PyAutoFit: Classy Probabilistic Programming for Data Science

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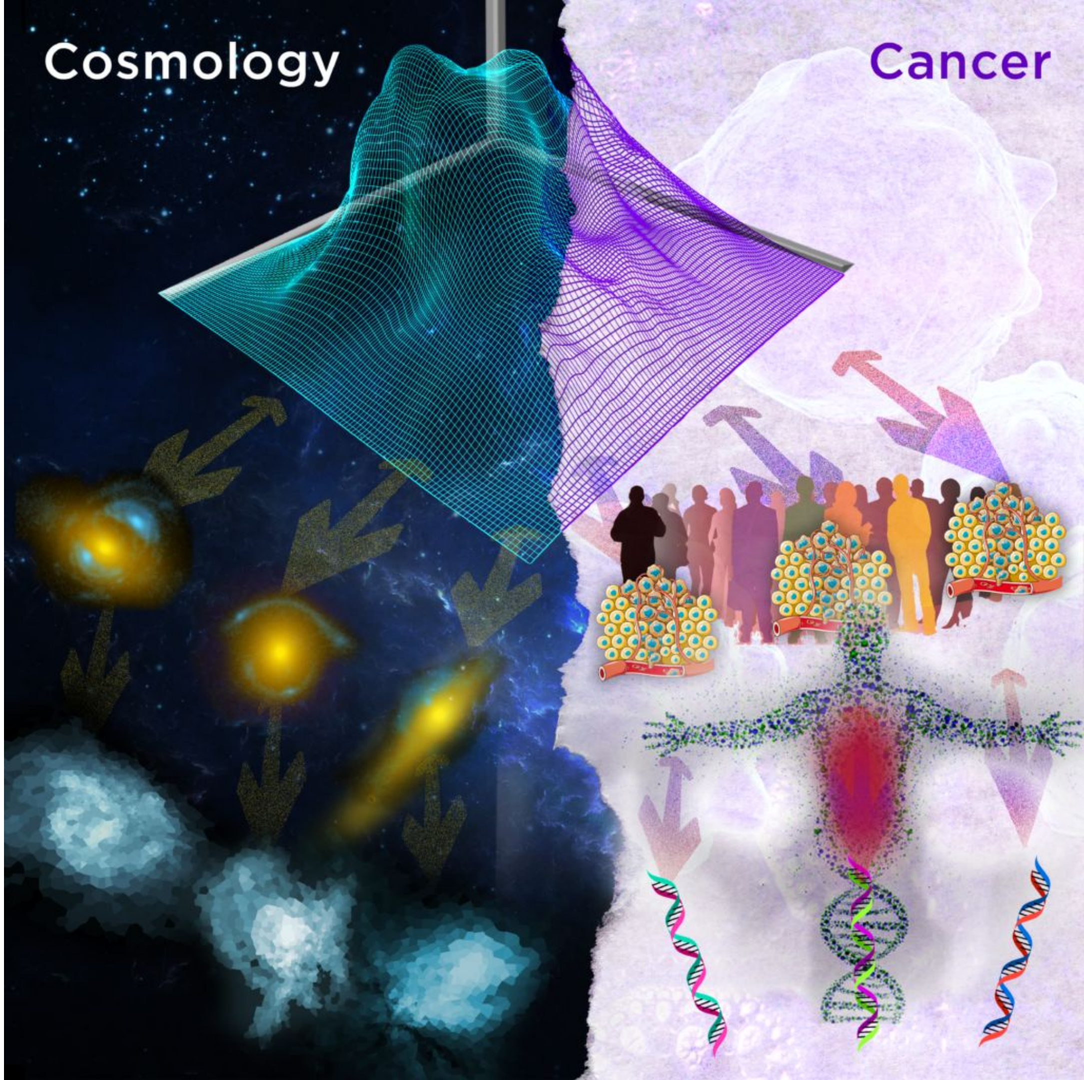
Durham University



Overview

PyAutoFit & Probabilistic Programming:

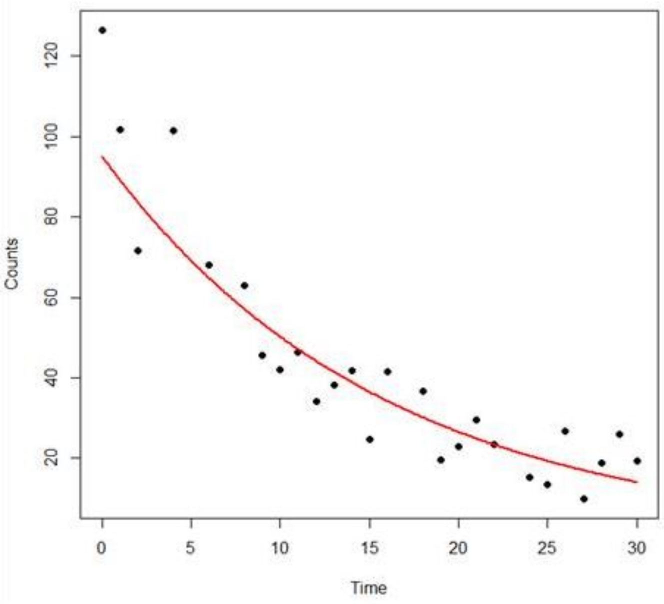
- What is probabilistic programming?
- What is PyAutoFit?
- Why PyAutoFit?

Cosmology:

- Description of example use-case - strong gravitational lensing.
- Application to Astronomy data.
- Building multi-level models via Python classes.

Model Fitting

Given some data and a model, finding the set of model parameters that provide the best fit to the data.



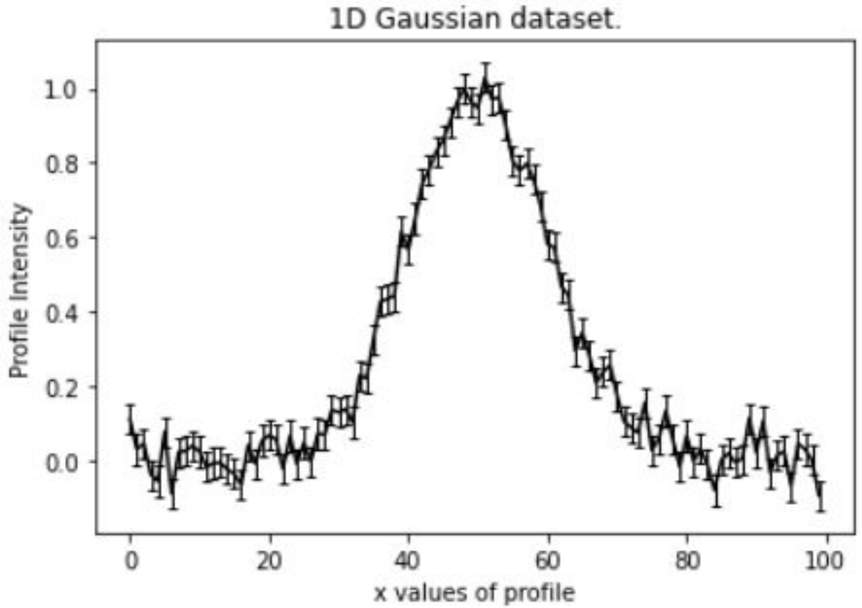
$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$$

Model Fitting

Model -> Gaussian:

- Centre
- Normalization
- Sigma

1) Draw a set of parameters.
2) Create Model Gaussian.
3) Fit to Dataset.
4) Compute Likelihood.
5) Repeat using non-linear search.



Model Fitting

Model -> Gaussian:

- Centre **= 60.0**
- Intensity **= 20.0**
- Sigma **= 15.0**

1) **Draw a set of parameters.**
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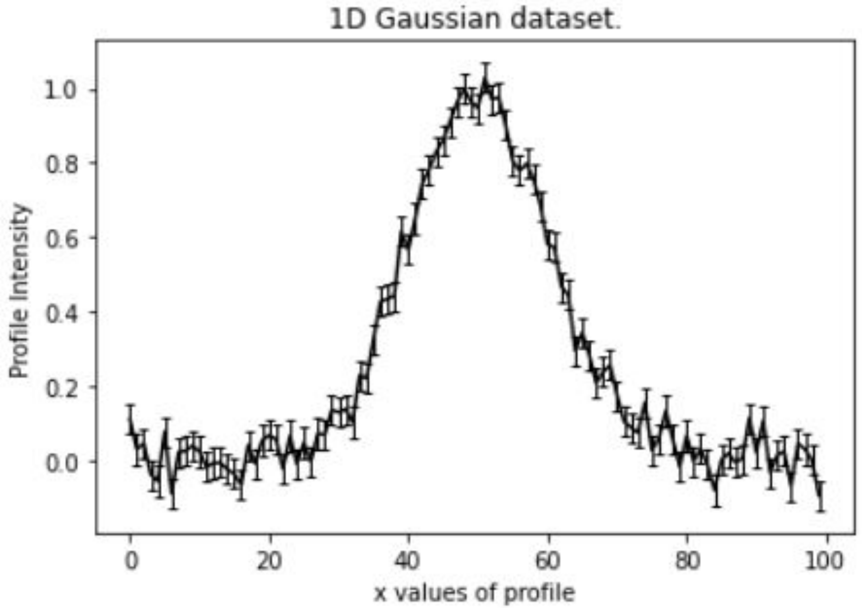

