

Introduction to MCALF

Multi-Component Atmospheric Line Fitting

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Queen's University Belfast

Solar Physics PhD

Sep 2019 —

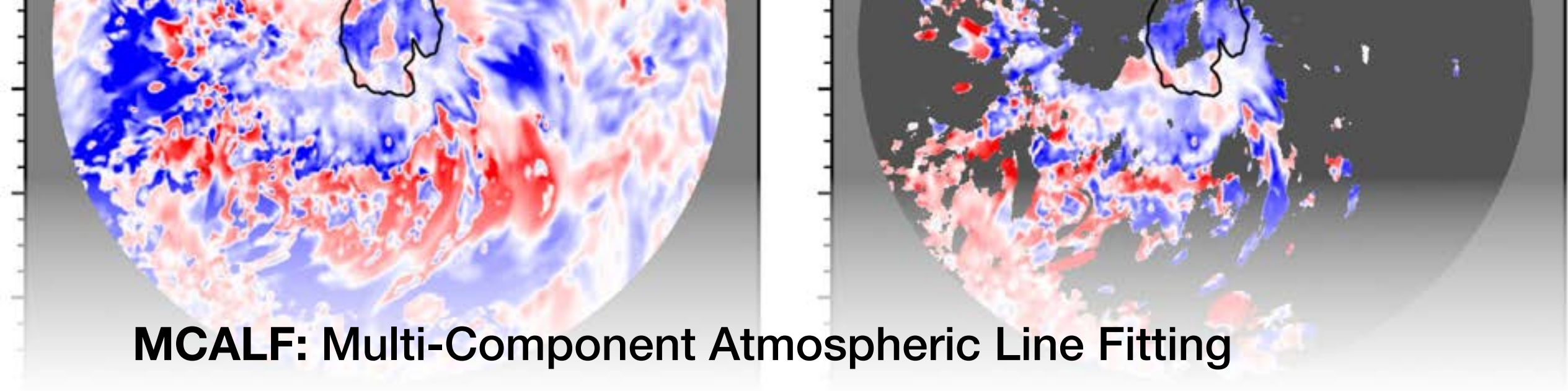
Energy Dissipation in Solar Physics

Supervisor: David Jess

University of St Andrews

MPhys Mathematics and Theoretical Physics

Sep 2015 — Jun 2019



MCALF: Multi-Component Atmospheric Line Fitting

MCALF is an open-source Python package for accurately constraining velocity information from spectral imaging observations using machine learning techniques.



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David Jess

Reader, Queen's University Belfast

GitHub

github.com/ConorMacBride/mcalf

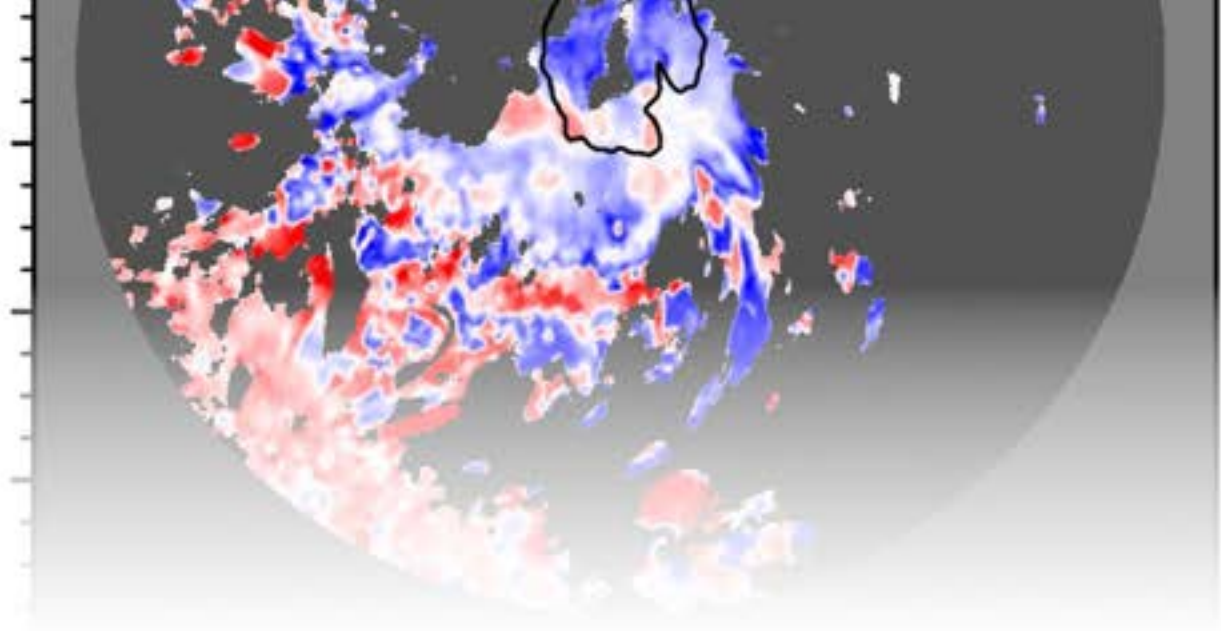
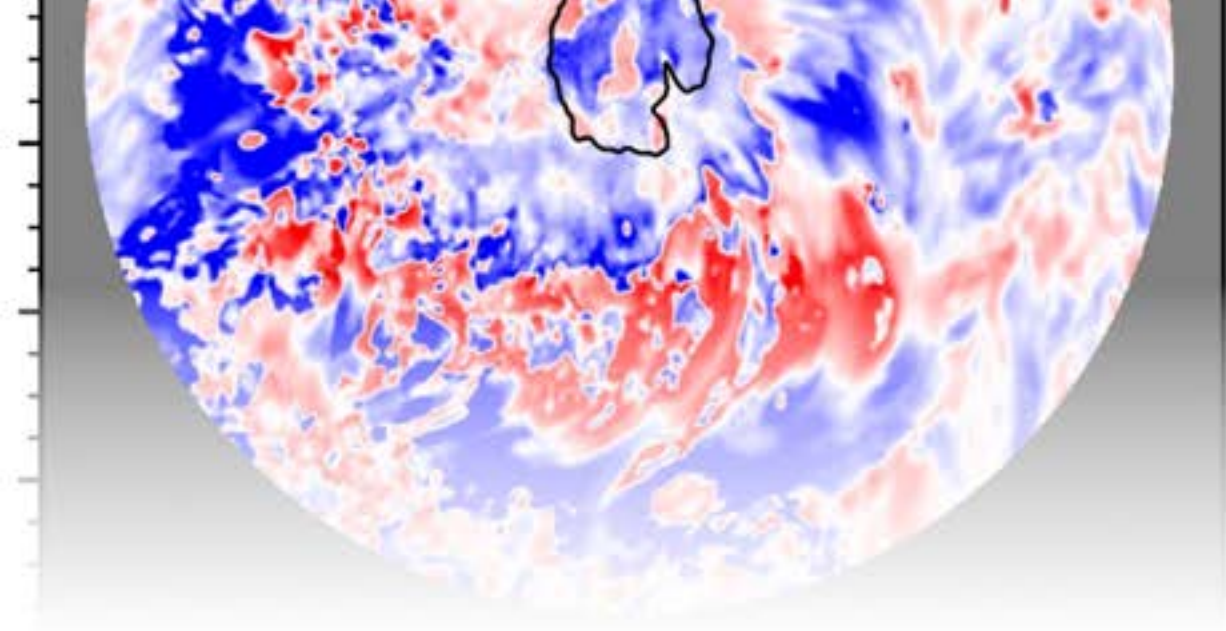
Documentation

