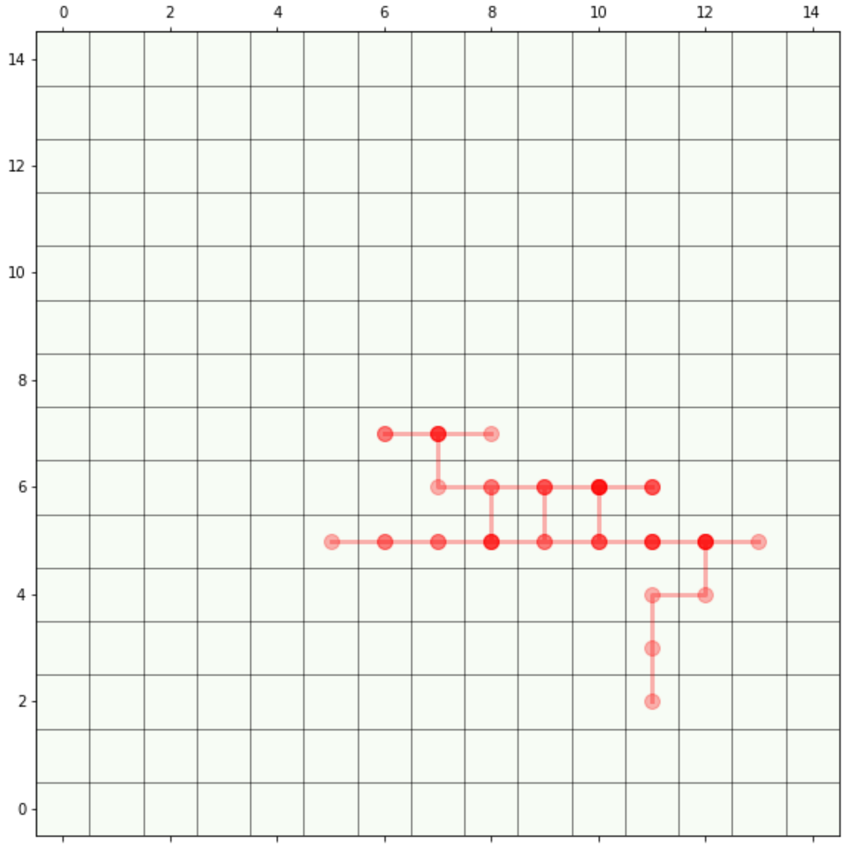


It randomly selects one step

Excursion: let’s walk!



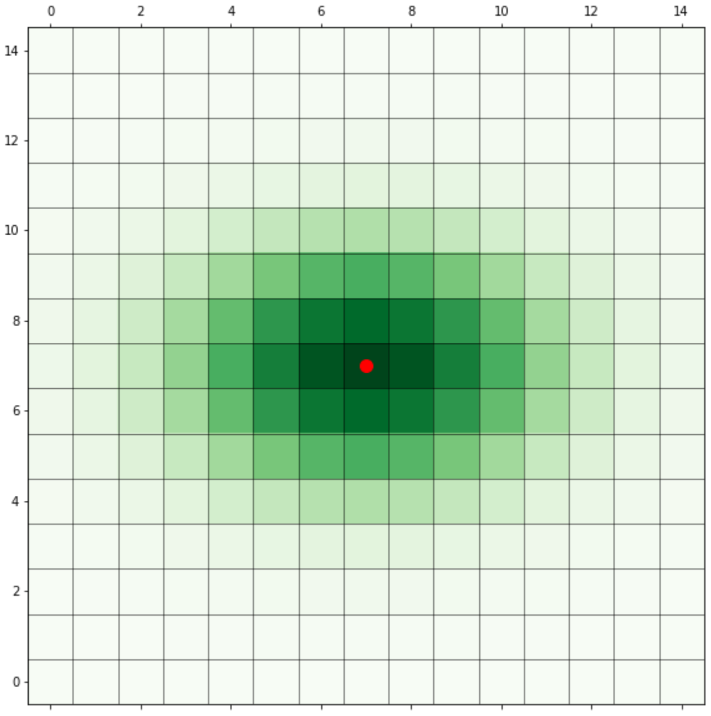
In the next step it has the same stepping options



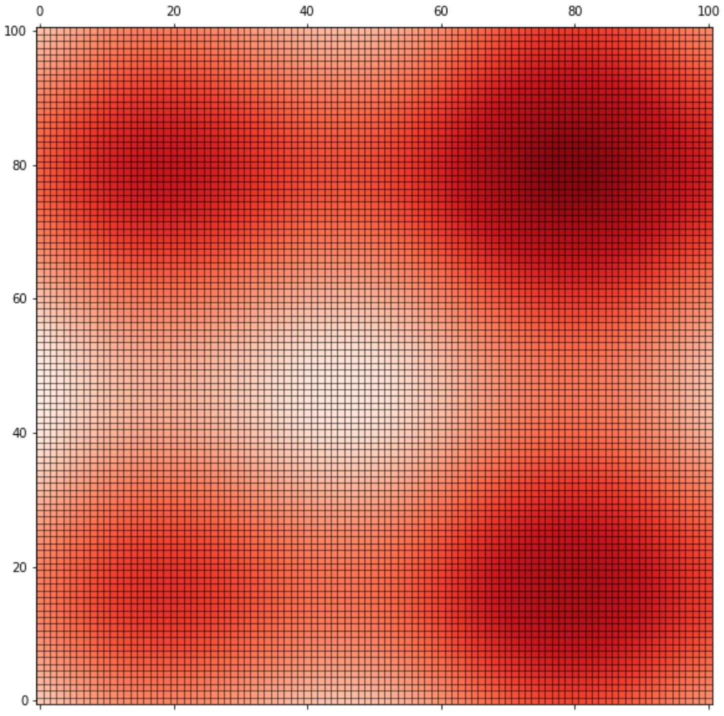
By iterating this procedure, we get a trajectory

Excursion: let’s walk!

- To make the behavior a little bit more interesting the walker in the exercise…
  - Choses its next step from a probability distribution
  - Can also walk over a non-uniform background, that influences how likely it is to go there



Stepping Probability

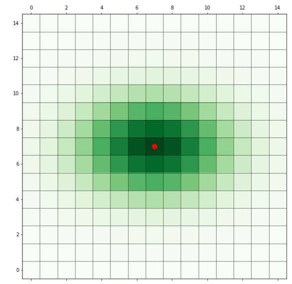


Background Activation

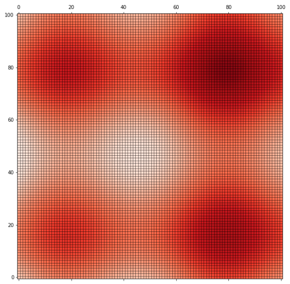
The walker Functions

Live Coding

walker/Step_0_Introduction/

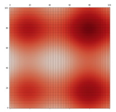
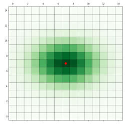


```
next_step_proposal(current_i, current_j, sigma_i, sigma_j, size)
```



```
create_context_map(size, map_type='flat')
```

```
sample_next_step(current_i, current_j, sigma_i, sigma_j, context_map,
random_state=np.random)
```

Combines  and  , and probabilistically selects the next location

Hands-on
General Notes

Exercise
walker/Step_1_classes/

- All the exercises in this class are about **reformatting code!** You are not expected to go into detail about how the code works- copy&pasting is fine!
- There are many ways to solve the exercises. **It is more important to think about the implementation choices with your partner than to finish**. We will give you working code to start from at each step, so don't worry about finishing!