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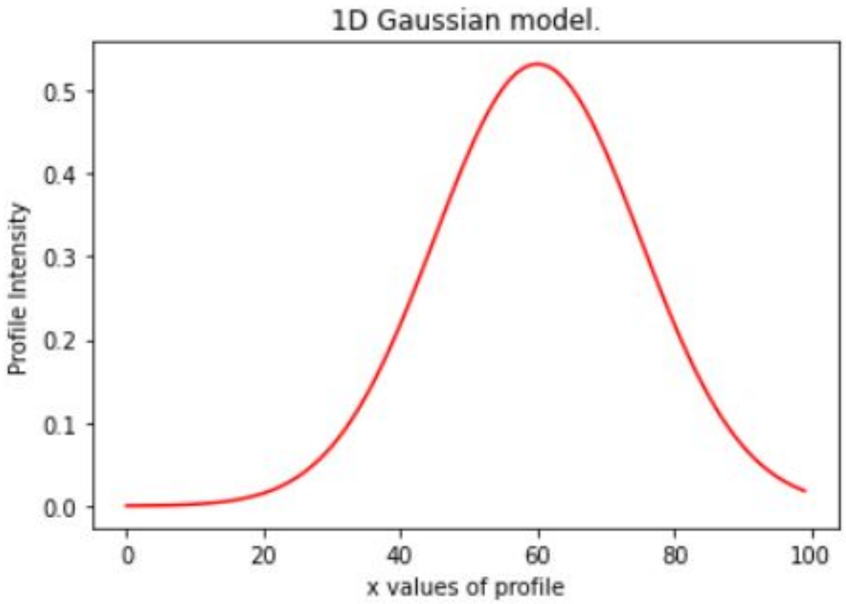

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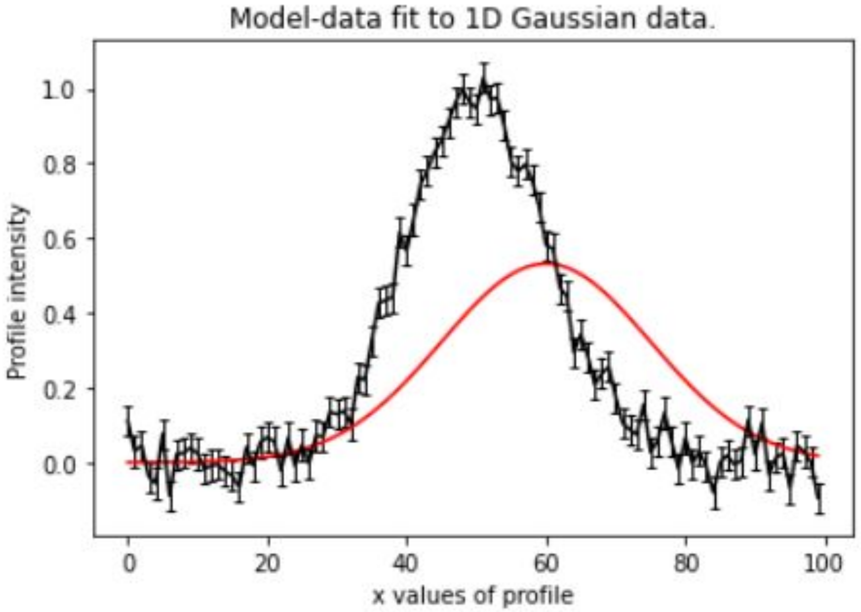

Model Fitting

Model -> Gaussian:

- Centre **= 60.0**
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1) Draw a set of parameters.
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3) Fit to Dataset.
4) **Compute Likelihood.**
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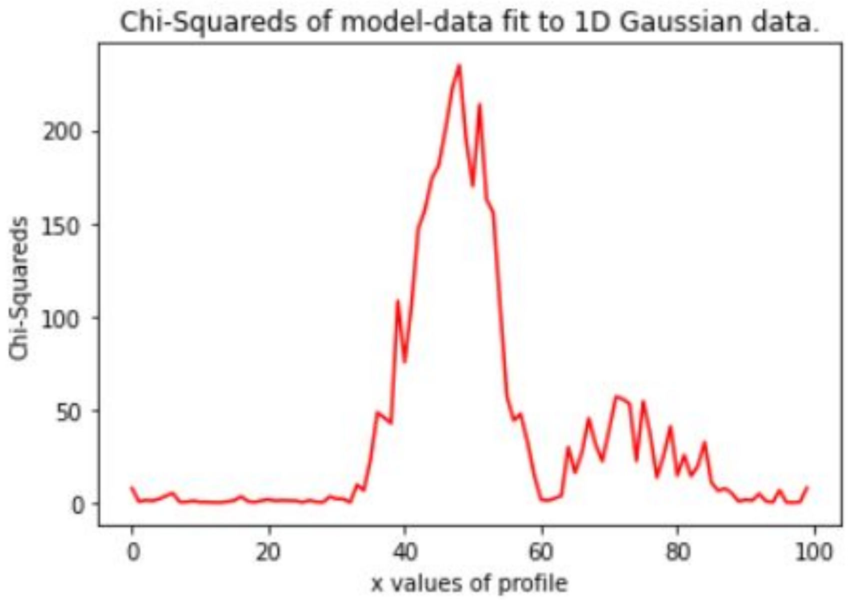
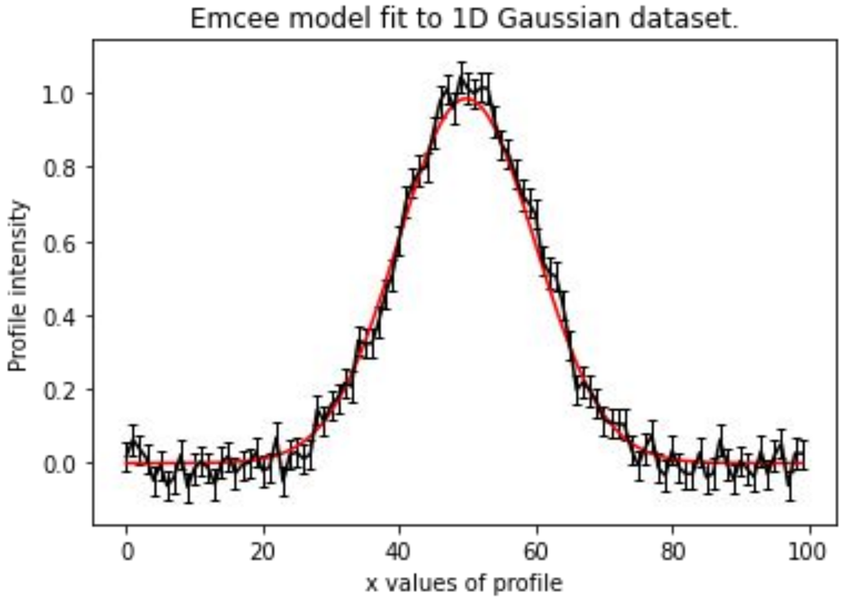


Model Fitting

Model -> Gaussian:

- Centre **= 50.0**
- Intensity **= 10.0**
- Sigma **= 5.0**

1) Draw a set of parameters.
2) Create Model Gaussian.
3) Fit to Dataset.
4) Compute Likelihood.
5) **Repeat using non-linear search.**



Probabilistic Programming

What is Probabilistic Programming?

Probabilistic programming languages (PPL) provide a framework that allows users to easily specify a probabilistic model and perform inference automatically.

- There are a plethora of PPL's available (e.g. **PyMC3, STAN, Pyro**).
- All are suited to different problems, have different core features, etc.

They are some of the Github mega projects, so why on Earth are we developing our own PPL?

```python
import pymc3 as pm

X, y = linear_training_data()
with pm.Model() as linear_model:
    weights = pm.Normal("weights", mu=0, sigma=1)
    noise = pm.Gamma("noise", alpha=2, beta=1)
    y_observed = pm.Normal(
        "y_observed",
        mu=X @ weights,
        sigma=noise,
        observed=y,
    )

    prior = pm.sample_prior_predictive()
    posterior = pm.sample()
    posterior_pred = pm.sample_posterior_predictive(posterior)
```

PyAutoFit: A PPL for Astronomers (and data science!)

Existing PPL's not suited to the model fitting challenges we faced when in Astronomy, for example:

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Existing PPL's not suited to the model fitting challenges we faced when in Astronomy, for example:

- Fitting large and homogenous datasets with an identical model fitting procedure, with tools for processing the large libraries of results output.
- Problems where likelihood evaluations are expensive (e.g. run times of days per model-fit), necessitating highly customizable model-fitting pipelines with support for massively parallel computing.

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- Fitting many different models to the same dataset with tools that streamline model comparison.