mcalf.macbride.me

Install

```
pip install mcalf
```

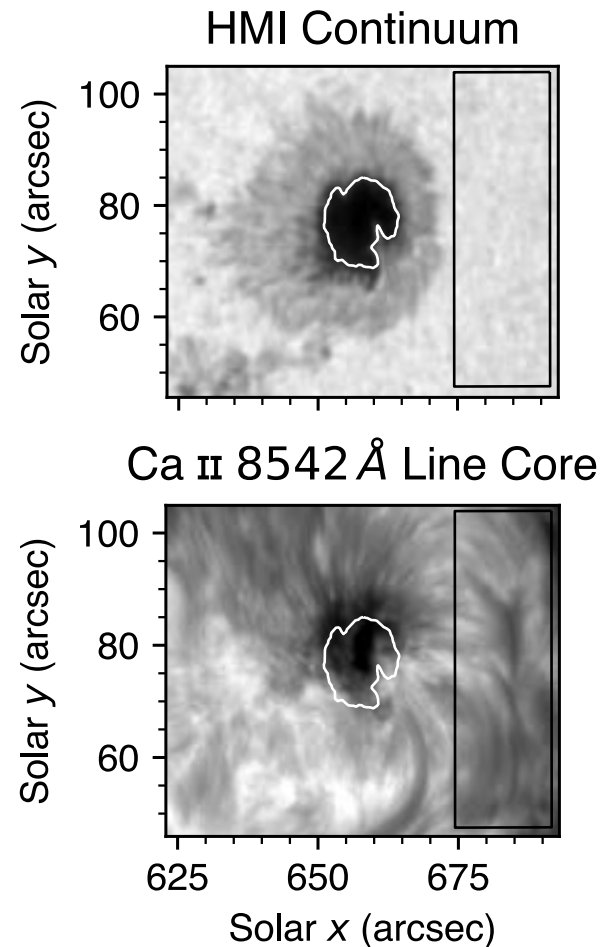
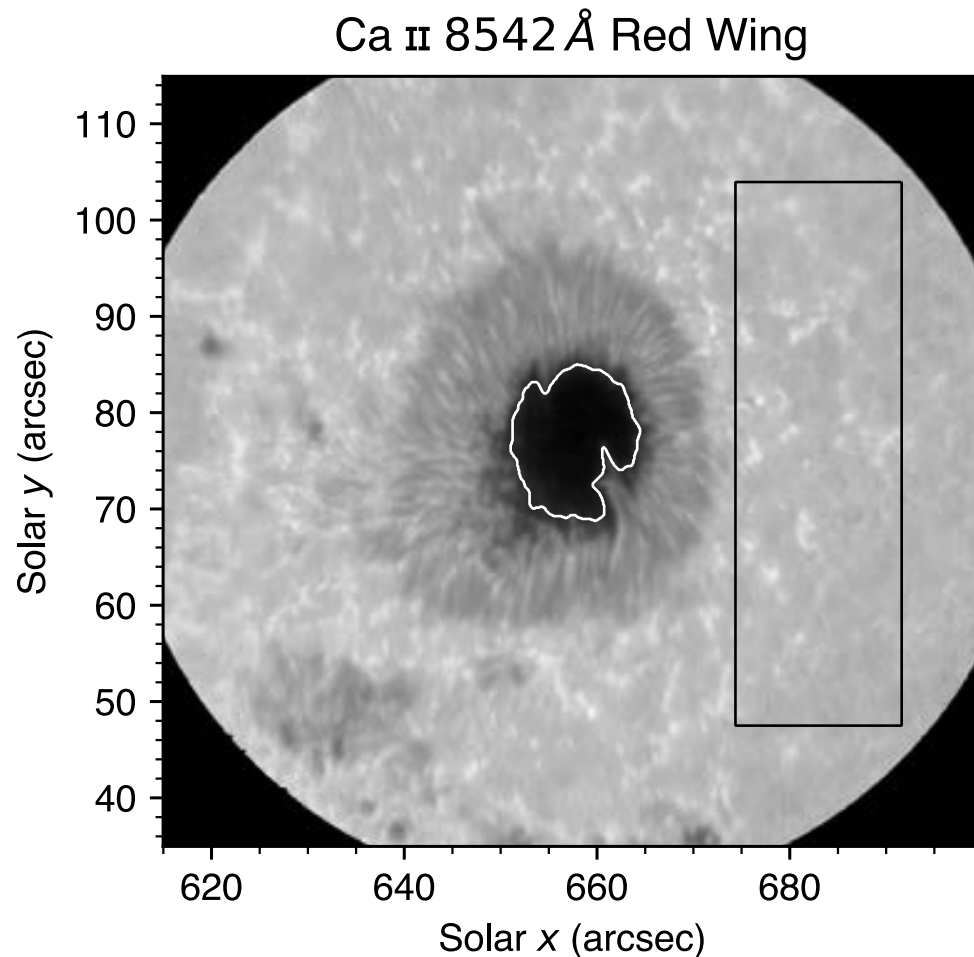
```
conda install mcalf
```

