Test -Driven Development in Astronomy

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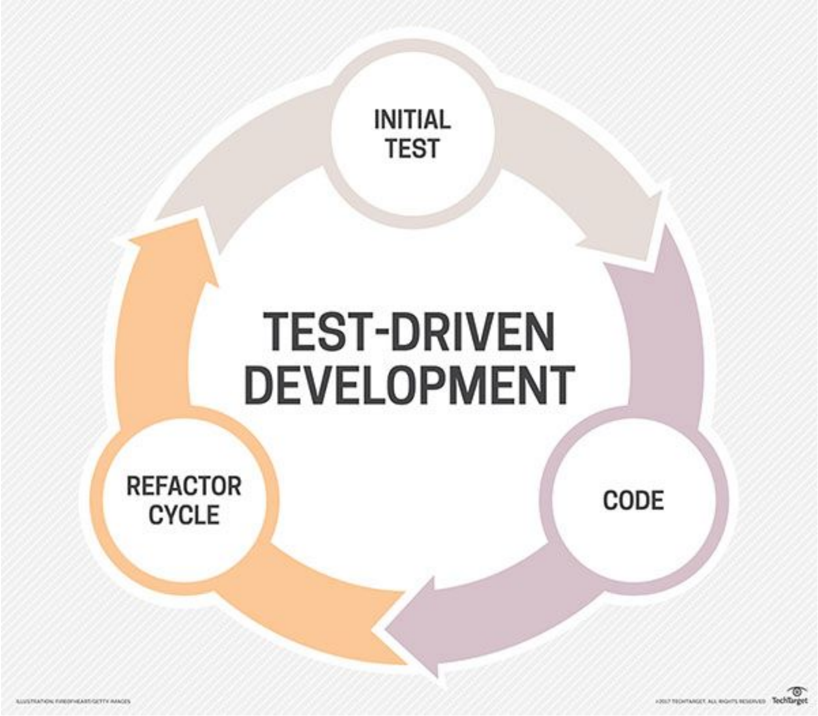
Credit:

Richard Hayes



The Astronomer’s Development Cycle

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- **Step 1:** Write Code.

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The Astronomer’s Development Cycle

- **Step 1:** Write Code.
- **Step 2:** Write more code.
- **Step 3:** Keep writing code, it’ll eventually work.
- **Step 4:** I think it does what its supposed to, I better not change it.
- **Step 5 (6 months later):** :(

```fortran
! Allocate variables to store each pixels neighbours
allocate (CompPix(maxval(g_degree(:)+1)), dist_fast(maxval(g_degree(:)+1)) )

! Subpix counts which subpixel we are currently on
subpix = 0

!Use NN to allocate all subgridded pixels to nearest cluster centre
do I = 1, Image_Pix(ImNo)
   do J = 1, Src_isub(ImNo)**2

      ! The subpixels 'host' image / source pixel (the source pixel that was allocated to the sub pixels host image pixel)
      if ( (Src_Cluster_Sparse .eq. 'Off') ) then
         CompPix(1) = cluster_index(I)
      elseif ( Src_Cluster_Sparse .eq. 'On') then
         CompPix(1) = cluster_index_Sparse(Src_Sparse_Grid_IpPair(I,ImNo))
      end if

      ! Calculate the distance of this sub-pix to its 'host' source pixel ...
      subpix = subpix + 1
20    dist_fast(1) =  (Source_XY_isub_Arc(1,subpix,ImNo) - centers(1,CompPix(1)))**2 +  (Source_XY_isub_Arc(2,subpix,ImNo) - centers(2,CompPix(1)))**2

      ! ... and all of that source pixels neighbours
      do K = 2, g_degree(CompPix(1))+1
         if (g_neighbour(g_start(CompPix(1))+K-2) .gt. 0) then
            CompPix(K) = g_neighbour(g_start(CompPix(1)) + K-2)
            dist_fast(K) =  (Source_XY_isub_Arc(1,subpix,ImNo) - centers(1,CompPix(K)))**2 +  (Source_XY_isub_Arc(2,subpix,ImNo) - centers(2,CompPix(K)))**2
         else
            dist_fast(K) = 1.e8
         end if

      end do

      ! Find the sub-pixels closest source pixel
      list = CompPix(minloc(dist_fast(1:K-1)))

      ! If the closest source pixel was a neighbouring pixel and not its 'host' pixel, then we don't know this is its nearest neighbour.
      ! Therefore, set this new source pixel as its 'host' and redo the calc above, until the host is the closest
      if (CompPix(1) .ne. list(1)) then
         CompPix(1) = list(1)
         go to 20
      end if

      ! If the host was the closter, allocate in 'cluster_index_isub' and go on to next sub-pixel
      cluster_index_isub(subpix) = list(1)

   end do

   if ( Src_Cluster_Sparse .eq. 'On') then

21    dist_fast(1) =  (Source_XY_Arc(1,I,ImNo) - centers(1,CompPix(1)))**2 +  (Source_XY_Arc(2,I,ImNo) - centers(2,CompPix(1)))**2
```