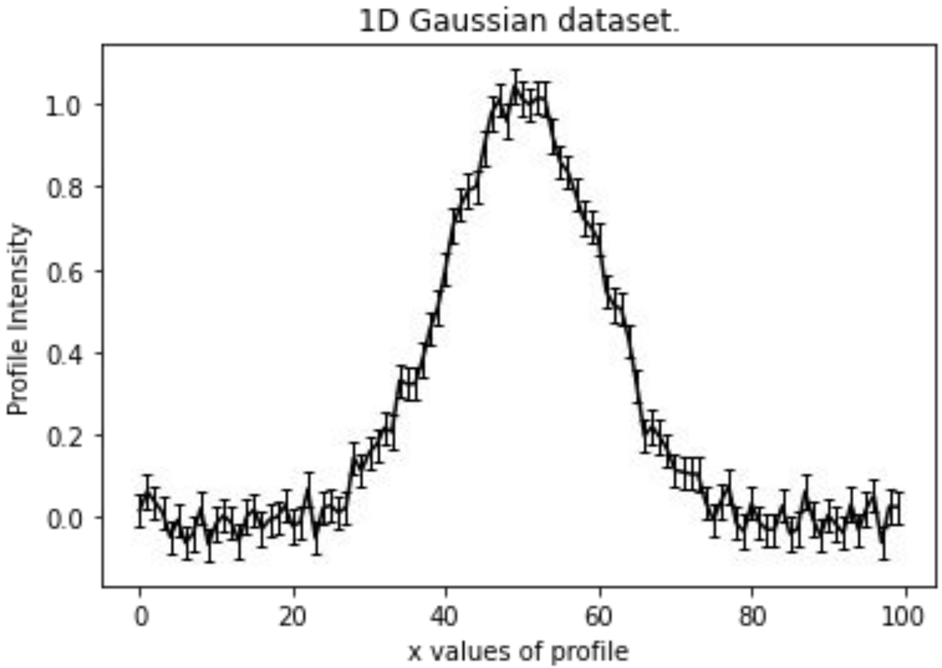
PyAutoFit: highly customizable model-fitting software, for big data challenges in the many model regime.

PyAutoFit: Classy Interface

PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

Aim: use **PyAutoFit** to fit a Gaussian to the dataset via a non-linear search.



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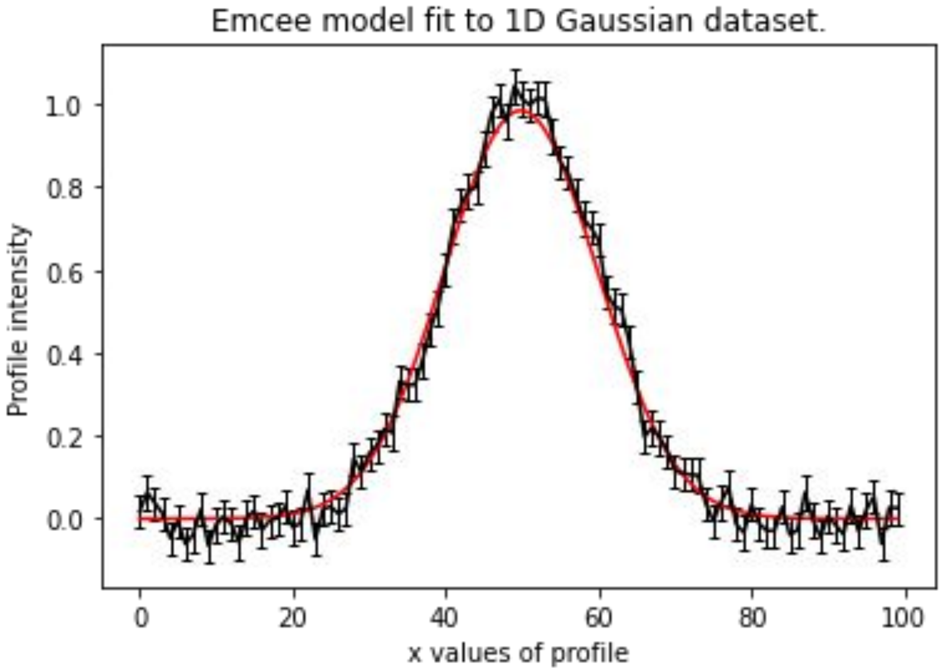


PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

- Write a Python class to define the **model component.**

```
class Gaussian:

    def __init__(
        self,
        centre=0.0,       # <- PyAutoFit recognises these
        intensity=0.1,    # <- constructor arguments are
        sigma=0.01,       # <- the Gaussian's parameters.
    ):
        self.centre = centre
        self.intensity = intensity
        self.sigma = sigma

    """
    An instance of the Gaussian class will be available during model fitting.

    This method will be used to fit the model to ``data`` and compute a likelihood.
    """

    def profile_from_xvalues(self, xvalues):

        transformed_xvalues = xvalues - self.centre

        return (self.intensity / (self.sigma * (2.0 * np.pi) ** 0.5)) * \
                np.exp(-0.5 * transformed_xvalues / self.sigma)
```

PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

- Write a Python class to define the **model component.**
- Write an Analysis class with the **data** and **likelihood function.**

```python
class Analysis(af.Analysis):

    def __init__(self, data, noise_map):

        self.data = data
        self.noise_map = noise_map

    def log_likelihood_function(self, instance):

        """
        The 'instance' that comes into this method is an instance of the Gaussian class
        above, with the parameters set to values chosen by the non-linear search.
        """

        print("Gaussian Instance:")
        print("Centre = ", instance.centre)
        print("Intensity = ", instance.intensity)
        print("Sigma = ", instance.sigma)

        """
        We fit the ``data`` with the Gaussian instance, using its
        "profile_from_xvalues" function to create the model data.
        """

        xvalues = np.arange(self.data.shape[0])

        model_data = instance.profile_from_xvalues(xvalues=xvalues)
        residual_map = self.data - model_data
        chi_squared_map = (residual_map / self.noise_map) ** 2.0
        log_likelihood = -0.5 * sum(chi_squared_map)

        return log_likelihood
```

PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

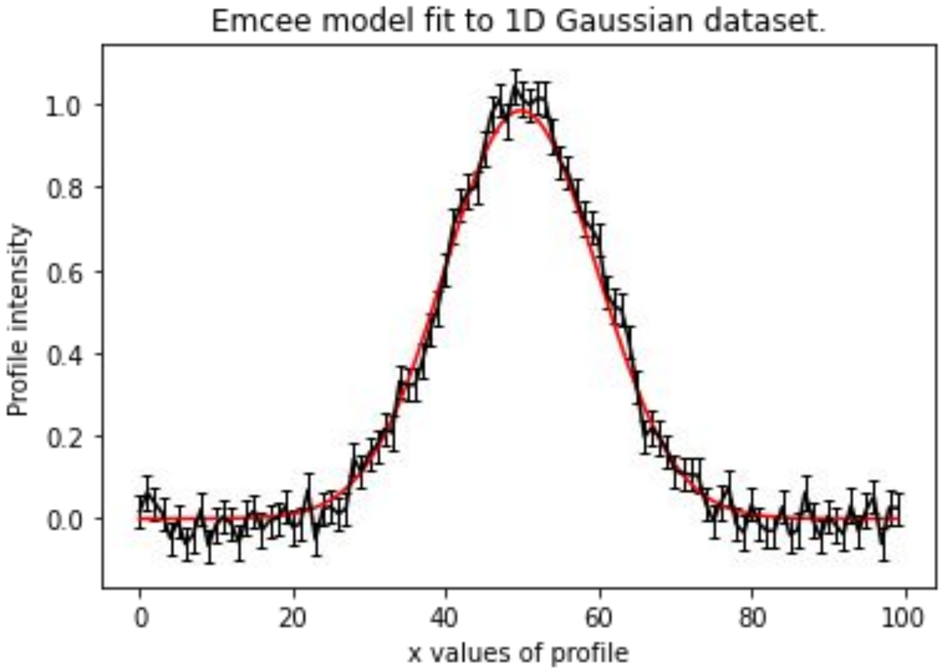
- Write a Python class to define the **model component.**
- Write an Analysis class with the **data** and **likelihood function.**
- Combine with your favourite **non-linear search** to fit the model to the data.

```
model = af.Model(Gaussian)

analysis = Analysis(data=data, noise_map=noise_map)

emcee = af.Emcee(nwalkers=50, nsteps=2000)

result = emcee.fit(model=model, analysis=analysis)
```

PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

Aim: use **PyAutoFit** to fit a Gaussian to the dataset via a non-linear search.



PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

- Write a Python class to define the **model component.**
- Write an Analysis class with the **data** and **likelihood function.**
- Combine with your favourite **non-linear search** to fit the model to the data.
- **Result** object contains all the information you need on your model-fit.

```
samples = result.samples

print("Final 10 Parameters:")
print(samples.parameter_lists[-10:])

print("Sample 10`s third parameter value (Gaussian -> sigma)")
print(samples.parameter_lists[9][2], "\n")

median_pdf_vector = samples.median_pdf_vector

vector_at_upper_sigma = samples.vector_at_upper_sigma(sigma=3.0)
vector_at_lower_sigma = samples.vector_at_lower_sigma(sigma=3.0)

print("Upper Parameter values w/ error (at 3.0 sigma confidence):")
print(vector_at_upper_sigma)
print("lower Parameter values w/ errors (at 3.0 sigma confidence):")
print(vector_at_lower_sigma, "\n")
```

PyAutoFit: Classy Probabilistic Programming

Illustrative example, fitting noisy 1D data of a Gaussian.