Hands-on

Turning the walker code into a class

Exercise

walker/Step_1_classes/

- Open the notebook “Step_1_classes_exercise” and follow the instructions
- Submit a PR for Issue #2 on GitHub.

From…

```
i, j = 100, 50  # initial position
sigma_i, sigma_j = 3, 4  # parameters of the next step map
size = 200  # size of the image
context_map = create_context_map(size, 'hills')  # fixed context map

# Sample a next step 1000 times
trajectory = []
for _ in range(1000):
    i, j = sample_next_step(i, j, sigma_i, sigma_j, context_map)
    trajectory.append((i, j))
```

To… ?

```
walker = Walker(sigma_i=3, sigma_j=4, ...)

# Sample a next step 1000 times
…
```

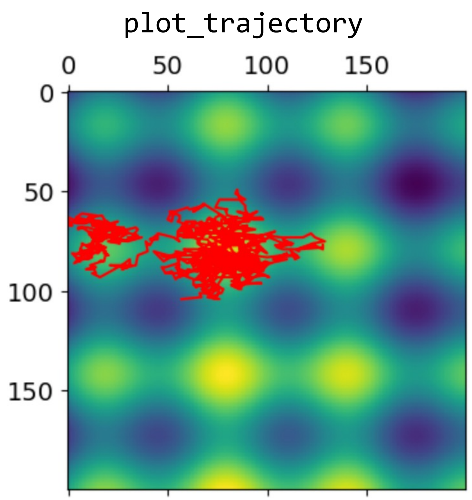
Plotting does not belong to the Walker

Live Coding
walker/Step_2_plotting/

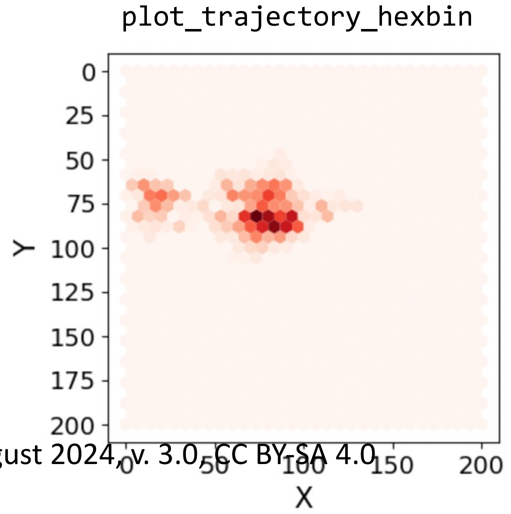
```python
import numpy as np
import matplotlib.pyplot as plt


class Walker:
    """ The Walker knows how to walk at random on a context map. """

    def __init__(self, sigma_i, sigma_j, size, map_type='flat'):
        # ...

    def plot_trajectory(self, trajectory):
        """ Plot a trajectory over a context map. """
        trajectory = np.asarray(trajectory)
        plt.matshow(self.context_map)
        plt.plot(trajectory[:, 1], trajectory[:, 0], color='r')
        plt.show()

    def plot_trajectory_hexbin(self, trajectory):
        """ Plot an hexagonal density map of a trajectory. """
        trajectory = np.asarray(trajectory)
        plt.hexbin(
            trajectory[:, 1], trajectory[:, 0],
            gridsize=30, extent=(0, 200, 0, 200),
            edgecolors='none', cmap='Reds'
        )
        plt.gca().invert_yaxis()
        plt.xlabel('X')
        plt.ylabel('Y')
```

1. Changing or adding new way of plotting (e.g. by a colleague) would require modifying the Walker’s code, without changing its behavior
2. Changing the Walker behavior will typically not modify the plotting code
3. Using your walker requires you to install matplotlib

These are smells of the fact that plotting varies independently of the Walker



vs.



The smells of the Walker constructor

```python
def __init__(self, sigma_i, sigma_j, size, map_type='flat'):
    self.sigma_i = sigma_i
    self.sigma_j = sigma_j
    self.size = size

    if map_type == 'flat':
        context_map = np.ones((size, size))
    elif map_type == 'hills':
        grid_ii, grid_jj = np.mgrid[0:size, 0:size]
        i_waves = np.sin(grid_ii / 130) + np.sin(grid_ii / 10)
        i_waves /= i_waves.max()
        j_waves = np.sin(grid_jj / 100) + np.sin(grid_jj / 50) + \
            np.sin(grid_jj / 10)
        j_waves /= j_waves.max()
        context_map = j_waves + i_waves
    elif map_type == 'labyrinth':
        context_map = np.ones((size, size))
        context_map[50:100, 50:60] = 0
        context_map[20:89, 80:90] = 0
        context_map[90:120, 0:10] = 0
        context_map[120:size, 30:40] = 0
        context_map[180:190, 50:60] = 0

        context_map[50:60, 50:200] = 0
        context_map[179:189, 80:130] = 0
        context_map[110:120, 0:190] = 0
        context_map[120:size, 30:40] = 0
        context_map[180:190, 50:60] = 0
    context_map /= context_map.sum()
    self.context_map = context_map

    # Pre-compute a 2D grid of coordinates for efficiency
    self._grid_ii, self._grid_jj = np.mgrid[0:size, 0:size]
```

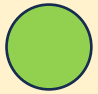
The smells of the Walker constructor

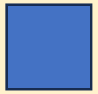
```python
def __init__(self, sigma_i, sigma_j, size, map_type='flat'):
    self.sigma_i = sigma_i
    self.sigma_j = sigma_j
    self.size = size

    if map_type == 'flat':
        context_map = np.ones((size, size))
    elif map_type == 'hills':
        grid_ii, grid_jj = np.mgrid[0:size, 0:size]
        i_waves = np.sin(grid_ii / 130) + np.sin(grid_ii / 10)
        i_waves /= i_waves.max()
        j_waves = np.sin(grid_jj / 100) + np.sin(grid_jj / 50) + \
            np.sin(grid_jj / 10)
        j_waves /= j_waves.max()
        context_map = j_waves + i_waves
    elif map_type == 'labyrinth':
        context_map = np.ones((size, size))
        context_map[50:100, 50:60] = 0
        context_map[20:89, 80:90] = 0
        context_map[90:120, 0:10] = 0
        context_map[120:size, 30:40] = 0
        context_map[180:190, 50:60] = 0

        context_map[50:60, 50:200] = 0
        context_map[179:189, 80:130] = 0
        context_map[110:120, 0:190] = 0
        context_map[120:size, 30:40] = 0
        context_map[180:190, 50:60] = 0
    context_map /= context_map.sum()
    self.context_map = context_map

    # Pre-compute a 2D grid of coordinates for efficiency
    self._grid_ii, self._grid_jj = np.mgrid[0:size, 0:size]
```

1. The constructor will become longer with more map types
2. We cannot contribute a new map type without modifying the code
3. It is difficult to test
4. It is not flexible, e.g. what happens if we want to create an instance from a context map saved on file?