The Astronomer’s Development Cycle

- **Structure and Planning is the difference between surgery...**

The Astronomer’s Development Cycle

- Structure and Planning is the difference between surgery and cutting people’s bodies open.

The Astronomer’s Development Cycle

- Structure and Planning is the difference between surgery and cutting people’s bodies open.
- We as astronomers are not taught or encouraged to write code in a way that uses structure or planning.
- Enter – Test-Driven Development.

The Test-Driven Development Cycle

The Test-Driven Development Cycle

- **Step 1: Write a unit test.**

code.py | test_code.py

```python
import pytest

import code

def test__add_integers__input_one_and_one__result_is_two():

    result = code.add_integers(1,1)

    assert result == 2
```

The Test-Driven Development Cycle

- **Step 1: Write a unit test.**
- **Step 2: Run the test, check it fails.**

```
==================================== FAILURES ====================================
_____________ test__add_integers__input_one_and_one__result_is_two _____________

    def test__add_integers__input_one_and_one__result_is_two():

>       result = code.add_integers(1,1)
E       AttributeError: module 'code' has no attribute 'add_integers'

test_code.py:7: AttributeError
=========================== 1 failed in 0.03 seconds ===========================
Process finished with exit code 0
```

The Test-Driven Development Cycle

- **Step 1: Write a unit test.**
- **Step 2: Run the test, check it fails.**
- **Step 3: Write the Code.**

code.py × test_code.py ×

```python
def add_integers(integer_one, integer_two):
    return integer_one + integer_two
```

The Test-Driven Development Cycle

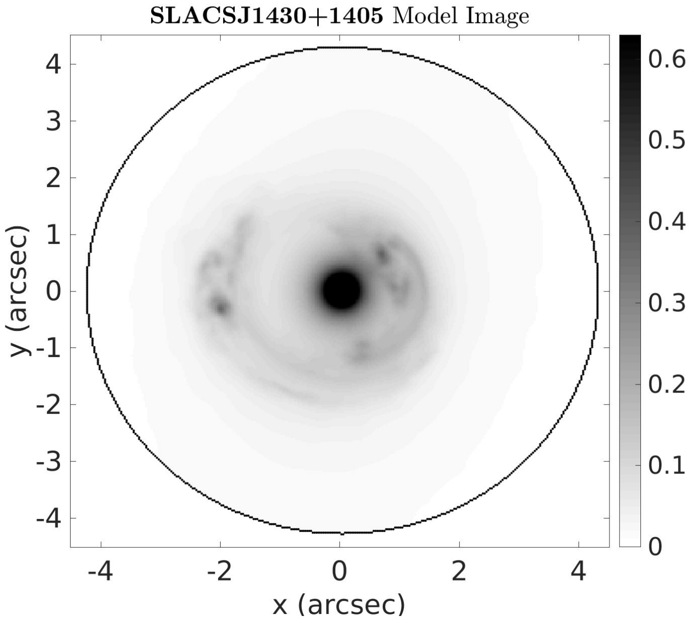
- **Step 1: Write a unit test.**
- **Step 2: Run the test, check it fails.**
- **Step 3: Write the Code.**
- **Step 4: Check the test (and all other tests) pass.**