- Write a Python class to define the **model component.**
- Write an Analysis class with the **data** and **likelihood function.**
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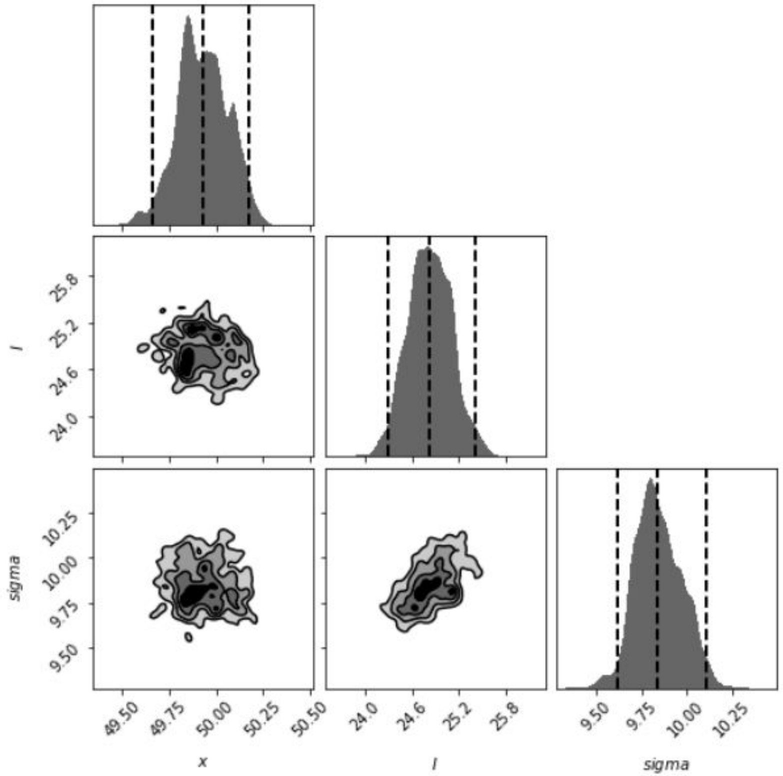


PyAutoFit: Links / Overview

PyAutoFit

GitHub: https://github.com/rhayes777/PyAutoFit

Readthedocs: https://pyautofit.readthedocs.io/en/latest/

JOSS Paper: https://joss.theoj.org/papers/10.21105/joss.02550

Binder: https://mybinder.org/v2/gh/Jammy2211/autofit_workspace/HEAD

HowToFit

Teach **anyone** how to compose and fit a probabilistic model with **PyAutoFit**.

We can also use it to get a model instance of the `median_pdf` model, which is the model where each parameter is the value estimated from the probability distribution of parameter space.

In [14]:
```
mp_instance = result.samples.median_pdf_instance
print()
print("Median PDF Model:\n")
print("Centre = ", mp_instance.centre)
print("Intensity = ", mp_instance.intensity)
print("Sigma = ", mp_instance.sigma)
```

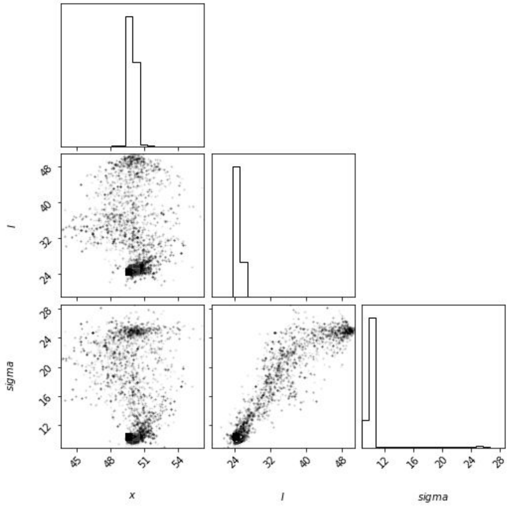
```
Median PDF Model:

Centre =  49.92285569756167
Intensity =  24.974961843717058
Sigma =  9.969794911012947
```

The Probability Density Functions (PDF's) of the results can be plotted using the Emcee's visualization tool `corner.py`, which is wrapped via the `EmceePlotter` object.

The PDF shows the 1D and 2D probabilities estimated for every parameter after the model-fit. The two dimensional figures can show the degeneracies between different parameters, for example how increasing σ and decreasing the intensity I can lead to similar likelihoods and probabilities.

In [15]:
```
emcee_plotter = aplt.EmceePlotter(samples=result.samples)
emcee_plotter.corner()
```

```
2021-07-26 16:42:47,675 - root - WARNING - Too few points to create valid contours
2021-07-26 16:42:47,712 - root - WARNING - Too few points to create valid contours
2021-07-26 16:42:47,737 - root - WARNING - Too few points to create valid contours
```

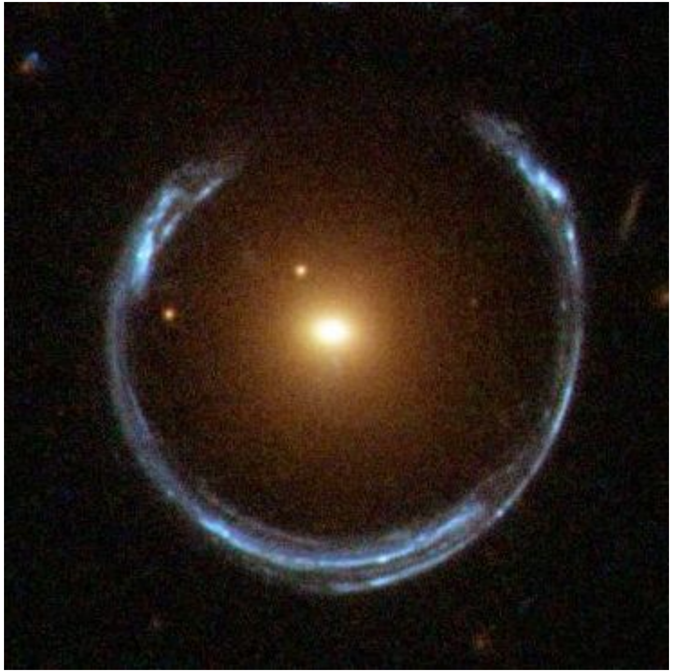


Cosmology: Strong Gravitational Lensing

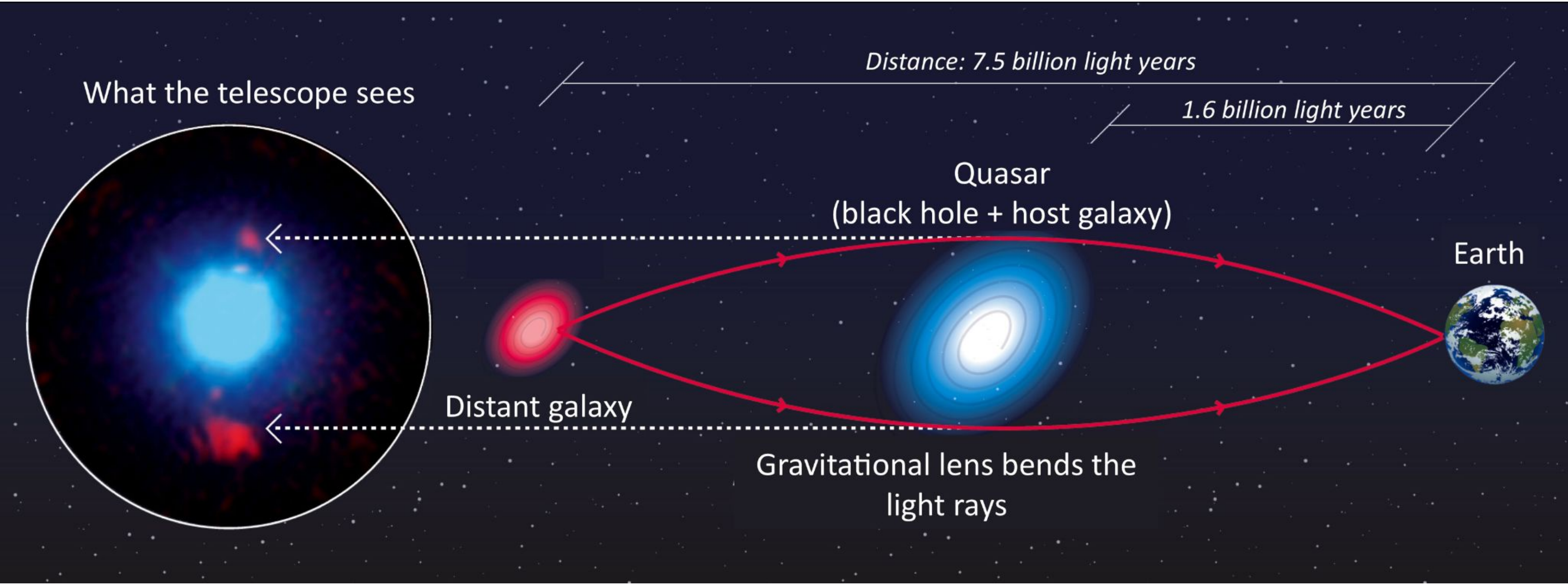
Strong Gravitational Lensing

“Normal” Galaxy:

Strong Gravitational Lens:



Strong Gravitational Lensing



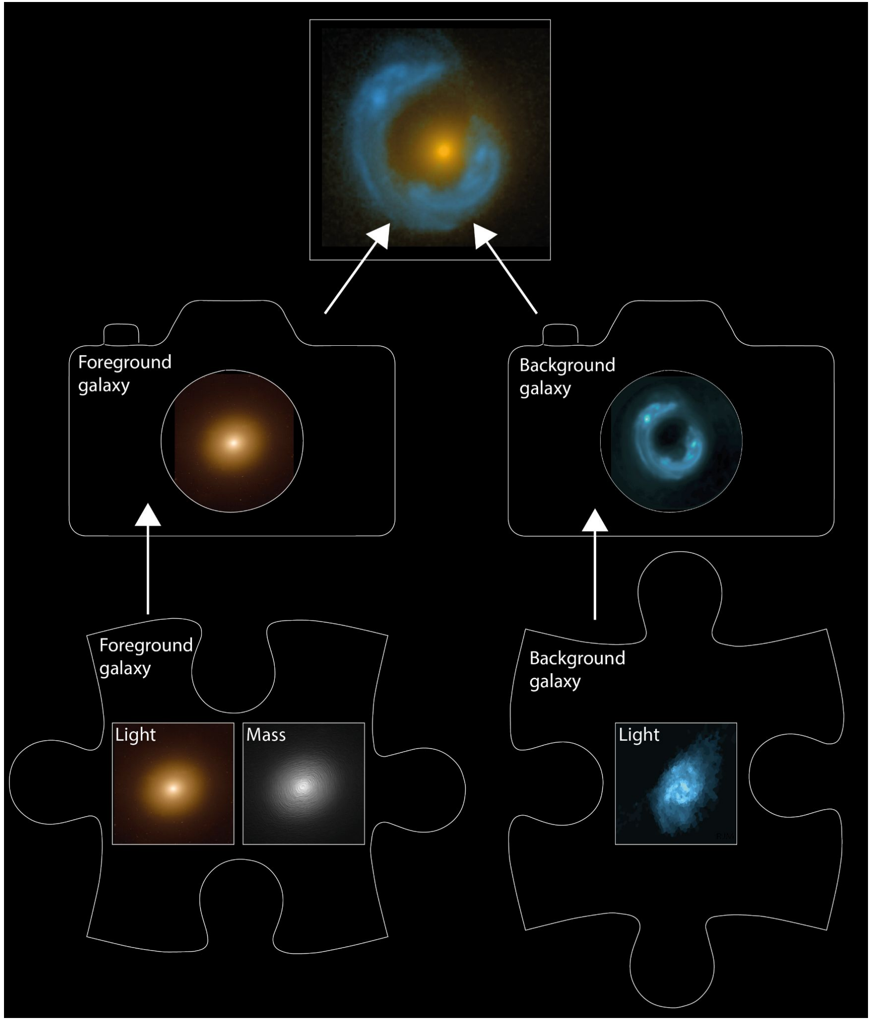
PyAutoFit: Model Composition

Model Composition

Break strong lens system into different model components:

Lens Galaxy: Light + Mass

Source Galaxy: Light



Light and Mass Profile classes

Write the **model components** of the problem as **Python classes** using the same API shown previously.

Note how the **model specific** calculations of this problem are functions of the classes.

Light Profile:

```python
class LightDeVaucouleurs:

    def __init__(
        self,
        centre: typing.Tuple[float, float] = (0.0, 0.0),
        axis_ratio : float = 1.0,
        angle : float = 0.0,
        intensity: float = 0.1,
        effective_radius: float = 0.6,
    ):
        """The De Vaucouleurs light profile representing the bulge of galaxies...."""

        self.centre = centre
        self.axis_ratio = axis_ratio
        self.angle = angle
        self.intensity = intensity
        self.effective_radius = effective_radius

    def transform_grid_to_reference_frame(self, grid : np.ndarray):...

    def grid_to_elliptical_radii(self, grid : np.ndarray) -> np.ndarray:...

    def image_from_grid(self, grid : np.ndarray) -> np.ndarray:...
```

Light and Mass Profile classes

Mass Profile:

```python
class MassIsothermal:

    def __init__(
        self,
        centre: typing.Tuple[float, float] = (0.0, 0.0),
        axis_ratio : float = 1.0,
        angle : float = 0.0,
        mass: float = 1.0,
    ):
        """Represents an elliptical isothermal mass distribution...."""

        self.centre = centre
        self.axis_ratio = axis_ratio
        self.angle = angle
        self.mass = mass

    def transform_grid_to_reference_frame(self, grid : np.ndarray):...

    def rotate_grid_from_reference_frame(self, grid : np.ndarray) -> np.ndarray:...

    def psi_from(self, grid : np.ndarray) -> np.ndarray:...

    def deflections_from_grid(self, grid : np.ndarray) -> np.ndarray:...
```

Light Profile:

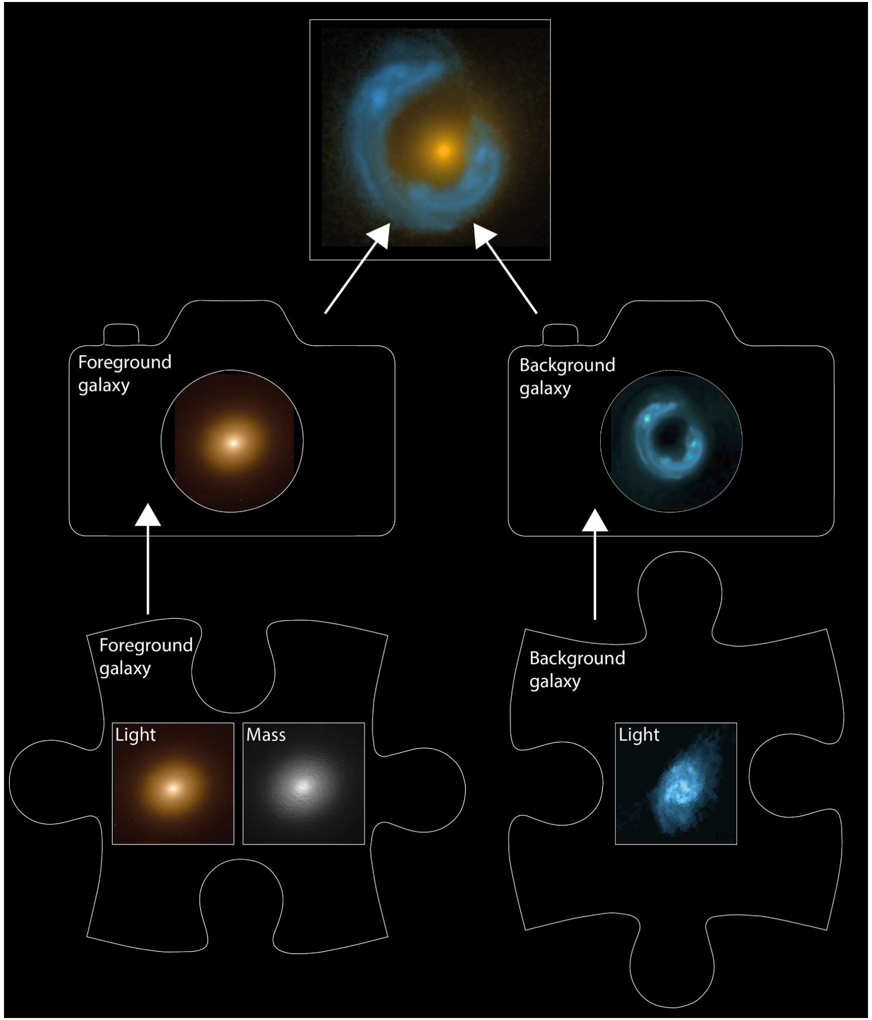
```python
class LightExponential:

    def __init__(
        self,
        centre: typing.Tuple[float, float] = (0.0, 0.0),
        axis_ratio : float = 1.0,
        angle : float = 0.0,
        intensity: float = 0.1,
        effective_radius: float = 0.6,
    ):
        """The Exponential light profile representing the disk of galaxies...."""

        self.centre = centre
        self.axis_ratio = axis_ratio
        self.angle = angle
        self.intensity = intensity
        self.effective_radius = effective_radius

    def transform_grid_to_reference_frame(self, grid : np.ndarray) -> np.ndarray:...

    def grid_to_elliptical_radii(self, grid : np.ndarray) -> np.ndarray:...

    def image_from_grid(self, grid : np.ndarray) -> np.ndarray:...
```

Model Composition

Break strong lens system into different model components:

Lens Galaxy: Light + Mass

Source Galaxy: Light



Python Classes

The use of Python Classes to define the has a crucial additional benefit.

- It allows for **multi-level model composition.**

Core for PyAutoFit's graphical modeling and hierarchical modeling functionality.

Galaxy Class

Combine the mass and light profiles **at a specific redshift** to make the lens galaxy and source galaxy.

Note how the **image_from_grid** and **deflections_from_grid** methods are included, which use the methods of the individual light and mass profiles.

Redshift = Distance from us in the Universe.