These are smells of the fact that the initialization of context_map varies independently of the Walker

`if … elif … else` chain is often the smell of independent plug-in blocks

```
def add_block(blocks, size, type):

    if type == ‘circle’:
        # build circle of given size
        block =
```


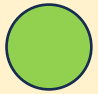
```
    elif type == ‘square’:
        # build square of given size
        block =
```


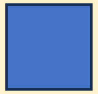
```
    elif type == ‘triangle’:
        # build triangle of given size
        block =
```


```
    blocks.append(block)
```

```
add_block(blocks, size=11,
             type=‘square’)
```

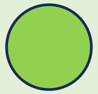
`if … elif … else` chain is often the smell of independent plug-in blocks

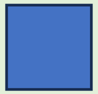
```
def add_block(blocks, size, type):

   if type == 'circle':
      # build circle of given size

      block =
```


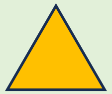
```
   elif type == 'square':
      # build square of given size

      block =
```


```
   elif type == 'triangle':
      # build triangle of given size

      block =
```


```
   blocks.append(block)
```

```
def build_circle(size):
   """ Build a circle. """

   return
```


```
def build_square(size):
   """ Build a square. """

   return
```


```
def build_triangle(size):
   """ Build a triangle. """

   return
```


```
def add_block(blocks, block):
   blocks.append(block)
```

```
add_block(blocks, size=11,
          type='square')
```

```
block = build_square(size=11)
add_block(blocks, block)
```

Hands-on

Move context map creation to separate module

Exercise

`Walker/Step_3_break_out ...`

- Go to the Notebook and follow the instructions there
- Submit a PR for Issue #3 on GitHub

New requirement: we need to use different next-step proposals for different experiments

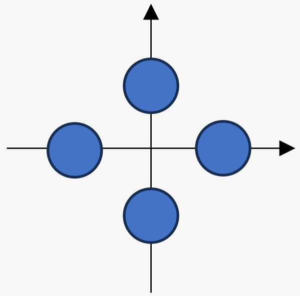
```python
class Walker:
    # ...

    def sample_next_step(self, current_i, current_j, random_state=np.random):
        """ Sample a new position for the walker. """
        # Combine the next-step proposal with the context map to get a
        # next-step probability map
        next_step_map = self._next_step_proposal(current_i, current_j)
        selection_map = self._compute_next_step_probability(next_step_map)

        # Draw a new position from the next-step probability map
        r = random_state.rand()
        cumulative_map = np.cumsum(selection_map)
        cumulative_map = cumulative_map.reshape(selection_map.shape)
        i_next, j_next = np.argwhere(cumulative_map >= r)[0]

        return i_next, j_next

    def _next_step_proposal(self, current_i, current_j):
        """ Create the 2D proposal map for the next step of the walker. """
        # 2D Gaussian distribution , centered at current position,
        # and with different standard deviations for i and j
        grid_ii, grid_jj = self._grid_ii, self._grid_jj
        sigma_i, sigma_j = self.sigma_i, self.sigma_j

        rad = (
            (((grid_ii - current_i) ** 2) / (sigma_i ** 2))
            + (((grid_jj - current_j) ** 2) / (sigma_j ** 2))
        )

        p_next_step = np.exp(-(rad / 2.0)) / (2.0 * np.pi * sigma_i * sigma_j)
        return p_next_step / p_next_step.sum()
```

- We would like to run some experiments with a Gaussian next step proposal, some with a rectangular proposal, etc.
- **How can we do that?**

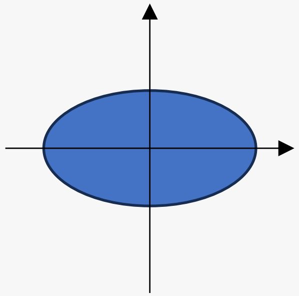
The inheritance solution

```python
class Walker:
    # ...

    def _next_step_proposal(self, current_i, current_j):
        """ Create the 2D proposal map for the next step of the walker. """
        raise NotImplementedError("`_next_step_proposal` not implemented")
```

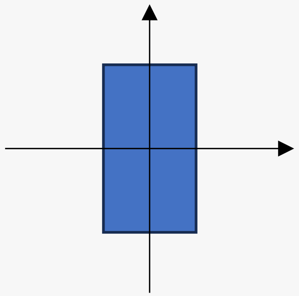
```python
class JumpingWalker(Walker):
    # ...

    def _next_step_proposal(self, current_i, current_j):
```



```python
class GaussianWalker(Walker):
    # ...

    def _next_step_proposal(self, current_i, current_j):
```



```python
class RectangularWalker(Walker):
    # ...

    def _next_step_proposal(self, current_i, current_j):
```



The problem with inheritance

New requirement: the way of combining next step proposal and context map can also vary

```
class Walker:
    # ...


    def _compute_next_step_probability(self, next_step_map):
        """ Compute the next step probability map from next step proposal and
        context map. """
        next_step_probability = next_step_map * self.context_map
        next_step_probability /= next_step_probability.sum()
        return next_step_probability
```

This combination can now be done through product, sum, or other

The problem with inheritance

The inheritance approach leads to a **combinatorial explosion of subclasses**

```
Gaussian                  Product
Rectangular        x      Sum
Jumping
```

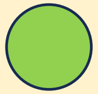
```python
class GaussianWalkerWithProductInteraction(Walker):
    def _next_step_proposal(self, current_i, current_j):
        # ...
    def _compute_next_step_probability(self, next_step_map):
        # ...


class GaussianWalkerWithSumInteraction(Walker):
    def _next_step_proposal(self, current_i, current_j):
        # ...
    def _compute_next_step_probability(self, next_step_map):
        # ...


class RectangularWalkerWithProductInteraction(Walker):
    def _next_step_proposal(self, current_i, current_j):
        # ...
    def _compute_next_step_probability(self, next_step_map):
        # ...


class RectangularWalkerWithSumInteraction(Walker):
    def _next_step_proposal(self, current_i, current_j):
        # ...
    def _compute_next_step_probability(self, next_step_map):
        # ...
```

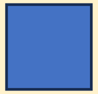
Passing varying behavior (e.g. functions) as an argument is usually a better alternative

```
class Walker:
    def __init__(self, size, context_map, next_step_proposal, next_step_proposal_arguments):
        self.next_step_proposal = next_step_proposal
        # ...


    def sample_next_step(self, current_i, current_j, random_state=np.random):
        """ Sample a new position for the walker. """
        # Combine the next-step proposal with the context map to get a
        # next-step probability map
        next_step_map = self.next_step_proposal(current_i, current_j, **next_step_proposal_arguments)
        selection_map = self._compute_next_step_probability(next_step_map)

        # Draw a new position from the next-step probability map
        r = random_state.rand()
        cumulative_map = np.cumsum(selection_map)
        cumulative_map = cumulative_map.reshape(selection_map.shape)
        i_next, j_next = np.argwhere(cumulative_map >= r)[0]

        return i_next, j_next
```