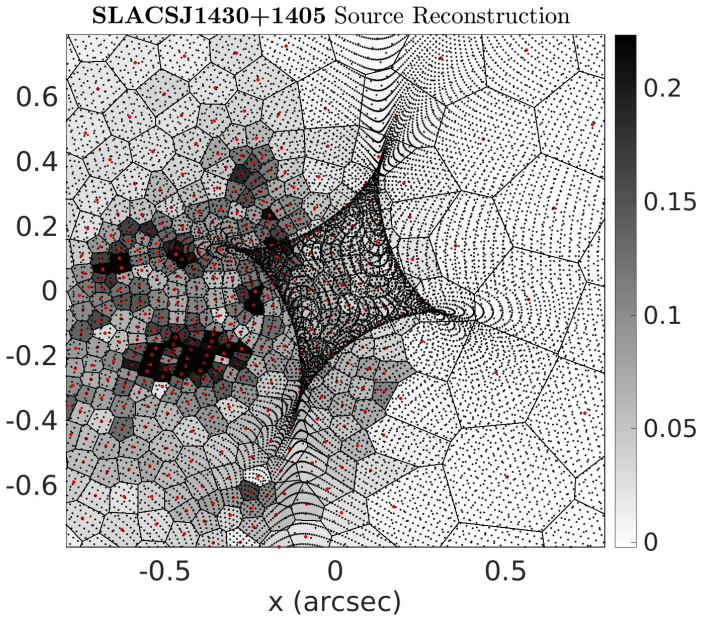
1 test passed - 0ms

```
Testing started at 19:57 ...
/home/jammy/Euclid/VirtualEnvs/AutoLensPy3/bin/python /home/jammy/PyCharm/pycharm-community-2017.3.2/helpers/pycharm/_jb_pytest_runner.py --target test_code
Launching py.test with arguments test_code.py::test__add_integers__input_one_and_one__result_is_two in /home/jammy/PycharmProjects/TDDTalk

============================== test session starts ===============================
platform linux -- Python 3.6.3, pytest-3.4.2, py-1.5.2, pluggy-0.6.0
rootdir: /home/jammy/PycharmProjects/TDDTalk, inifile:
collected 1 item
test_code.py .                                                            [100%]

============================ 1 passed in 0.01 seconds ============================
Process finished with exit code 0
```

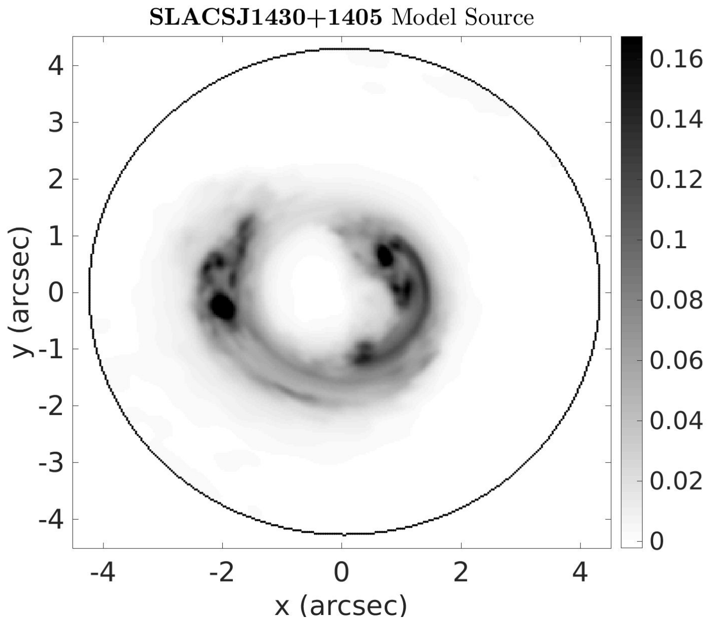
TDD – A (brief) case study

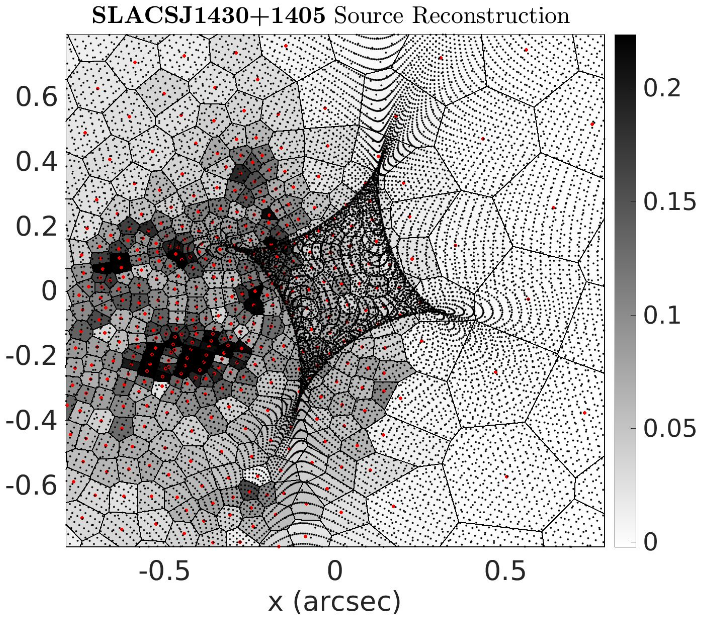
PyAutoLens – Open-source Strong Lens modeling