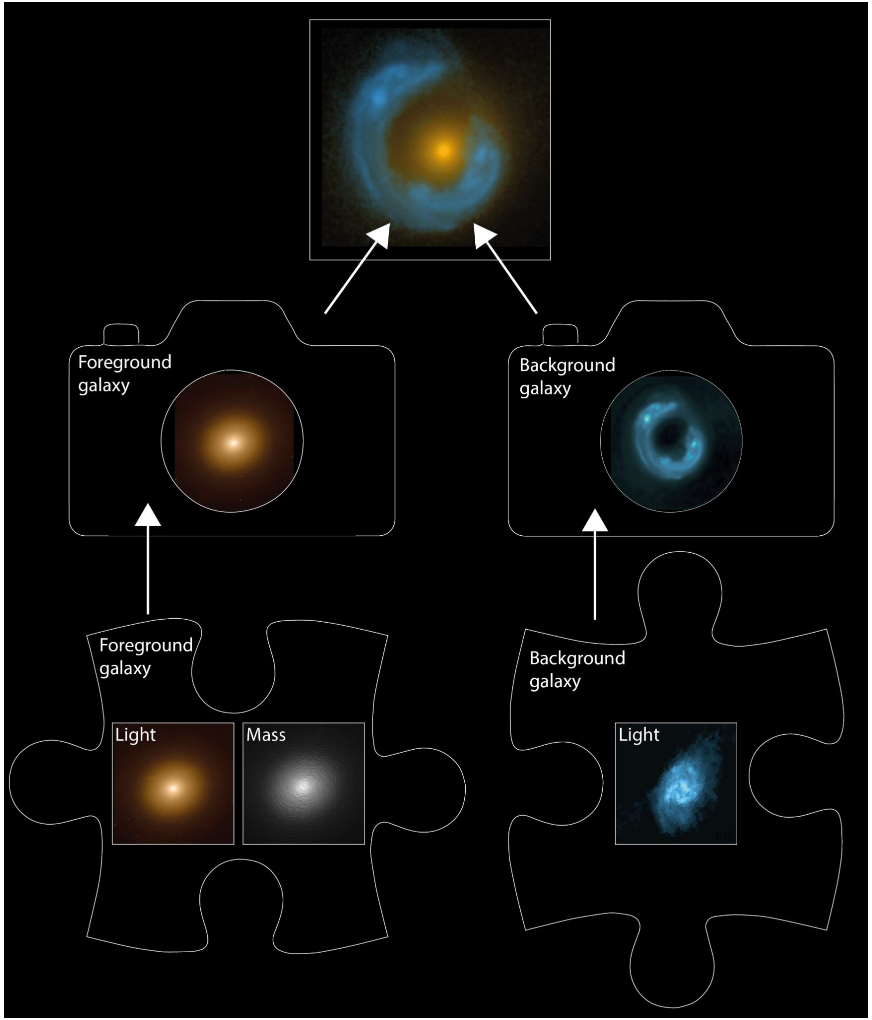
```
class Galaxy:

    def __init__(
            self,
            redshift: float,
            light_profiles: Optional[List] = None,
            mass_profiles: Optional[List] = None,
    ):
        """A galaxy, which contains light and mass profiles at a specified redshift...

        self.redshift = redshift
        self.light_profiles = light_profiles
        self.mass_profiles = mass_profiles

    def image_from_grid(self, grid : np.ndarray) -> np.ndarray:
        """..."""
        if len(self.light_profiles) > 0:
            return sum(
                map(lambda p: p.image_from_grid(grid=grid), self.light_profiles)
            )
        return np.zeros((grid.shape[0],))

    def deflections_from_grid(self, grid : np.ndarray) -> np.ndarray:
        """..."""
        if len(self.mass_profiles) > 0:
            return sum(
                map(lambda p: p.deflections_from_grid(grid=grid), self.mass_profiles)
            )
        return np.zeros((grid.shape[0], 2))
```

Model Composition

Break strong lens system into different **model components**:

Lens Galaxy: Light + Mass

Source Galaxy: Light



Composing the Model

Scans every light and mass profile to determine this model has 16 free parameters that the non-linear search fits.

- A user can easily extend the model with more light profiles, mass profiles, etc.

This is the API a user of your model-fitting software is greeted with!

```python
import autofit as af

lens_galaxy_model = af.Model(
    Galaxy,
    redshift=0.5,
    bulge=LightDeVaucouleurs,
    mass=MassIsothermal
)
source_galaxy_model = af.Model(
    Galaxy,
    redshift=1.0,
    disk=LightExponential
)

model = af.Collection(
    lens=lens_galaxy_model,
    source=source_galaxy_model
)
```

Writing the Analysis

By using Python classes as the model components, this means we can write a concise likelihood function.

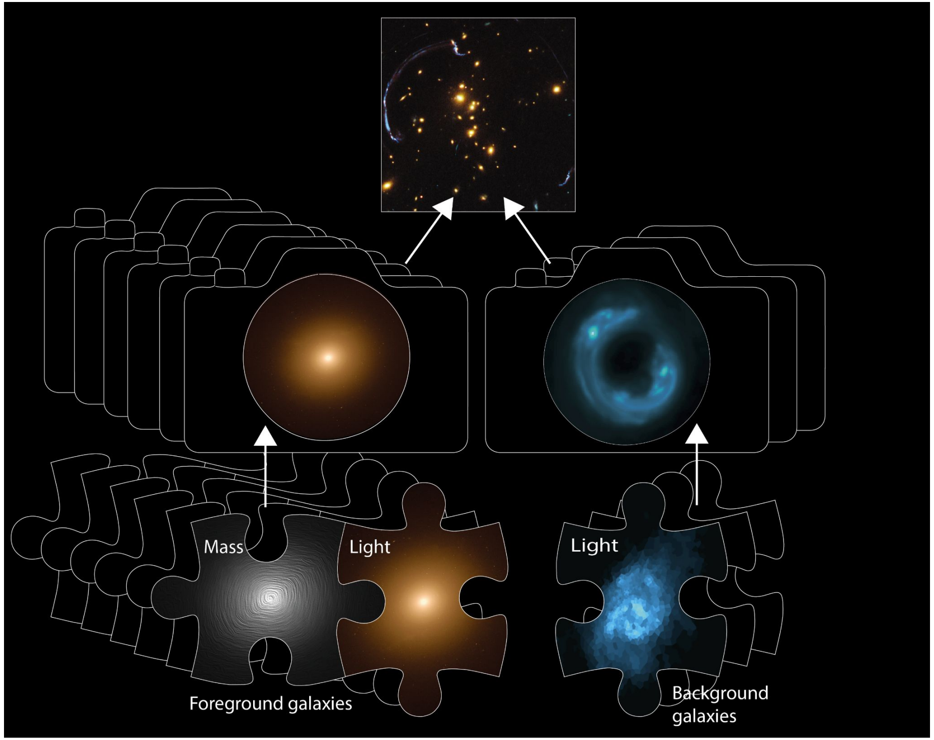
- Cleanly separate the model-specific code (e.g. light profiles, mass profiles, lensing) from the model-fitting code.
- Easy to extend and customize the Analysis class for bespoke model-fitting.

```python
class Analysis(af.Analysis):

    def __init__(self, image, noise_map, psf, grid):

        self.image = image
        self.noise_map = noise_map
        self.psf = psf
        self.grid = grid

    def log_likelihood_function(self, instance):

        """
        The 'instance' that comes into this method contains the `Galaxy`'s
        we setup in the model.
        """

        print("Lens Model Instance:")
        print("Lens Galaxy = ", instance.lens)
        print("Lens Galaxy Bulge = ", instance.lens.bulge)
        print("Lens Galaxy Bulge Centre = ", instance.lens.bulge.centre)
        print("Lens Galaxy Mass Centre = ", instance.lens.mass.centre)
        print("Source Galaxy = ", instance.sources)

        """
        The methods of the `Galaxy` class are available, making it easy to fit
        the lens model.
        """

        lens_image = instance.lens.image_from_grid(grid=self.grid)
        deflections = instance.lens.deflections_from_grid(grid=self.grid)
        source_grid = self.grid - deflections
        source_image = instance.source.image_from_grid(grid=source_grid)

        model_image = lens_image + source_image
        model_image = self.psf.convolve(model_image)

        residual_map = self.image - model_image
        chi_squared_map = (residual_map / self.noise_map) ** 2.0
        log_likelihood = -0.5 * sum(chi_squared_map)

        return log_likelihood
```

Model Composition

Straightforward for complex models to be composed and fitted in a scalable and streamlined way:

- Easy to extend model galaxies with many light and mass profiles.
- Or extend the model with many more galaxies.



PyAutoLens: Open Source Strong Gravitational Lensing

All code publically available (pip / conda), object oriented design, extensive documentation.