Method & Proof of Concept

Description of the method behind the `mcalf.models.IBIS8542Model` class

IBIS observations



IBIS settings

Spatial resolution

0".098
per pixel

Temporal resolution

5.8
seconds

Spectral resolution

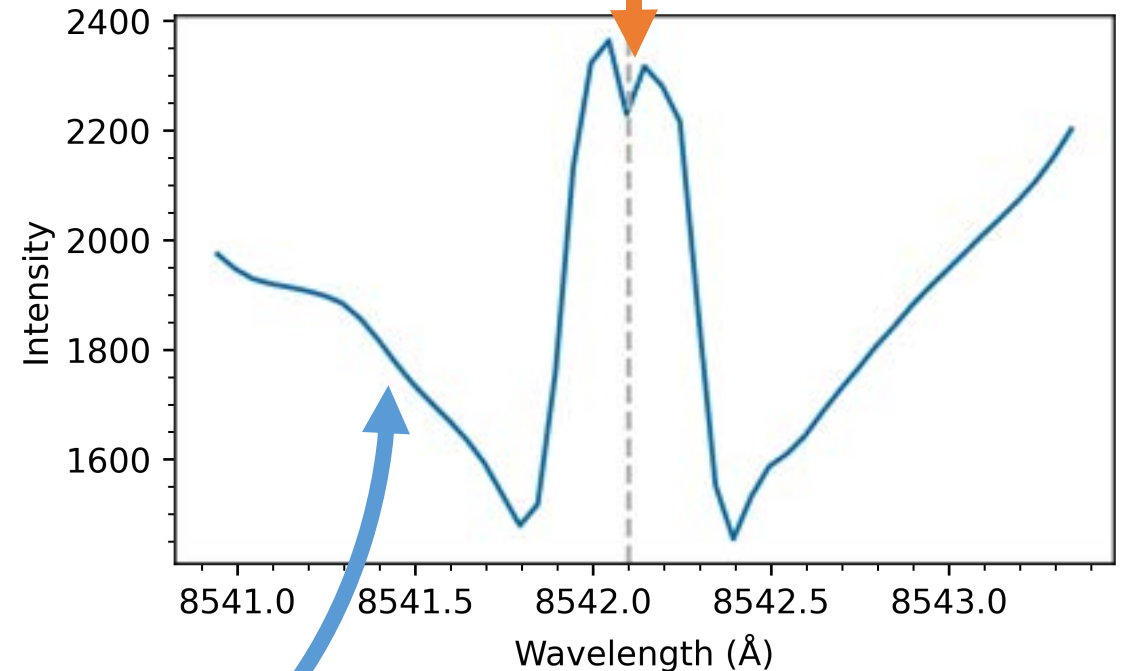
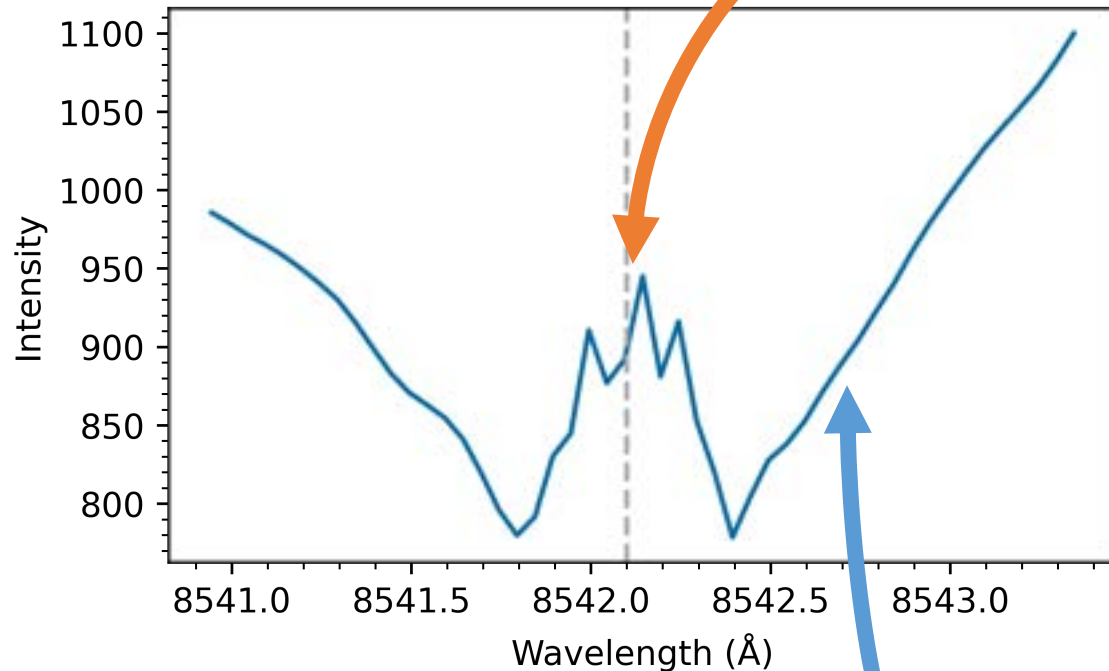
27
points over