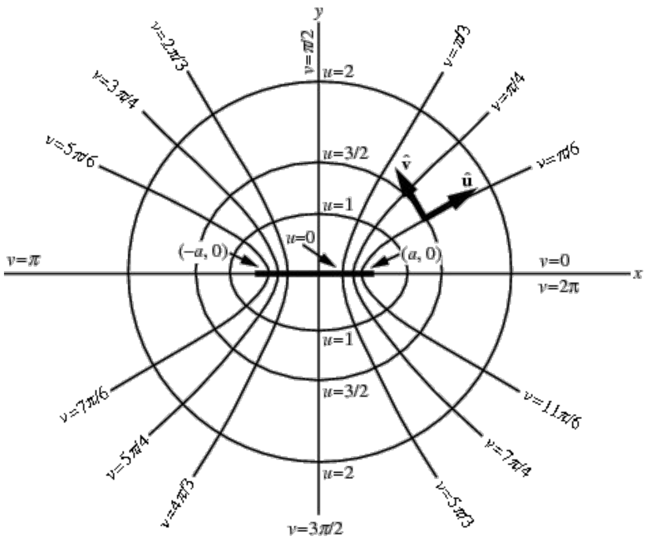
PyAutoLens – Open-source Strong Lens modeling





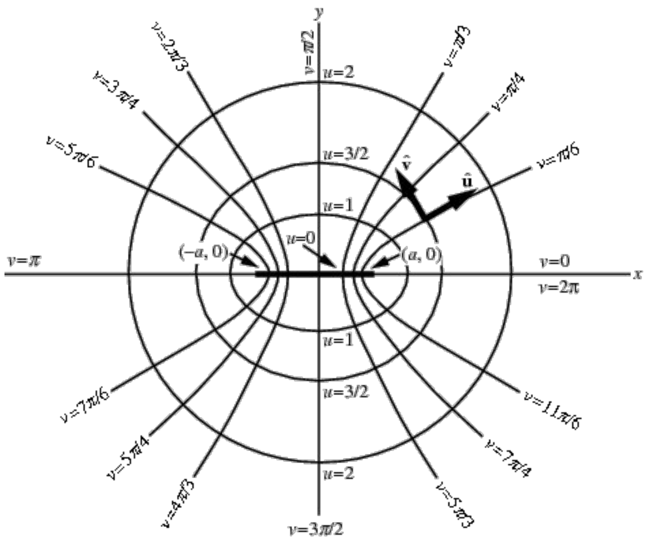
Coordinate Transform

- **Image** – Cartesian Coordinates.
- **Galaxy** – Elliptical Coordinates.



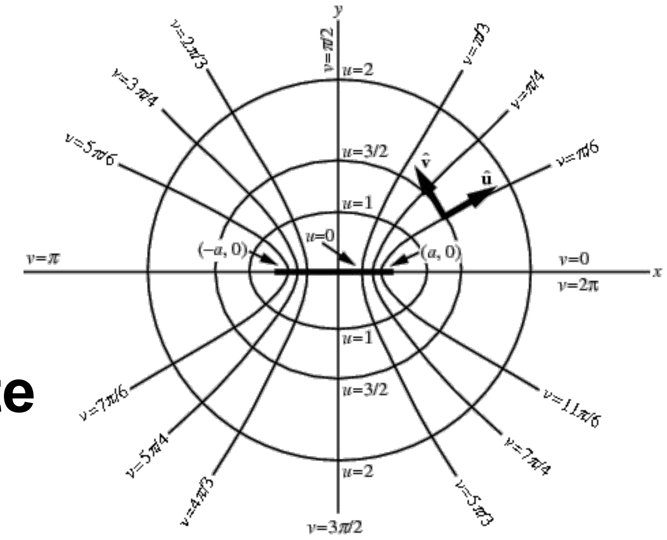
TDD - Coordinate Transform

- **TDD forces you to break the problem down.**
- I don’t know how to write a unit test to perform this transformation.