In this way, we can **define the behavior independently** of the class, avoiding the combinatoric explosion

`if … elif … else` chain is often the smell of independent plug-in blocks

```
def add_block(blocks, size, type):

    if type == ‘circle’:
        # build circle of given size

        block =
```


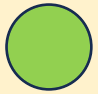
```
    elif type == ‘square’:
        # build square of given size

        block =
```


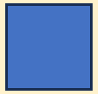
```
    elif type == ‘triangle’:
        # build triangle of given size

        block =
```


```
    blocks.append(block)
```

```
add_block(blocks, size=11,
          type=‘triangle’)
```

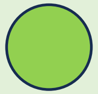
`if … elif … else` chain is often the smell of independent plug-in blocks

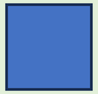
```
def add_block(blocks, size, type):

    if type == ‘circle’:
        # build circle of given size

        block =
```


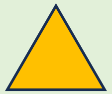
```
    elif type == ‘square’:
        # build square of given size

        block =
```


```
    elif type == ‘triangle’:
        # build triangle of given size

        block =
```


```
    blocks.append(block)
```

```
def build_circle(size):
    """ Build a circle. """

    return
```


```
def build_square(size):
    """ Build a square. """

    return
```


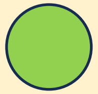
```
def build_triangle(size):
    """ Build a triangle. """

    return
```


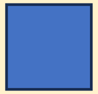
```
def add_block(blocks, block):
    blocks.append(block)
```

```
add_block(blocks, size=11,
          type=‘triangle’)
```

```
block = build_triangle(size=11)
add_block(blocks, block)
```

`if … elif … else` chain is often the smell of independent plug-in blocks

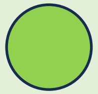
```
def add_block(blocks, size, type):

    if type == ‘circle’:
        # build circle of given size
        block =
```


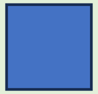
```
    elif type == ‘square’:
        # build square of given size
        block =
```


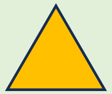
```
    elif type == ‘triangle’:
        # build triangle of given size
        block =
```


```
    blocks.append(block)
```

```
add_block(blocks, size=11,
              type=‘square’)
```

```
def build_circle(size):
    """ Build a circle. """
    return
```


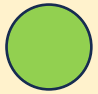
```
def build_square(size):
    """ Build a square. """
    return
```


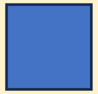
```
def build_triangle(size):
    """ Build a triangle. """
    return
```


```
def add_block(blocks, size, block_builder):
    block = block_builder(size)
    blocks.append(block)
```

```
add_block(blocks, size=11,
              build_triangle)
```

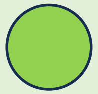
`if … elif … else` chain is often the smell of independent plug-in blocks

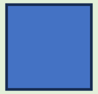
```
def add_block(blocks, size, type):

    if type == ‘circle’:
        # build circle of given size

        block =
```


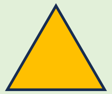
```
    elif type == ‘square’:
        # build square of given size

        block =
```


```
    elif type == ‘triangle’:
        # build triangle of given size

        block =
```


```
    blocks.append(block)
```

```
def build_circle(size):
    """ Build a circle. """

    return
```


```
def build_square(size):
    """ Build a square. """

    return
```


```
def build_triangle(size, angle):
    """ Build a triangle. """

    return
```


```
def add_block(blocks, size, block_builder, kw_args):
    block = block_builder(**kw_args)
    blocks.append(block)
```

```
add_block(blocks, size=11,
          type=‘square’)
```

```
add_block(blocks, size=11,
          build_triangle, {‘angle’: 35})
```

Hands-on
Implement two next-step proposals

Exercise

`walker/Step_4_break_out ...`

- Follow the instructions in the Notebook!
- Submit a PR for Issue #4 on GitHub.

The Walker: what have we achieved?

- We can run simulations with **different combinations** of context maps and next step proposals
- New context maps and next step proposals can be **contributed** by external people **without changing the code** in your package, or even knowing how it works
- We achieved **flexibility** and **openness to change**

Chapter 3: Separate what varies at the level of projects

The holy trinity of scientific computing

1. Provenance
2. Reproducibility
3. Organization

The holy trinity of scientific computing

1. Provenance

It needs to be clear **where** data and plots come from, **when** and **how** they were generated

2. Reproducibility

All information necessary to **get the same result** needs to be saved

3. Organization

For your own sanity, you should have a **consistent system** for all this **data** and **artefacts**

1. Provenance

- Data Provenance, or lineage, documents **where** data comes from
- Recording **when** and **by which** code the dataset has been changed
- But HOW?
  - External software? Usually not specific for scientific use case.
  - Folder structure/Filenames?
  - Code generated meta-information files? (see next slide)
- In case of plots:
  - data that generated the plots
  - For work in progress plots: plt.annontate()
  - Save .ipynb as pdf (with all the paths/version information in the notebook)
  - Could use metadata in images https://github.com/dfm/savefig

2. Reproducibility

- Save all information necessary to get the same result again
  - All input parameters to the code
  - Randomness- if used, save the seed
  - Which version of the code was used?

- Serialization of intermediate steps in the code (estimation and analysis)

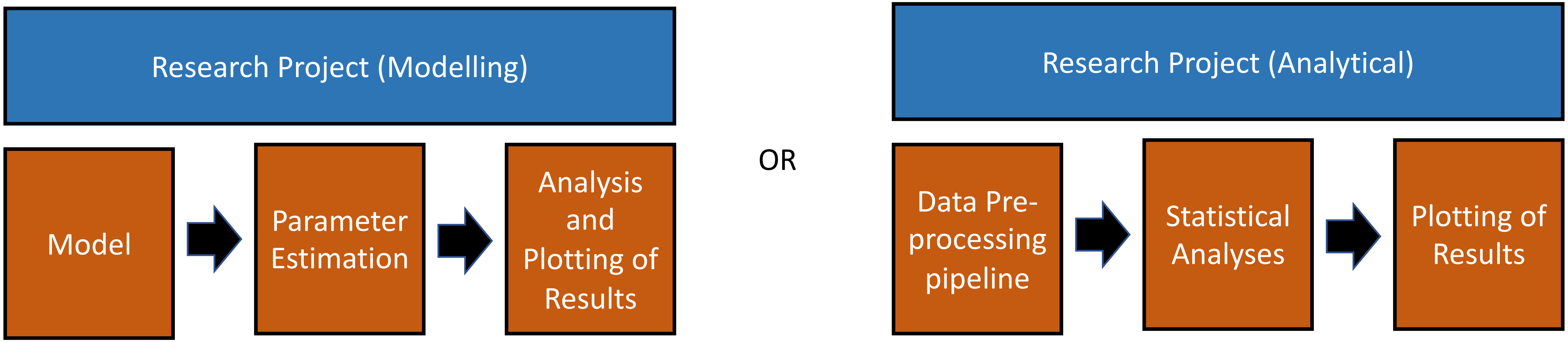
```python
import git
import time

curr_time = time.strftime("%Y%m%d-%H%M%S")

repo = git.Repo(search_parent_directories=True)
sha = repo.head.object.hexsha

with open('meta.txt', 'w') as f:
    f.write(f'I estimated parameters at {curr_time}.\n')
    f.write(f'The git repo was at commit {sha}')
```