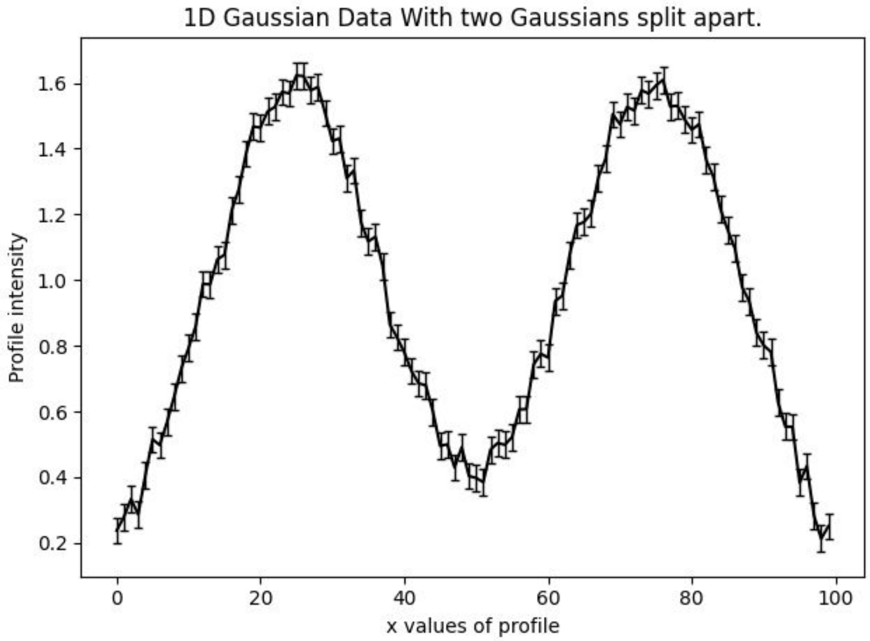
GitHub: https://github.com/Jammy2211/PyAutoLens
Readthedocs: https://pyautolens.readthedocs.io/en/latest/
JOSS paper: https://joss.theoj.org/papers/10.21105/joss.02825

The HowToLens Jupyter notebook lectures teach strong lens modeling to beginners (pitched at undergrads and above)!

PyAutoFit: Advanced Features

Search Chaining

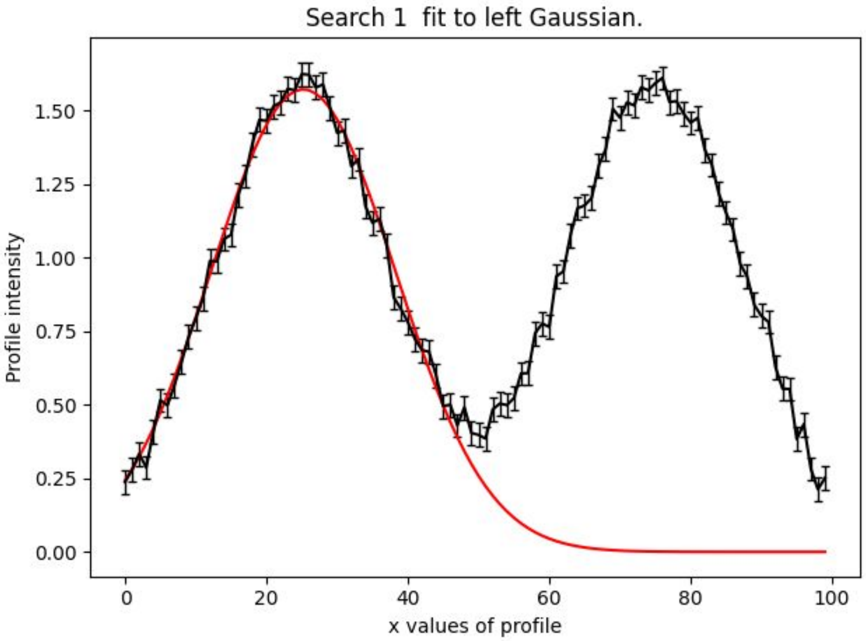
Break a model-fit into a **chained sequence** of searches:



Search Chaining

Break a model-fit into a chained sequence of searches:

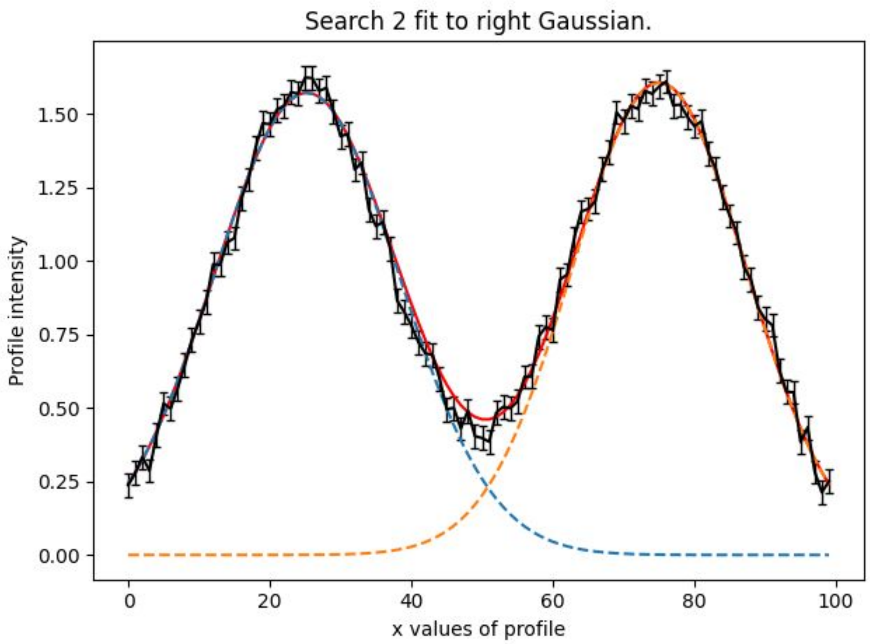
- Search 1: fit model to left Gaussian with **fast non-linear search**.



Search Chaining

Break a model-fit into a chained sequence of searches:

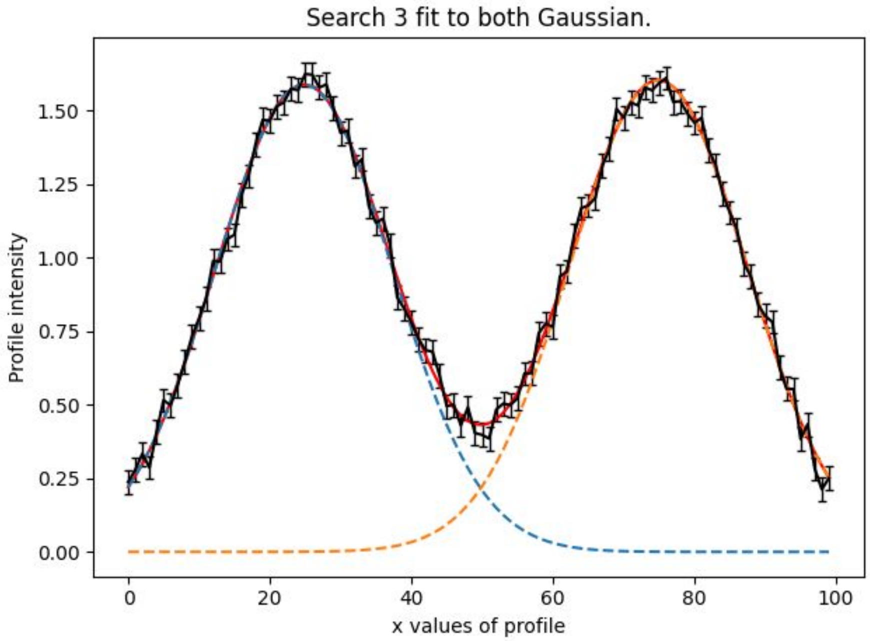
- Search 1: fit model to left Gaussian with **fast non-linear search**.
- Search 2: fit model to right Gaussian with fast non-linear search and result of search 1.



Search Chaining

Break a model-fit into a chained sequence of searches:

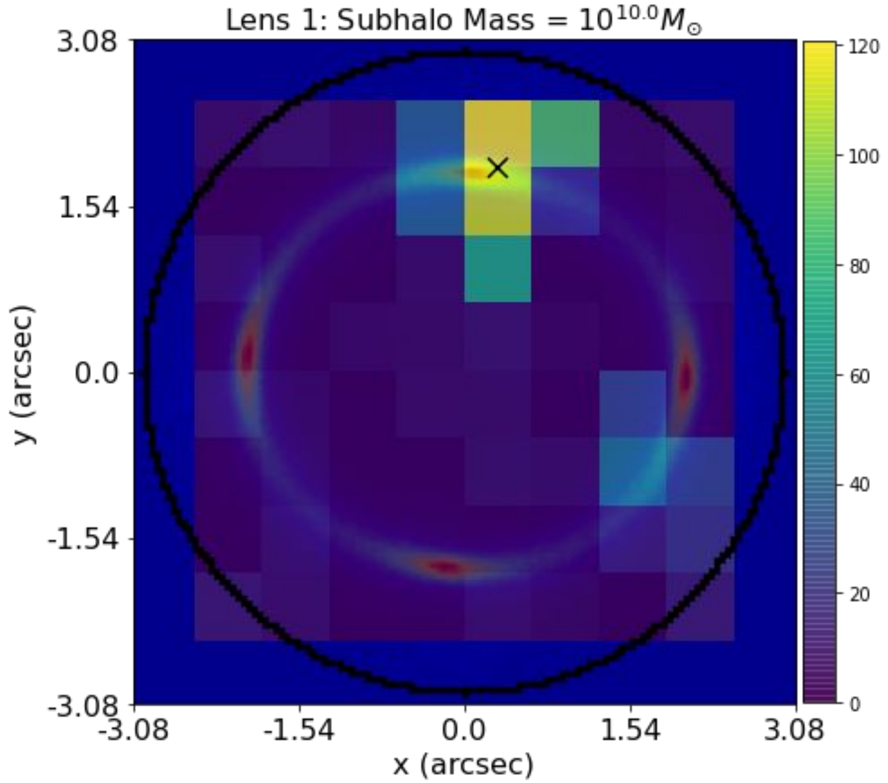
- Search 1: fit model to left Gaussian with **fast non-linear search**.
- Search 2: fit model to right Gaussian with **fast non-linear search** and result of search 1.
- Search 3: Fit both Gaussians simultaneously with **thorough non-linear search and a parameter space starting point** inferred from first two searches.