TDD - Coordinate Transform

- **TDD forces you to break the problem down.**
- I don’t know how to write a unit test to perform this transformation.
- However, I will need to **translate the coordinates to the galaxy’s centre.**
- **I know how to test this.**



TDD - Coordinate Transform

```python
def test__coordinates_to_centre__input_coordinates_and_centre__shifts_coordinates_to_centre():

    coordinates_shift = geometry.coordinates_to_centre(coordinates=(0.0, 0.0), centre=(1.0, 1.0))

    assert coordinates_shift == (-1.0, -1.0)
```

TDD - Coordinate Transform

geometry.py | test_geometry.py

```python
def coordinates_to_centre(coordinates, centre):
    """
    Converts coordinates to a reference frame centre.

    Parameters
    ----------
    coordinates : (float, float)
        The x and y coordinates.
        coordinates : (float, float)
        The x and y centre.

    Returns
    ----------
    The coordinates at the reference frame's centre
    """
    return (coordinates[0] - centre[0], coordinates[1] - centre[1])
```

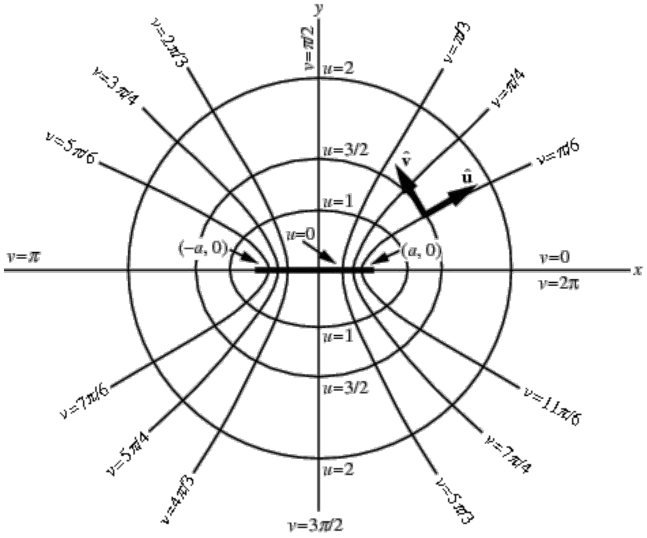
TDD - Coordinate Transform

geometry.py × test_geometry.py ×

```python
import pytest

import geometry

def test__coordinates_to_centre__input_coordinates_and_centre__shifts_coordinates_to_centre():

    coordinates_shift = geometry.coordinates_to_centre(coordinates=(0.0, 0.0), centre=(1.0, 1.0))

    assert coordinates_shift == (-1.0, -1.0)

def test__coordinates_to_centre__different_centre_and_coordinates():

    coordinates_shift = geometry.coordinates_to_centre(coordinates=(5.0, 2.0), centre=(4.0, 3.0))

    assert coordinates_shift == (1.0, -1.0)

def test__coordinates_to_centre__shift_only_x__only_x_shifts():

    coordinates_shift = geometry.coordinates_to_centre(coordinates=(0.0, 0.0), centre=(1.0, 0.0))

    assert coordinates_shift[1] == 0.0
    assert coordinates_shift == (-1.0, 0.0)

def test__coordinates_to_centre__shift_only_y__only_y_shifts():

    coordinates_shift = geometry.coordinates_to_centre(coordinates=(0.0, 0.0), centre=(0.0, 1.0))

    assert coordinates_shift[0] == 0.0
    assert coordinates_shift == (0.0, -1.0)
```

TDD - Coordinate Transform

- **TDD forces you to break the problem down.**
- The angle between the coordinate and the x-axis.
- The angle between the coordinate and galaxy.
- Rotating the coordinate by that angle.