2.4 Å

*centred at Ca II IR 8542 Å
with greater density
around the line core*

Multiple spectral components

Emission



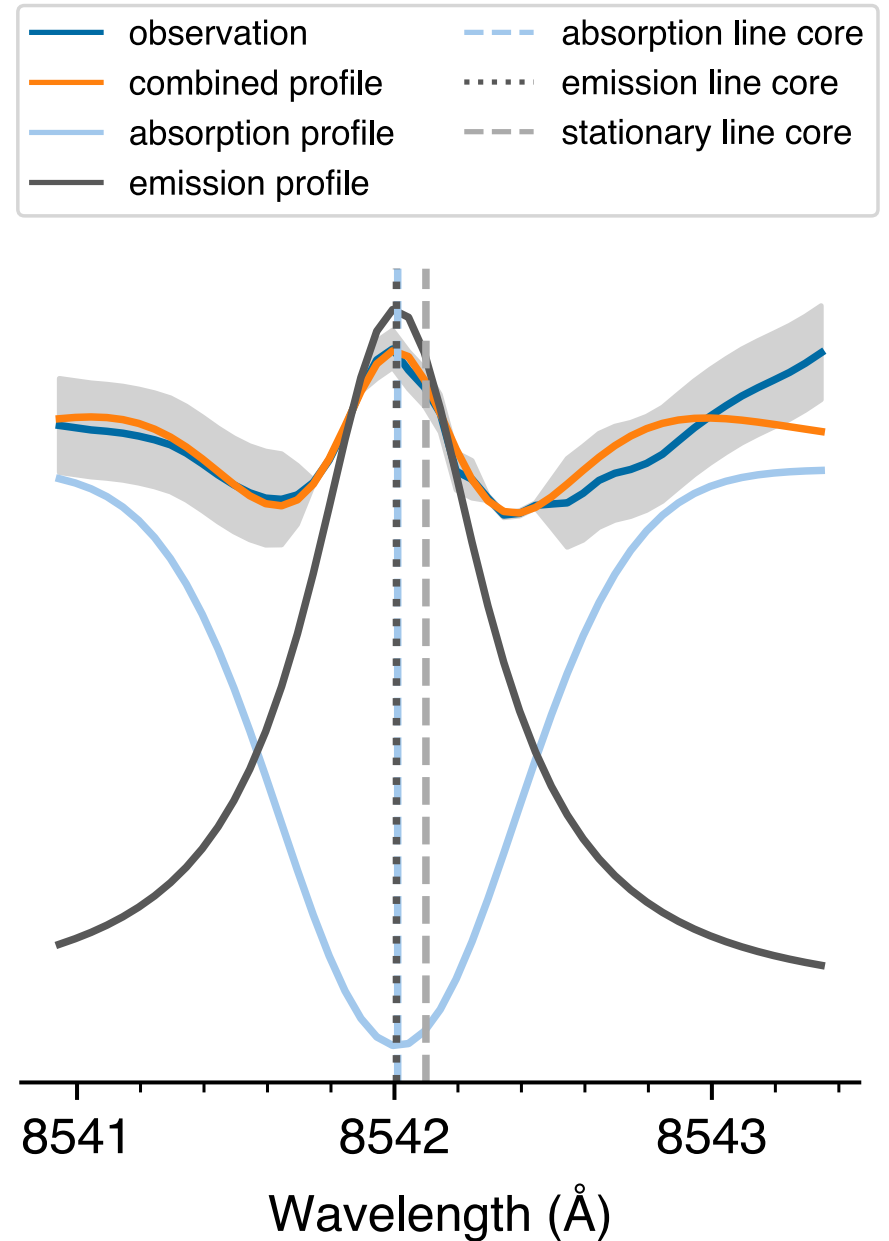
Absorption

Using the Voigt function

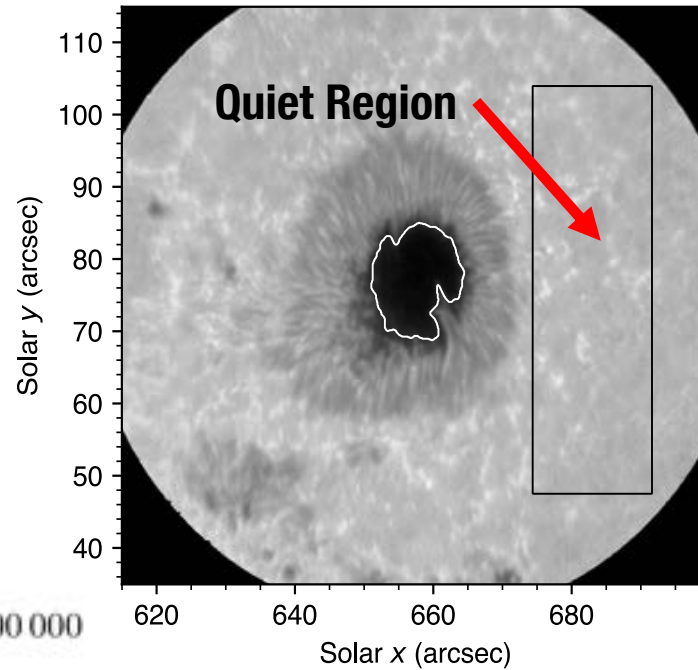
$$V(x; A, \sigma, \gamma) = A \int_{-\infty}^{\infty} G(u; \sigma) L(x - u; \gamma) du$$

$$G(x; \sigma) = \exp(-x^2 / (2\sigma^2)) / (\sigma \sqrt{2\pi})$$

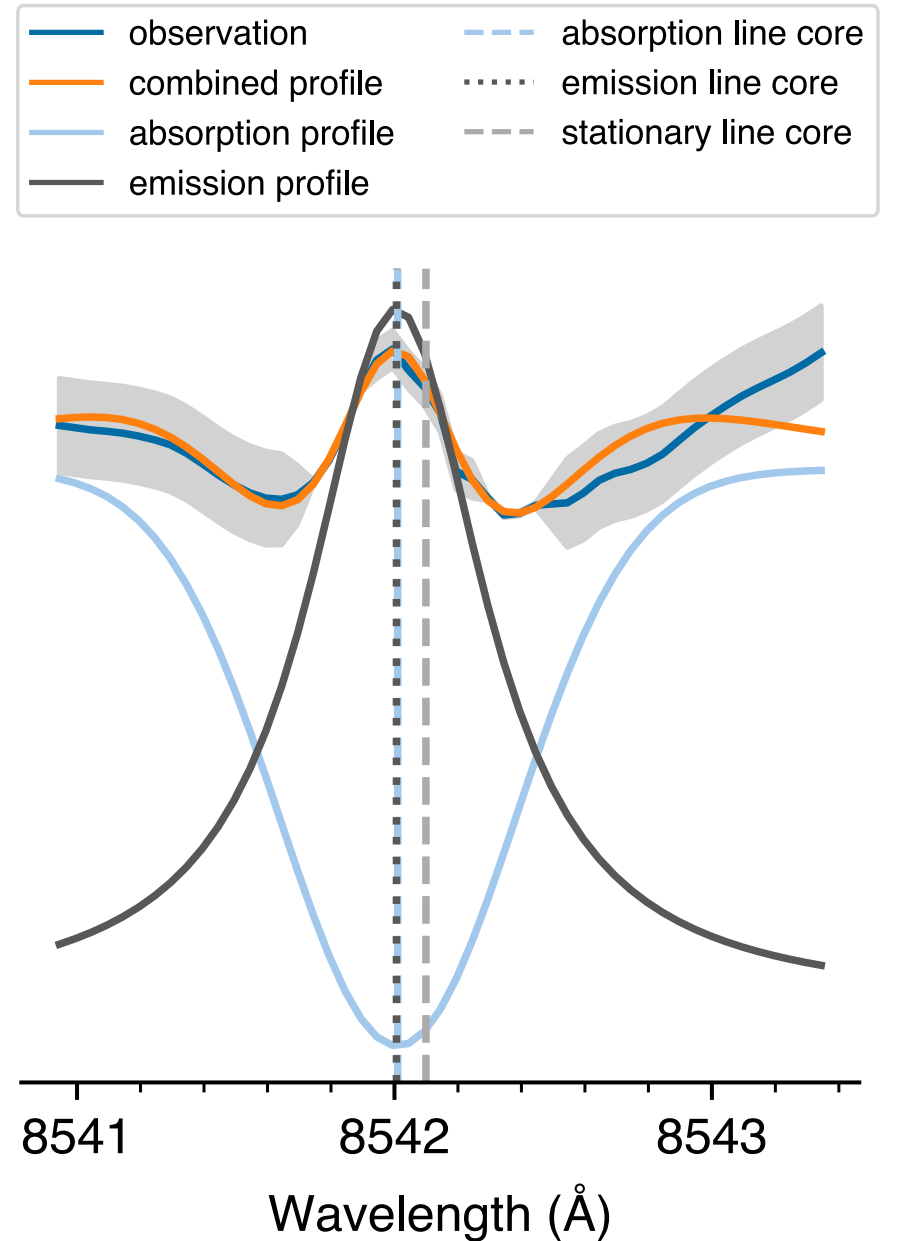
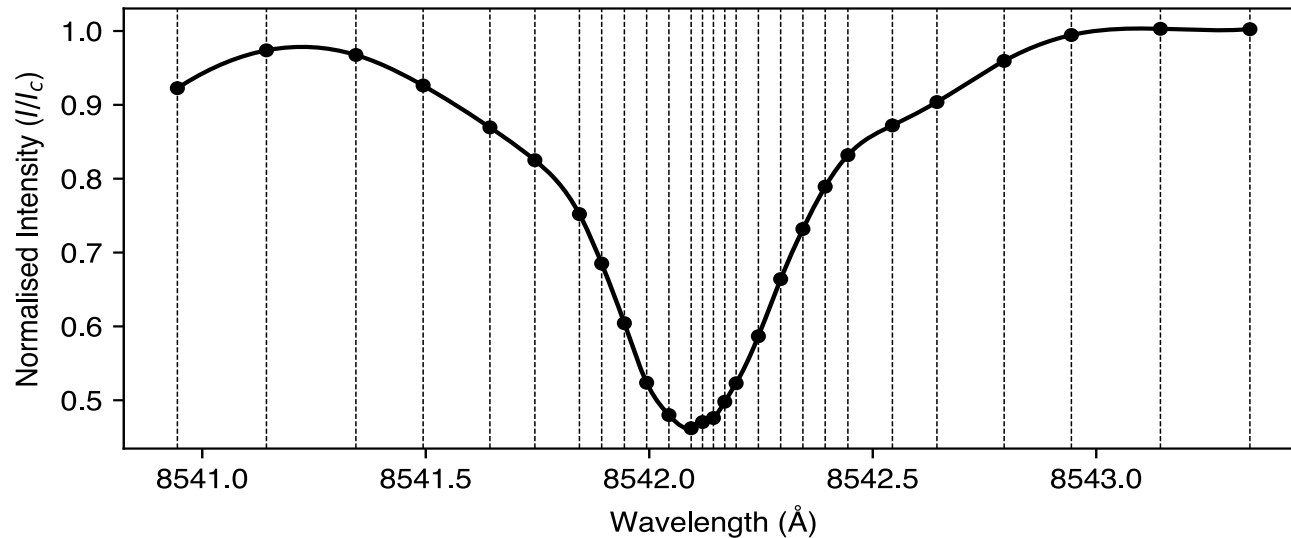
$$L(x; \gamma) = \gamma / (\pi(x^2 + \gamma^2))$$