2. Reproducibility

- We also recommend using file names containing a version number or a time stamp, so that two subsequent runs do not overwrite previous results

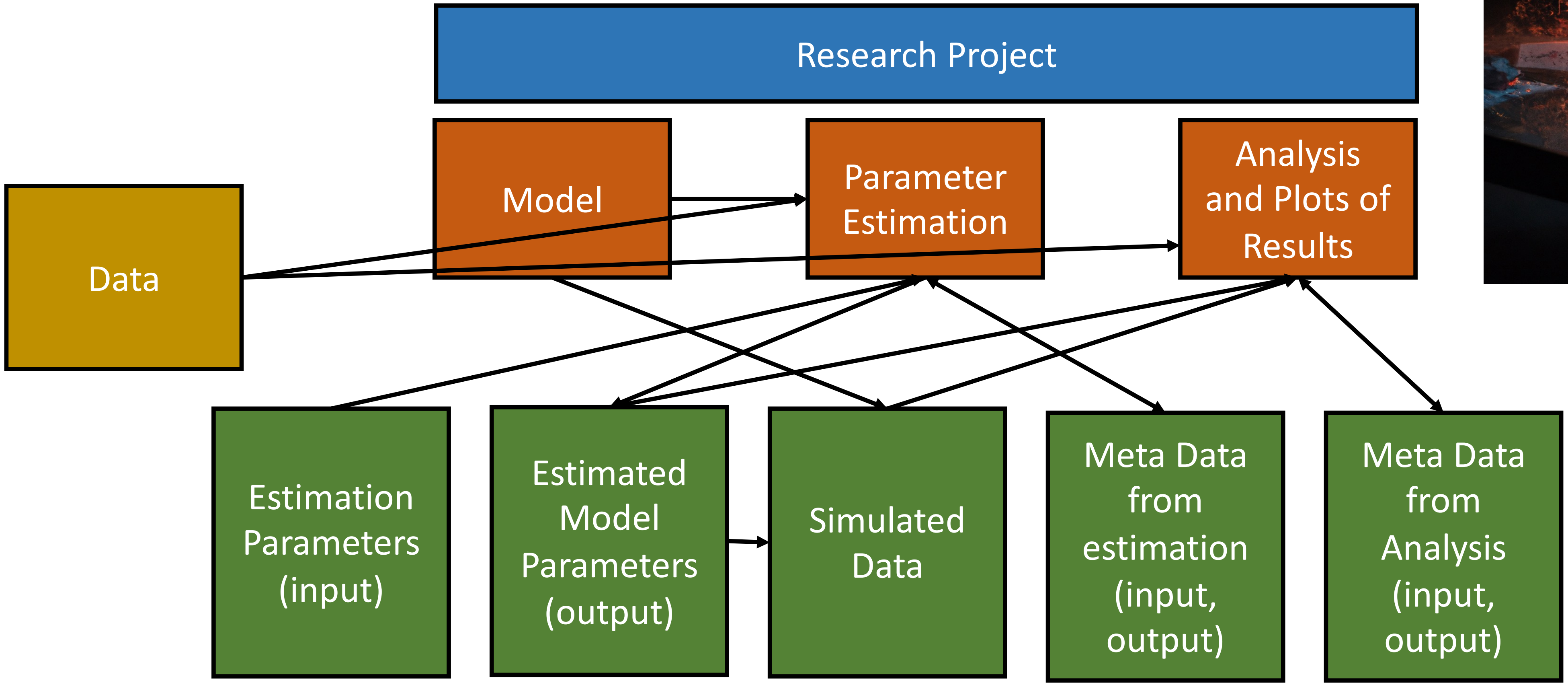
```python
# STEP 4: Save the trajectory
curr_time = time.strftime("%Y%m%d-%H%M%S")
np.save(f"sim_{curr_time}", trajectory)
```

3. Organization



- Your research project may look something like this (or maybe you have different steps or a subset of steps)
- In any case it is likely that you will go through the steps many times before you‘re ready to publish your work

3. Organization

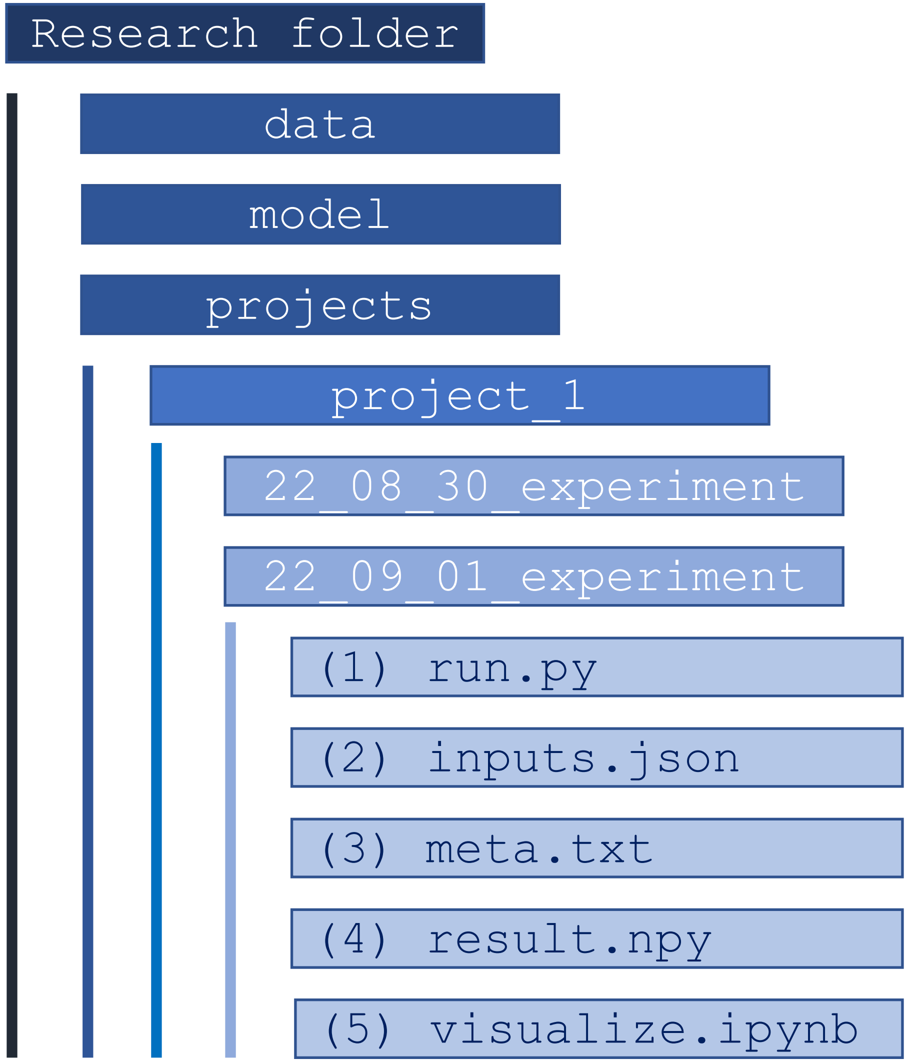


Each run has a bunch of associated data resulting folders and folders of data where no one knows which version of the code generated it or is using it!