TDD - Coordinate Transform

geometry.py × | test_geometry.py ×

```python
import numpy as np

def coordinates_to_centre(coordinates, centre):...

def coordinates_to_radius(coordinates):...

def coordinates_angle_from_x(coordinates):...

def coordinates_angle_to_galaxy(coordinates, theta, galaxy_theta):...

def rotate_coordinates_to_galaxy(cos_theta, sin_theta):...
```

TDD - Coordinate Transform

geometry.py test_geometry.py

```python
import geometry

def test__transform_to_galaxy_reference_frame__use_simple_functions():

    coordinates = (1.0, 1.0)
    centre = (2.0, 2.0)
    galaxy_theta = 45

    shifted_coordinates = geometry.coordinates_to_centre(coordinates, centre)

    radius = geometry.coordinates_to_radius(shifted_coordinates)

    theta_from_x = geometry.coordinates_angle_from_x(shifted_coordinates)

    cos_theta, sin_theta = geometry.coordinates_angle_to_galaxy(radius, theta_from_x, galaxy_theta)

    rotated_coordinates = geometry.rotate_coordinates_to_galaxy(cos_theta, sin_theta)

    assert rotated_coordinates == geometry.transform_to_galaxy_reference_frame(coordinates, centre, galaxy_theta)
```

TDD - Coordinate Transform

geometry.py | test_geometry.py

```python
import numpy as np

def coordinates_to_centre(coordinates, centre):...

def coordinates_to_radius(coordinates):...

def coordinates_angle_from_x(coordinates):...

def coordinates_angle_to_galaxy(coordinates, theta, galaxy_theta):...

def rotate_coordinates_to_galaxy(cos_theta, sin_theta):...

def transform_to_galaxy_reference_frame(coordinates, centre, galaxy_theta):
    """..."""

    shifted_coordinates = coordinates_to_centre(coordinates, centre)

    theta_from_x = coordinates_angle_from_x(shifted_coordinates)

    cos_theta, sin_theta = coordinates_angle_to_galaxy(shifted_coordinates, theta_from_x, galaxy_theta)

    return rotate_coordinates_to_galaxy(cos_theta, sin_theta)

```

TDD - Coordinate Transform

geometry.py | test_geometry.py

```python
import geometry

def test__transform_to_galaxy_reference_frame__use_simple_functions__():...

def test__transform_to_galaxy_reference_frame__x_aligned_with_galaxy__no_rotation__():...

def test__transform_to_galaxy_reference_frame__x_offset_180_degrees__coordinates_change_sign__():...

def test__transform_to_galaxy_reference_frame__answer_calculated_on_paper():...
```

TDD - Coordinate Transform

geometry.py | test_geometry.py

```python
import numpy as np

def coordinates_to_centre(coordinates, centre):...

def coordinates_to_radius(coordinates):...

def coordinates_angle_from_x(coordinates):...

def coordinates_angle_to_galaxy(coordinates, theta, galaxy_theta):...

def rotate_coordinates_to_galaxy(cos_theta, sin_theta):...

def transform_to_galaxy_reference_frame(coordinates, centre, galaxy_theta):
    """..."""

    shifted_coordinates = coordinates_to_centre(coordinates, centre)

    theta_from_x = coordinates_angle_from_x(shifted_coordinates)

    cos_theta, sin_theta = coordinates_angle_to_galaxy(shifted_coordinates, theta_from_x, galaxy_theta)

    return rotate_coordinates_to_galaxy(cos_theta, sin_theta)
```

TDD - Coordinate Transform

- At 225 degrees, a test failed!
- The trigonometry reverted back to -45 degrees.
- **TDD forced me to make a design choice about my code (and coordinate system) immediately.**
- **I’d have thought about this a lot later, one a lot more code was in place!**