Doppler velocities

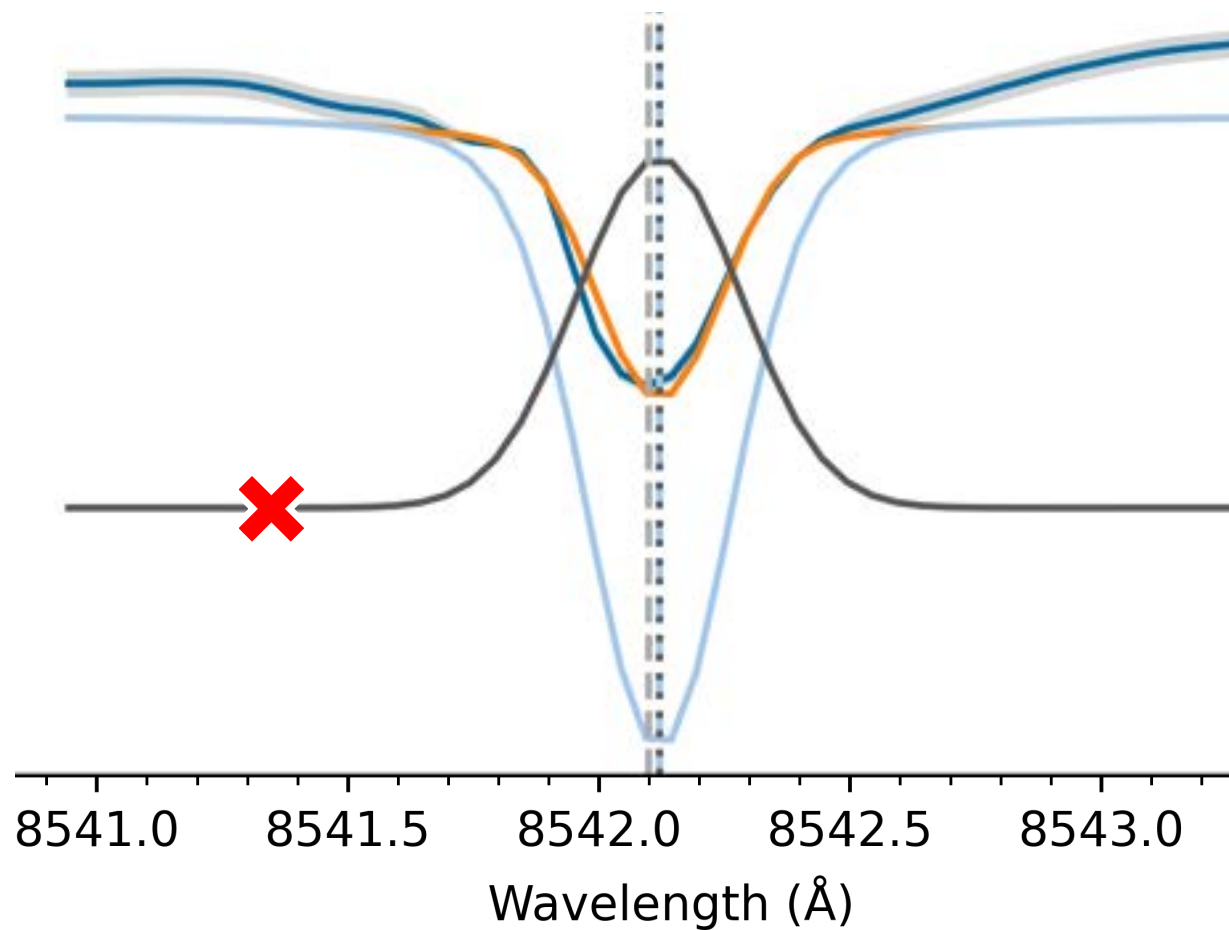
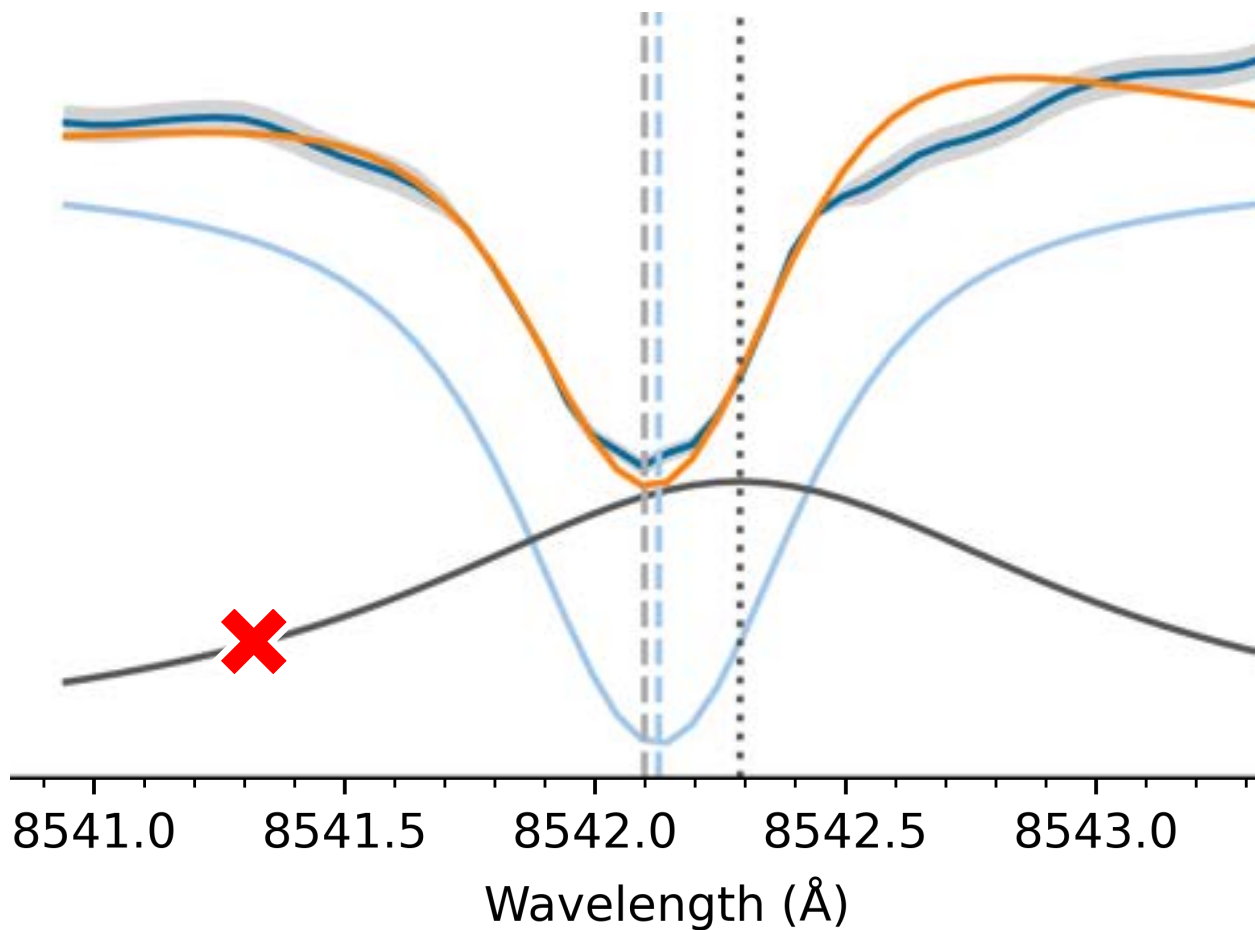