Grid Search of Non-linear Searches

Break a model-fit into a grid search of searches:

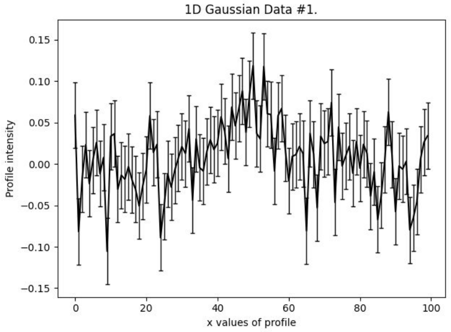
- Support for massively parallel fits.
- Database provides tools for analysing results efficiently.

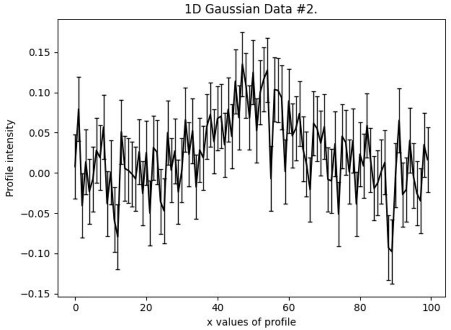


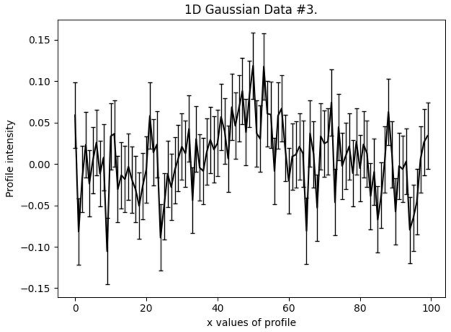
Graphical and Hierarchical Models

Compose multi-level models for fitting many datasets:

- Simple example of fitting three low signal to noise Gaussians simultaneously.
- Can assume all three Gaussians have same centre, but different intensity / sigma.







Graphical and Hierarchical Models

Can set up unique **Analysis** class, which will pair every dataset with components of the multi-level model:

```
analysis_0 = a.Analysis(data=data_0, noise_map=noise_map_0)
analysis_1 = a.Analysis(data=data_1, noise_map=noise_map_1)
analysis_2 = a.Analysis(data=data_2, noise_map=noise_map_2)
```

Model is built out of individual model components like before.

```
centre_shared_prior = af.GaussianPrior(mean=50.0, sigma=30.0)
```

```
gaussian_0 = af.Model(m.Gaussian)
gaussian_0.centre = centre_shared_prior
gaussian_0.intensity = af.GaussianPrior(mean=10.0, sigma=10.0)
gaussian_0.sigma = af.GaussianPrior(mean=10.0, sigma=10.0)  # This prior is used by all 3 Gaussians!

prior_model_0 = af.Collection(gaussian=gaussian_0)

gaussian_1 = af.Model(m.Gaussian)
gaussian_1.centre = centre_shared_prior
gaussian_1.intensity = af.GaussianPrior(mean=10.0, sigma=10.0)
gaussian_1.sigma = af.GaussianPrior(mean=10.0, sigma=10.0)  # This prior is used by all 3 Gaussians!

prior_model_1 = af.Collection(gaussian=gaussian_1)
```

PyAutoFit: Customization

Python Classes

The use of Python Classes to define the model, analysis and non-linear searches has downsides relative to other PPLs:

- It is a less concise interface.
- It requires a basic understanding of Python classes and object oriented programming (albeit good documentation can alleviate this).

The benefit is it provides a far more customizable model-fitting experience.

Customizing the Model

Full customization of the model parameterization, priors and valid regions of parameter space.

- Default priors can be specified in easy to set up configuration files, so a new user does not need to ‘think’ about them.

```
"""
Compose model with multiple-components.
"""

gaussian_0 = af.Model(Gaussian)
gaussian_1 = af.Model(Gaussian)

"""
Manually set prior on each parameter.
"""

gaussian_0.centre = af.UniformPrior(lower_limit=0.0, upper_limit=100.0)
gaussian_0.intensity = af.LogUniformPrior(lower_limit=0.0, upper_limit=1e2)
gaussian_0.sigma = af.GaussianPrior(mean=10.0, sigma=5.0, lower_limit=0.0, upper_limit=np.inf)

"""
Fix a parameter to a value (reducing dimensionality of parameter space by 1).
"""
gaussian_0.sigma = 0.5

"""
Link two parameters in a model (reducing dimensionality of parameter space by 1).
"""
gaussian_0.centre = gaussian_1.centre

"""
Make assertions removing regions of parameter space.
"""
gaussian_1.add_assertion(gaussian_1.sigma > 5.0)

"""
To make a model with multiple components we use a `Collection` object.
"""
model = af.Collection(gaussian_0=gaussian_0, gaussian_1=gaussian_1)
```

Customizing the Model

Full customization of the model parameterization, priors and valid regions of parameter space.

- Straightforward to add many different model-components via inheritance.
- **Composition** makes this concise and scalable.

```
class Gaussian:

    def __init__(
            self,
            centre=0.0,
            intensity=0.1,
            sigma=0.01,
    ):
        self.centre = centre
        self.intensity = intensity
        self.sigma = sigma

class GaussianKurtosis(Gaussian):

    def __init__(
            self,
            centre=0.0,
            intensity=0.1,
            sigma=0.01,
            kurtosis=0.1,
    ):

        super().__init__(
            centre=centre,
            intensity=intensity,
            sigma=sigma
        )

        self.kurtosis = kurtosis

class Exponential:
    def __init__(
        self,
        centre=0.0,
        intensity=0.1,
        rate=0.01,
    ):

        self.centre = centre
        self.intensity = intensity
        self.rate = rate
```

Customizing the Analysis

The Analysis class can be extended or provide model-specific on-the-fly visualization of the model-fit so far.

- Uses the maximum likelihood model of the search so far.
- For long model-fits can inform you if the fitting has gone wrong early.

```python
class Analysis(af.Analysis):
    def __init__(self, data, noise_map):

        self.data = data
        self.noise_map = noise_map

    def log_likelihood_function(self, instance):

        ...

    def visualize(self, paths, instance):

        """
        During a model-fit, the `visualize` method is called throughout the
        non-linear search. The `instance` is maximum log likelihood solution
        obtained so far and is used to output on-the-fly images.
        """
        xvalues = np.arange(self.data.shape[0])

        model_data = instance.profile_from_xvalues(xvalues=xvalues)
        residual_map = self.data - model_data

        plt.errorbar(
            x=xvalues, y=residual_map, color="k", ecolor="k",
        )
        plt.title("1D Residual Map")
        plt.xlabel("x value of profile")
        plt.ylabel("Residual")
        plt.savefig(path.join(paths.image_path, "residual_map.png"))
        plt.clf()
```

Customizing the Search

PyAutoFit supports many non-linear searches (MCMC, nested sampling, optimizers, etc.).

- Full customization of their settings.
- Defaults to configuration file values if not specified.

```
emcee = af.Emcee(
    name="example_mcmc",
    nwalkers=50,
    nsteps=2000,
    initializer=af.InitializerBall(lower_limit=0.49, upper_limit=0.51),
    auto_correlations_settings=af.AutoCorrelationsSettings(
        check_for_convergence=True,
        check_size=100,
        required_length=50,
        change_threshold=0.01,
    ),
)
```

PyAutoFit: Features

Database

Results of many model fits are output in an sqlite relational database:

- Allocated a **unique identifier** based on the model-fit, such that you can trivially fit many models.
- Database supports advanced queries (e.g. find all results, where this parameter is in this range).
- Results use memory-light Python generators.

You can therefore fit (very) large datasets on a HPC and access the results efficiently via a Jupyter notebook.

```
agg = af.Aggregator.from_database("database.sqlite")

bulge = agg.lens.bulge
agg_query = agg.query(bulge == LightDeVaucouleurs)

for samples in agg_query.values("samples"):

    print("Maximum Log Likelihood Instance:")
    print(samples.max_log_likelihood_instance)
```

Advanced Modeling Tools

Search Grid Search: Massively parallel grid searches of non-linear searches.

Search Chaining: Write highly customizable model-fitting pipelines that chain together multiple non-linear searches.

Sensitivity Mapping: Simulate and fit many datasets to determine when a more complex model would be accepted via model comparison.

Graphical / Hierarchical Models: Fit for global trends in large datasets by composing and fitting graphical models.