Astronomer’s Coordinate Transform

```
!    These common blocks pass other information to different model integrals
common /Int_coords_Arc/  npow, Xrot_Arc, Yrot_Arc
common /Int_eta/ eta

do I = 1, No_Defls

   R_Arc =  ((XYPos_Arc(1,I)-Lens_x_Arc)**2 + (XYPos_Arc(2,I)-Lens_y_Arc)**2)**0.5

   !    CAlculate cos theta / sin theta using trig (= x/r and y/r)
   costhe1=(XYPos_Arc(1,I)-Lens_x_Arc)/R_Arc
   sinthe1=(XYPos_Arc(2,I)-Lens_y_Arc)/R_Arc

   ! Perform rotation if ellpitical mass distribution
   dum=costhe1
   costhe=costhe1*Lens_cosphi+sinthe1*Lens_sinphi
   sinthe=sinthe1*Lens_cosphi-dum*Lens_sinphi

   ! Convert theta values to x and y using trig in rotated plane
   Xrot_Arc = R_Arc*costhe
   Yrot_Arc = R_Arc*sinthe

   !SIS Model is rotationally symmetric so treat seperately to avoid rotation

   If (Lens_Model_Defl .eq. trim('SIS')) then

      call Lens_Calc_Defl_Angles_SIS(XRot_Arc, YRot_Arc, Defl_Angles_Arc_Calc(:,I))

   elseif (Lens_Model_Defl .eq. trim('PtMass')) then

      call Lens_Calc_Defl_Angles_PtMass(costhe1, sinthe1, R_Arc, Defl_Angles_Arc_Calc(:,I))

   elseif ( Lens_Model_Defl .eq. trim('SIE')  ) then
```

TDD - Coordinate Transform ... and More!

geometry.py test_geometry.py

```python
class TransformedCoordinates(tuple):...


class CoordinatesException(Exception):...


class Profile(object):
    """Abstract Profile, describing an object with x, y cartesian image_grid"""

    def __init__(self, centre=(0.0, 0.0)):...

    # noinspection PyMethodMayBeStatic
    def transform_to_reference_frame(self, coordinates):...

    # noinspection PyMethodMayBeStatic
    def transform_from_reference_frame(self, coordinates):...

    def coordinates_to_centre(self, coordinates):...

    def coordinates_from_centre(self, coordinates):...

    def coordinates_to_radius(self, coordinates):...


class EllipticalProfile(Profile):...


class SphericalProfile(EllipticalProfile):
    """Generic circular profiles class to contain functions shared by light and mass profiles"""

    def __init__(self, centre=(0.0, 0.0)):
        """..."""
        super(SphericalProfile, self).__init__(centre, 1.0, 0.0)

```

TDD

Test-Driven Development

- TDD is NOT a **testing process.**
- The fact your code comes out fully tested is a **bonus.**

Test-Driven Development

- TDD Is a **development process.**
- You focus on what the code should do, **before you write it.**
- Leading to **versatile, clean and adaptable code.**
- That has a **specified purpose.**
- **If you add unit-tests after writing the code, you are not doing TDD!**

Example

https://github.com/Jammy2211/PyAutoGalaxy

Refactoring

The Test-Driven Development Cycle

- **Step 1:** Write a unit test.
- **Step 2:** Run the test, check it fails.
- **Step 3:** Write the Code.
- **Step 4:** Check the test (and all other tests) pass**.**
- **Step 5:** Refactor, refactor and refactor.

Refactoring

- In the Astronomers development cycle, **refactoring is terrifying.**
- You have **no idea** if your changes break the code.
- And even if you think they do, you cannot be **confident**.

Refactoring

- **With TDD, you receive instant feedback on if your code's functionality has changed.**
- Refactoring becomes **enjoyable.**
- You focus on **how to structure the code**, not **whether changing it will break it.**
- **The code design becomes part of the development cycle!**

Other TDD benefits

- The unit tests become **living, breathing documentation.**
- They make the API of your code visible.
- For **collaborative projects,** TDD ensures other developers know what your code does.
- And lets them know their changes don’t break it!

Summary

- **TDD is a development process that produces clean and versatile code.**
- **More astronomers should be using it!**
- https://github.com/Jammy2211/PyAutoLens

TDD and AI

Converting Code

- Needed to Convert loads of Python code written using numba (e.g. for loops) to JAX (vectorized code for GPU).

Convert this to numpy arithmitic:

```
def constant_zeroth_regularization_matrix_from(
    coefficient: float,
    coefficient_zeroth: float,
    neighbors: np.ndarray,
    neighbors_sizes: np.ndarray,
) -> np.ndarray:
    """
    From the pixel-neighbors array, setup the regularization matrix using
the instance regularization scheme.

    A complete description of regularizatin and the
`regularization_matrix can be found in the Regularization
    class in the module `autoarray.inversion.regularization.

    Parameters
    ----------
    coefficients
        The regularization coefficients which controls the degree of
smoothing of the inversion reconstruction.
    neighbors
        An array of length (total_pixels) which provides the index of all
neighbors of every pixel in
        the Voronoi grid (entries of -1 correspond to no neighbor).
    neighbors_sizes
        An array of length (total_pixels) which gives the number of
neighbors of every pixel in the
        Voronoi grid.

    Returns
    -------
    np.ndarray
        The regularization matrix computed using Regularization where
the effective regularization
        coefficient of every source pixel is the same.
    """
```

Convert this to numpy arithmitic:

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        Voronoi grid.