3. Organization

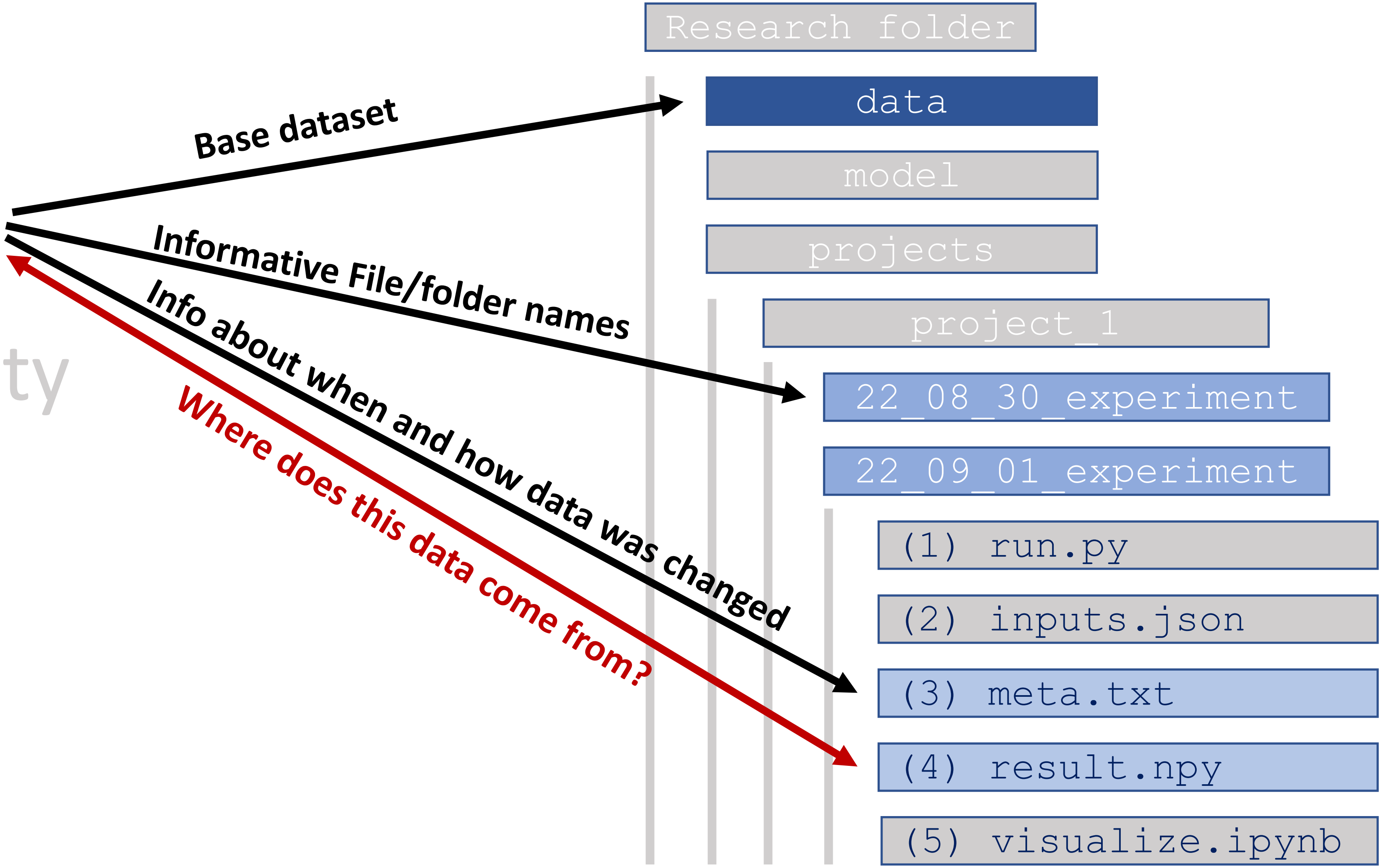
Suggestion:

- Data should always be separated from code
- The model or algorithms or things that are applied to your data should be packages (see packaging lecture)
- Think of “runs” as Experiments. Each experiment has its own folder. The folder contains:
  1. **Minimal code** that calls the model and saves the result
  2. All **inputs** necessary to produce the result saved separately
  3. **Meta information** about which version of your code was used (and maybe a note about what you were trying to achieve, if you want to be extra nice to future you)
  4. The **result**
  5. Maybe the visualization of the result