$$v \text{ (km/s)} = \frac{\lambda_{\text{observed}} - \lambda_{\text{stationary}}}{\lambda_{\text{stationary}}} \times 300\,000$$

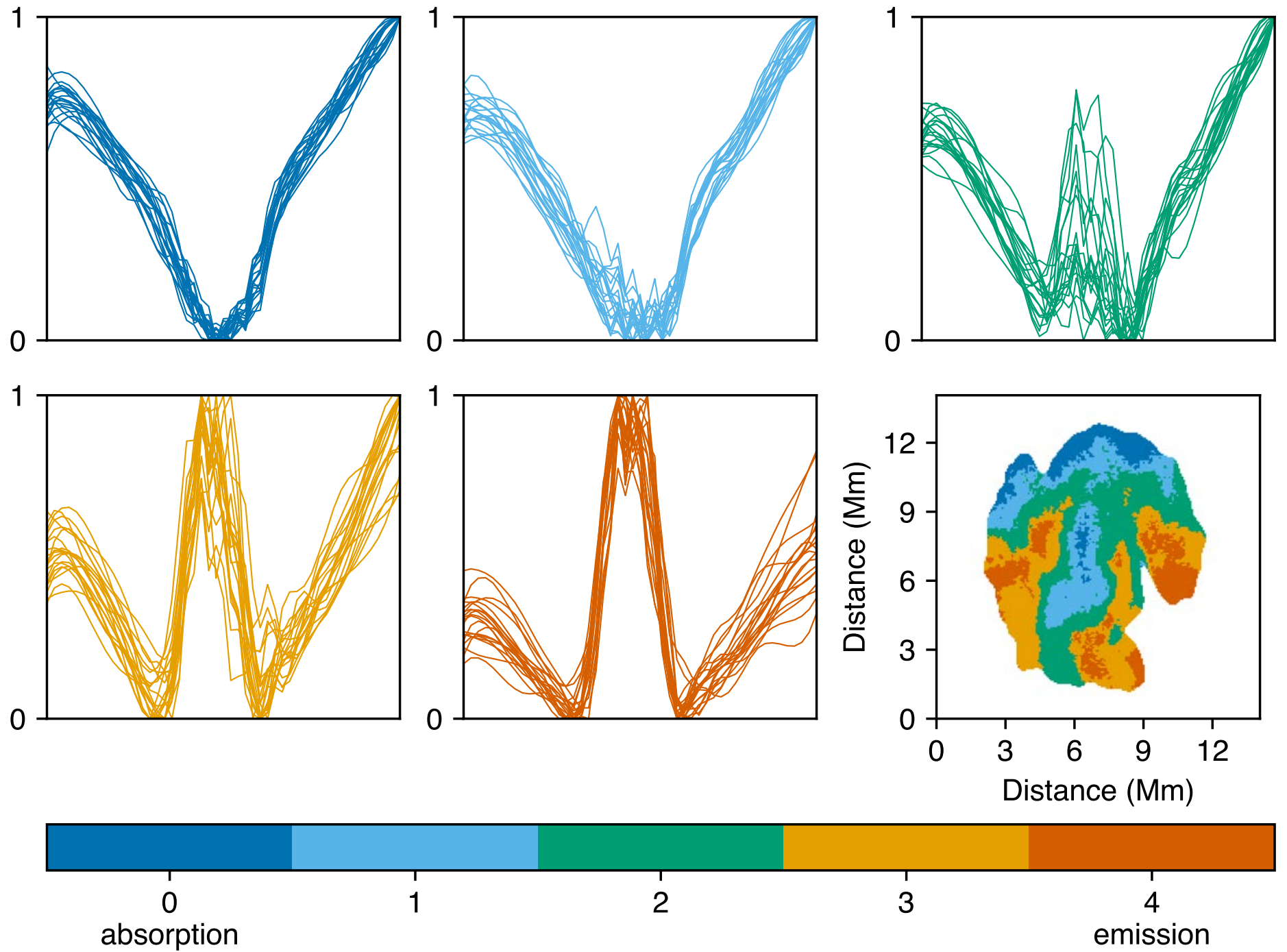


Overfitting

- observation
- combined profile
- absorption profile
- emission profile
- - - absorption line core
- emission line core
- - - stationary line core