    Returns
    -------
    np.ndarray
        The regularization matrix computed using Regularization where
the effective regularization
        coefficient of every source pixel is the same.
    """
```

```
    pixels = len(neighbors)

    regularization_matrix = np.zeros(shape=(pixels, pixels))

    regularization_coefficient = coefficient**2.0
    regularization_coefficient_zeroth = coefficient_zeroth**2.0

    for i in range(pixels):
        regularization_matrix[i, i] += 1e-8
        regularization_matrix[i, i] += regularization_coefficient_zeroth
        for j in range(neighbors_sizes[i]):
            neighbor_index = neighbors[i, j]
            regularization_matrix[i, i] += regularization_coefficient
            regularization_matrix[i, neighbor_index] -=
regularization_coefficient

    return regularization_matrix
```

Here's a JAX-friendly version of `constant_zeroth_regularization_matrix_from`, following the same "flatten + scatter" pattern as before:

python

Copy code

```python
import jax.numpy as jnp
from functools import partial

@partial(jax.jit, static_argnums=())
def constant_zeroth_regularization_matrix_from(
    coefficient: float,
    coefficient_zeroth: float,
    neighbors:      jnp.ndarray,  # shape (S, P), dtype=int32/int64; -1 = no neighbor
    neighbors_sizes:jnp.ndarray,  # shape (S,),   dtype=int32/int64
) -> jnp.ndarray:
    """
    Build the S×S regularization matrix with both "zeroth" and "first" order penalties:

      - Add 1e-8 + coefficient_zeroth**2 on every diagonal entry.
      - For each (i → j) neighbor:
          diag[i]                 += coefficient**2
          offdiag[i, j]           -= coefficient**2

    Any -1 entries in `neighbors` are treated as "no neighbor" and ignored.

    Parameters
    ----------
    coefficient
        strength of the first-order (gradient) regularization.
    coefficient_zeroth
        strength of the zeroth-order (value) regularization.
    neighbors
        an S×P array of neighbor-indices, with -1 meaning no neighbor.
    neighbors_sizes
        length-S array giving, for each i, how many of its first P columns are valid neighbors.
```

```
S, P = neighbors.shape
reg1 = coefficient**2
reg0 = coefficient_zeroth**2

# 1) Flatten (i,j) neighbor-pairs
I = jnp.repeat(jnp.arange(S), P)        # (S*P,)
J = neighbors.reshape(-1)               # (S*P,)

# 2) Remap “no neighbor” = -1 → OUT = S
OUT = S
J = jnp.where(J < 0, OUT, J)

# 3) Start on an (S+1)x(S+1) zero canvas
M = jnp.zeros((S+1, S+1), dtype=jnp.float32)

# 4) Diagonal baseline: 1e-8 + reg0  for i in [0..S-1]
diag_base = jnp.concatenate([jnp.full((S,), 1e-8 + reg0), jnp.zeros((1,))])
M = M.at[jnp.diag_indices(S+1)].add(diag_base)

# 5) Scatter the first-order reg1 into diag[i] for each neighbor (i→j):
#    M[i,i] += reg1
M = M.at[I, I].add(reg1)

# 6) Scatter the off-diagonals: M[i,j] -= reg1
M = M.at[I, J].add(-reg1)

# 7) Return only the top-left S×S block
return M[:S, :S]
```

Unit Test + AI

- The function returned by ChatGPT **was wrong.**
- My unit test immediately told me it was wrong.
- I then copy and pasted the error message into ChatGPT, explaining that it was wrong, and told it to fix it.

ChatGPT than gave me the **correct function**.

TDD + AI: The Future of Code

In the future, **I predict that no human will ever write code.**

Instead, I think we will write unit tests for our problem and agent based AI will follow the TDD cycle:

- AI agent writes the code.
- AI agent runs the code + unit test, checks error message.
- AI agent rewrites code if unit tests fail based on error.
- AI agent refactors the code + documentation.

So, why not get a head start and learn TDD today!