Organization

1. Provenance
2. Reproducibility
3. Organization

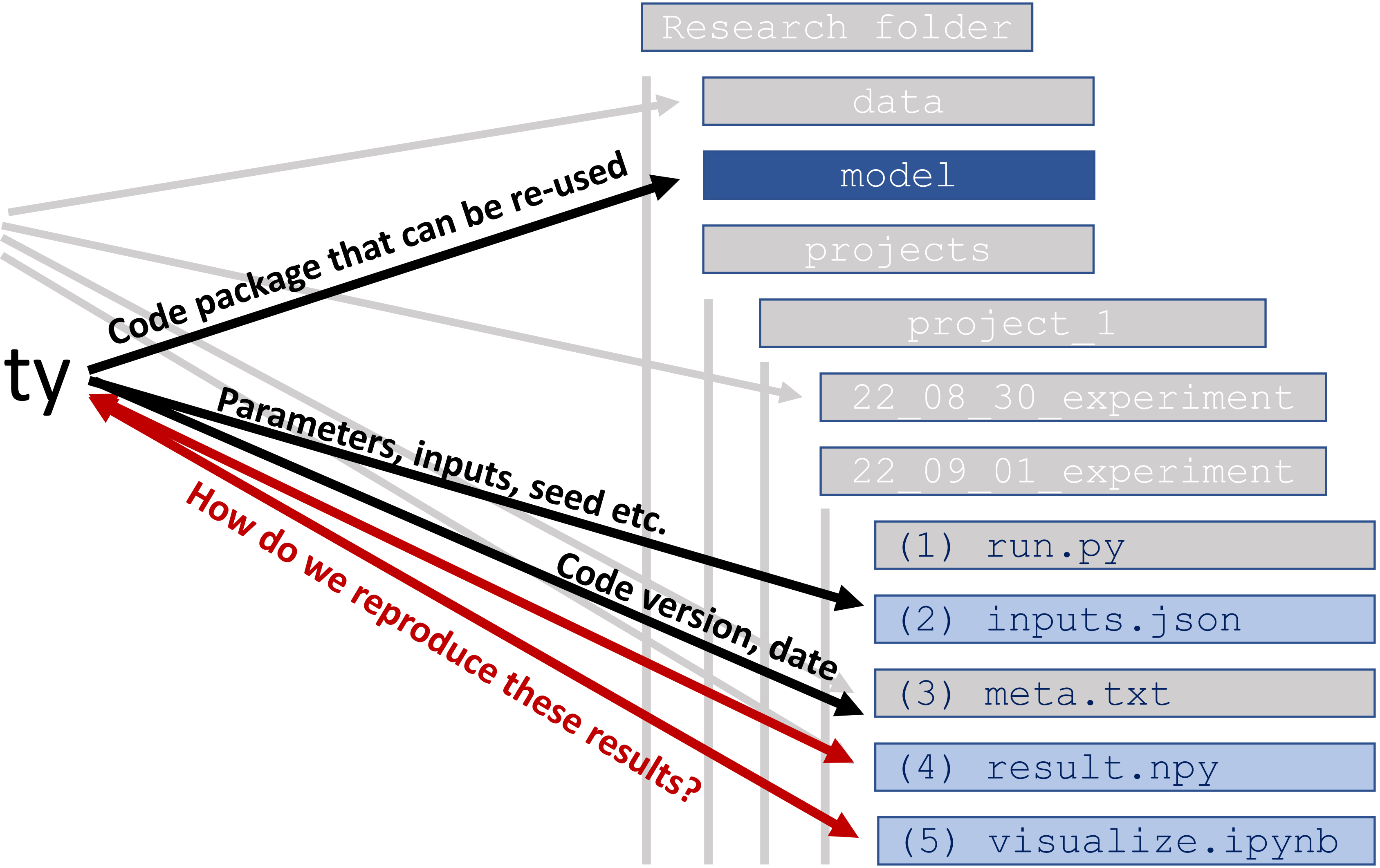


Organization

1. Provenance

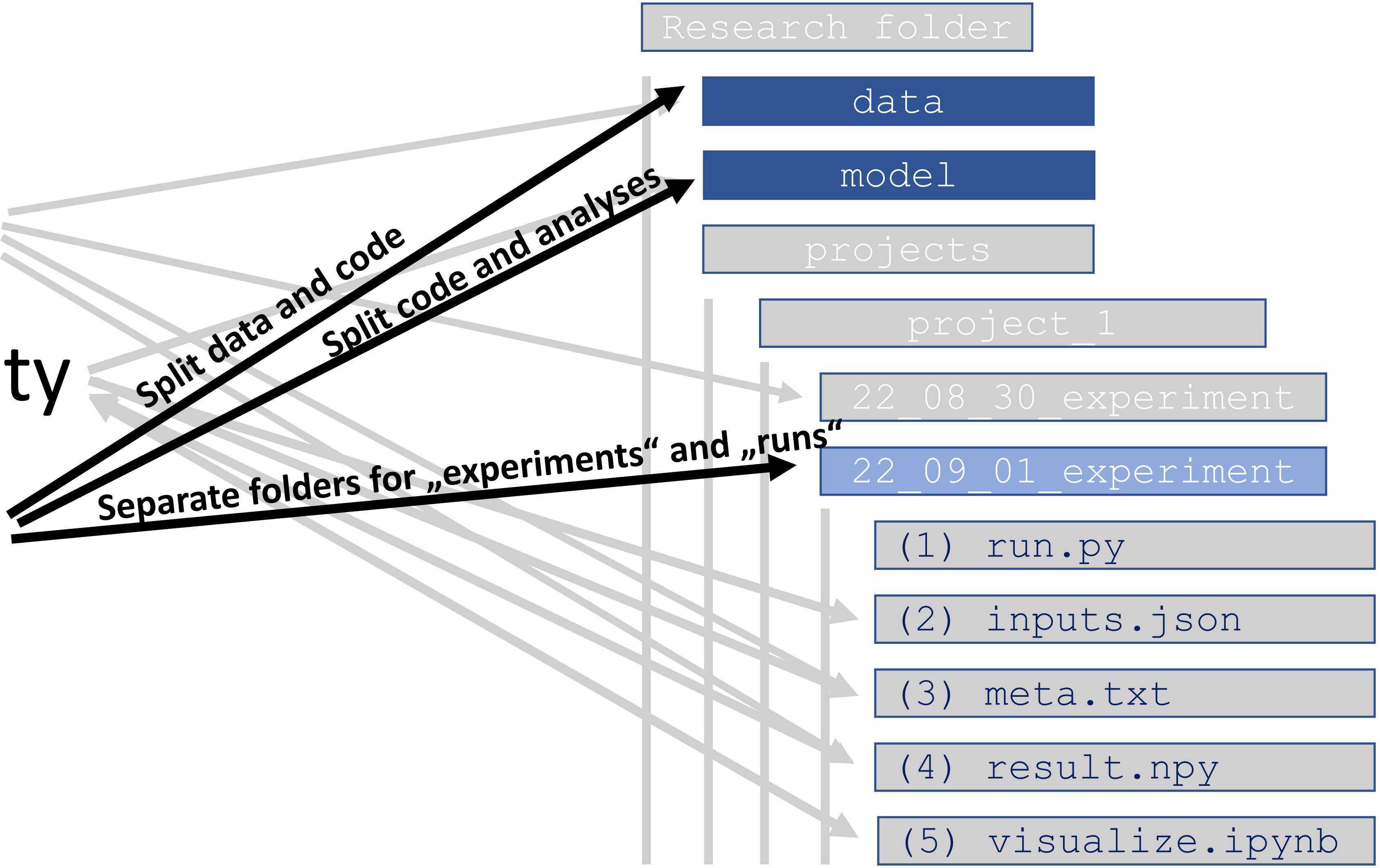
2. Reproducibility

3. Organization



Organization

1. Provenance
2. Reproducibility
3. Organization



Hands On
Provenance and Reproducibility

Exercise
`walker/Step_5_reproducibility/`

Go through the following steps:

1. Complete the run.py script
   - In the file, at the top we give the desired parameters for the run
   - create a context map and walker (see previous exercises for reference)
   - simulate a trajectory (see previous exercises for reference)
2. Save the trajectory using `np.save()`, and also save some metadata
3. Run the run.py script twice and confirm the results are identical by plotting them using the provided notebook
4. Submit PR for Issue #5 on GitHub