Neural networks

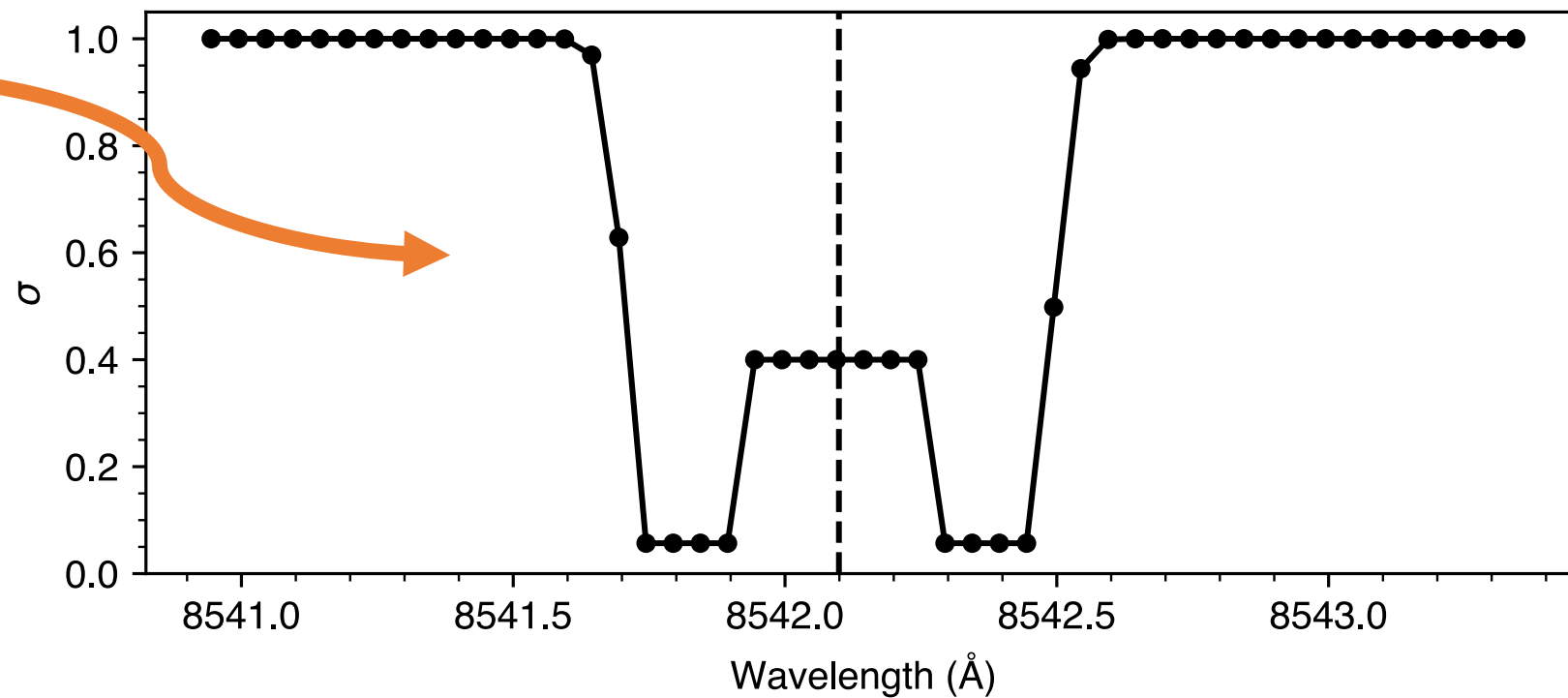
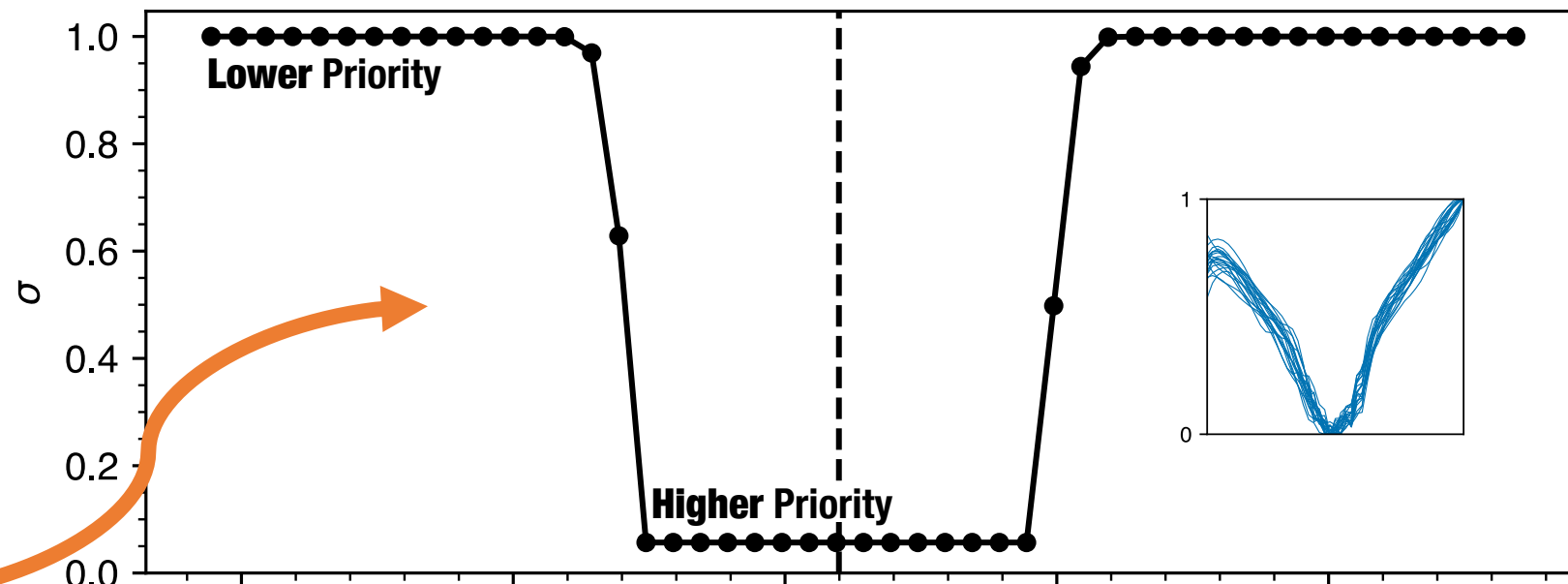