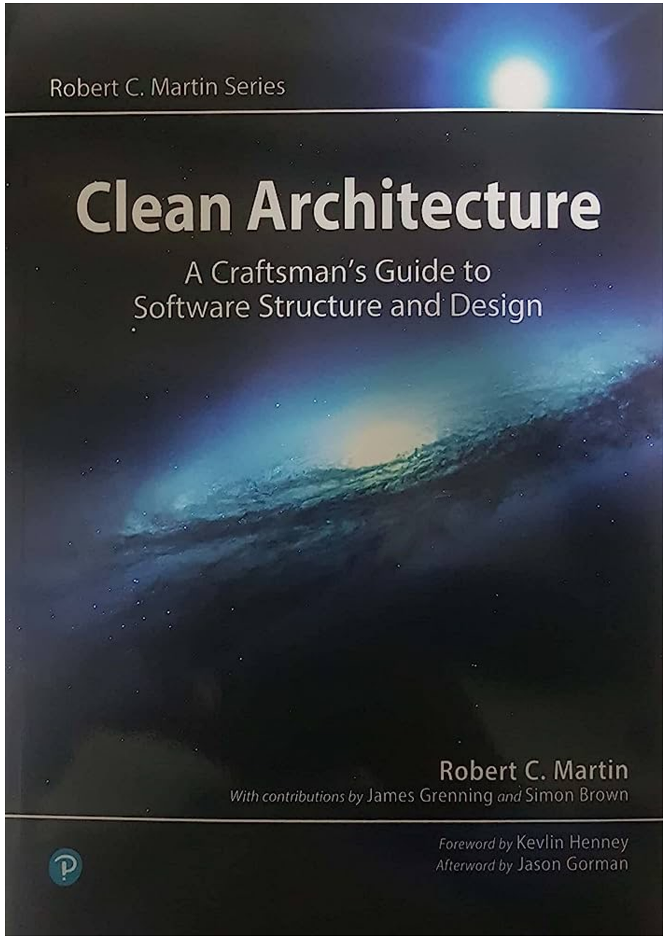
Live Coding

walker/Step_6_load_parameters_...

Provenance and Reproducibility

Where to go from here…

- Trust your nose! When your code smells, spend some time figuring out where the smell come from
- Don’t get carried away: over-engineering counts as premature optimization



Thank you!

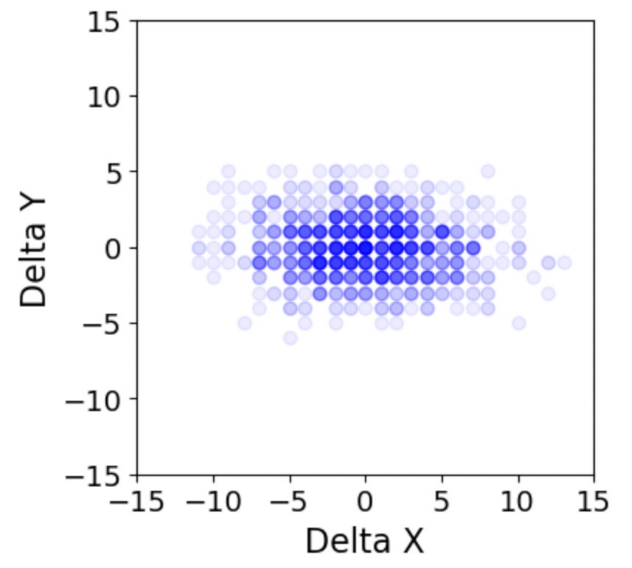
Hands-on

Move plotting code to a new module

Exercise

walker/Step 2 plotting/

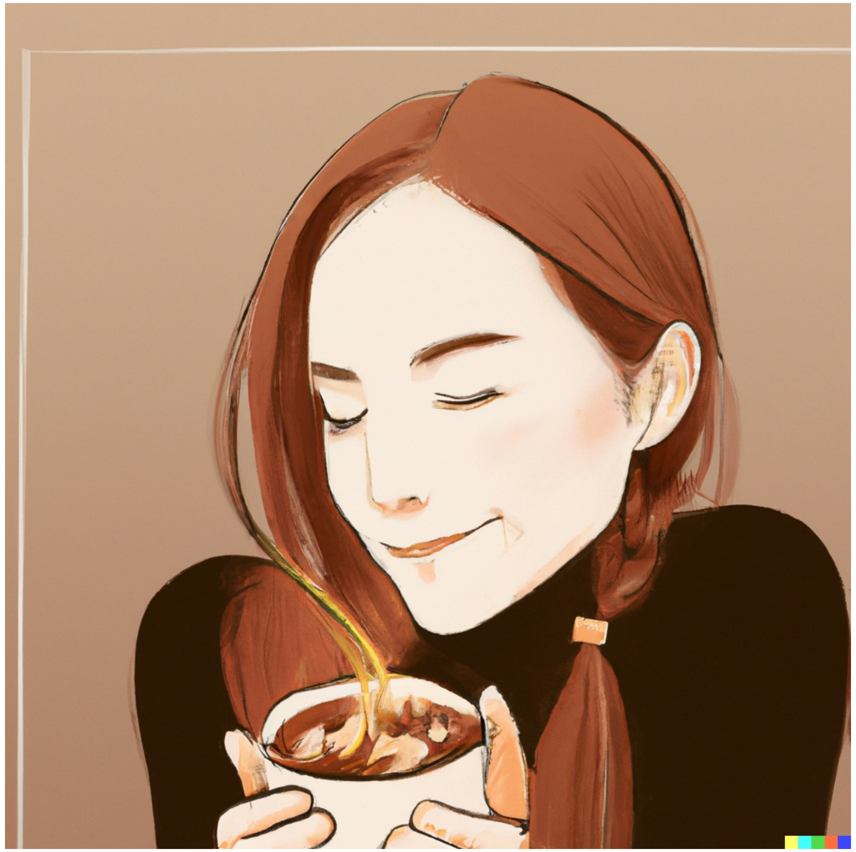
- Move plotting code to a separate plotting.py module
- Modify the notebook to import the plots and make sure it runs
- Add a new plotting function, `plot_delta_trajectory`, that plots a scatter plot of delta_x and delta_y for a (x, y) trajectory. Observe how we did not have to touch the walker.py file at all.
- Submit a PR for Issue #2 on GitHub.



Here is how to fix it, class dismissed

What are you missing? A few patterns that make your code odor as nice as a spring meadow

1. Group together things that belong together
2. Break out things that vary independently
3. Keep code open for extension



Keep things open for extension

Bonus material

Hooks patterns

Bonus material

- common cases:
  - in graph traversing algorithms (e.g., depth-first search) the graph traversing is generic, but the operation to be done with the data on the nodes is specific to the application. Graph libraries often implement the traverversing, and allow implementing the operation through hooks (hook when first visiting node, and when all children are visited on the way back)
  - in some UI frameworks, hooks can be added to react to certain UI events

Architecture discussion?

- walker.from_data(data)
- walker.fit(data)
- walker_from_data(data), return fitted instance
- fit(walker, data), return parameters

- trajectory from walker
- walker.trajectory(n_steps) (hooks might be useful)
- trajectory(walker, n_steps) (hooks not so useful – just write another trajectory creator)

What is an API?

- How is the interface between your code and your manager scripts?
- Other things to consider when writing your code:
  - Who will be using it?
    - Maybe your code has a practical application
    - Even if it‘s most likely no one, imagine someone trying to replicate your research after you publish
  - Are there parts of the code you may want to use in your next project?
    - E.g. a fitting algorithm can be reused when you move on to the next model
    - E.g. a class for your data may be reusable for the next dataset