Weighting the fit

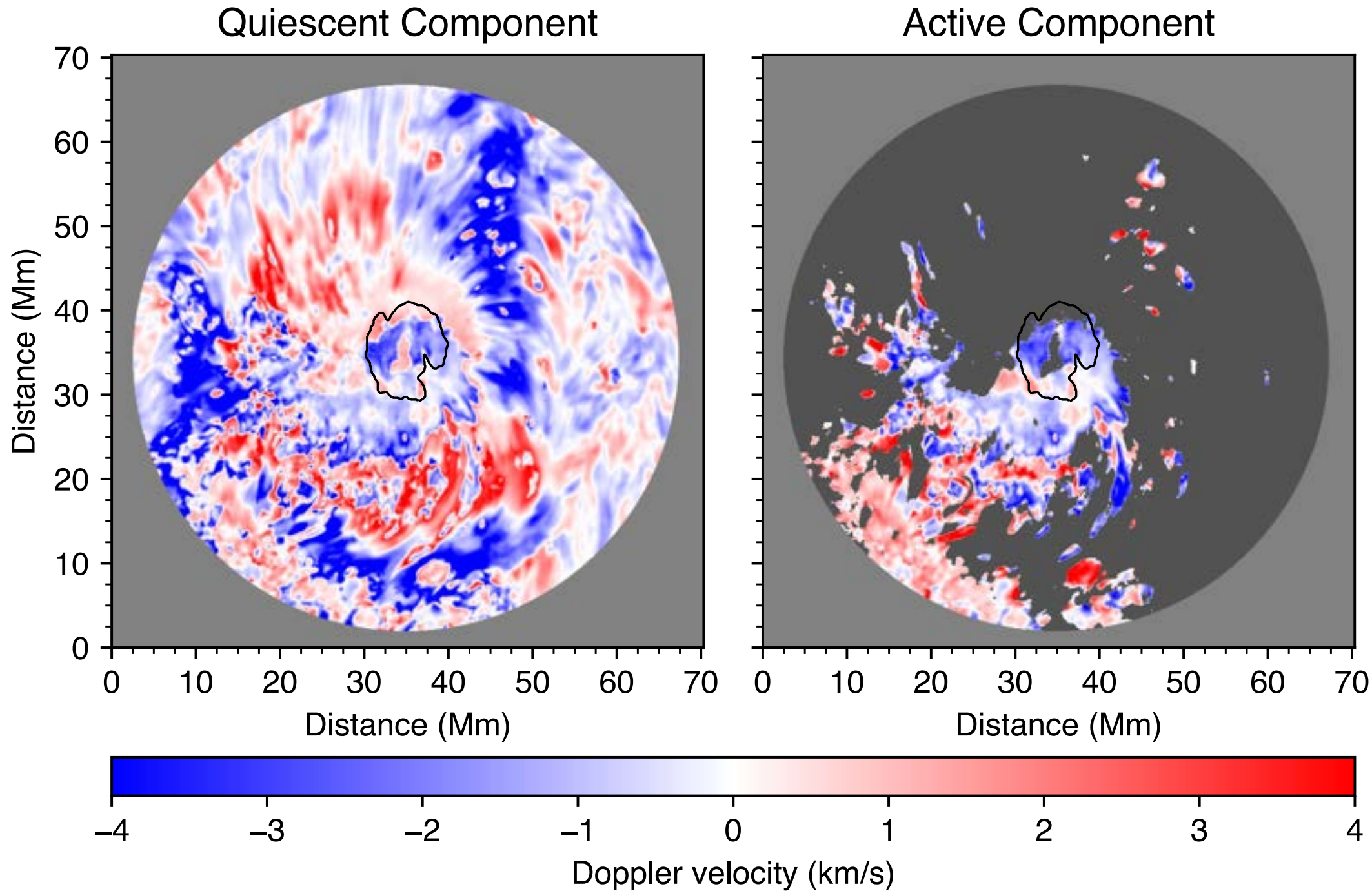
Classifications:

0

1 2 3 4



Doppler velocity plots



Modified χ^2

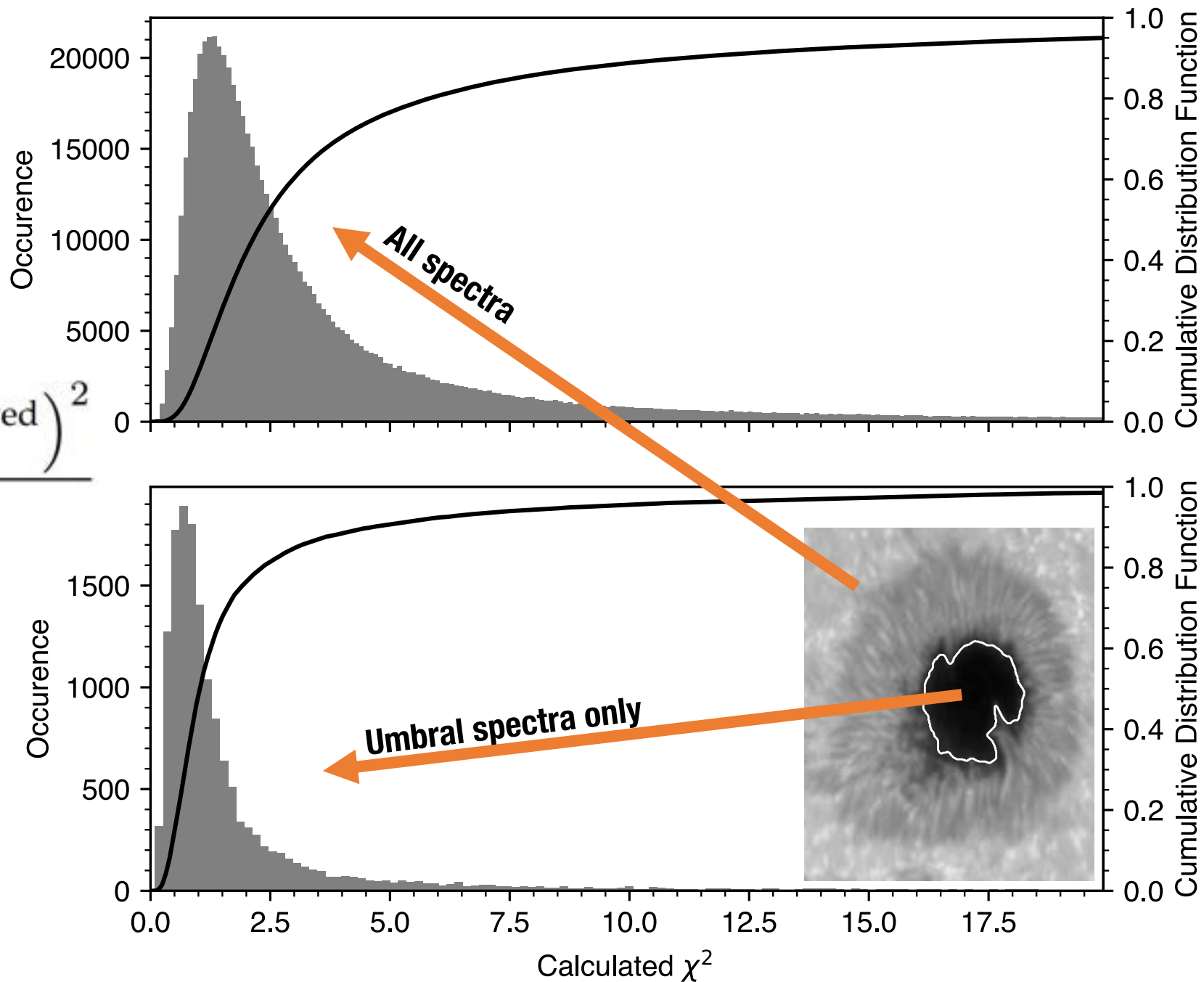
$$\chi^2 = \frac{s}{\nu} \sum_{\lambda \in \lambda_c} \frac{\left(I_{\lambda}^{\text{fitted}} - I_{\lambda}^{\text{observed}}\right)^2}{I_{\lambda}^{\text{observed}}}$$

Scaling factor

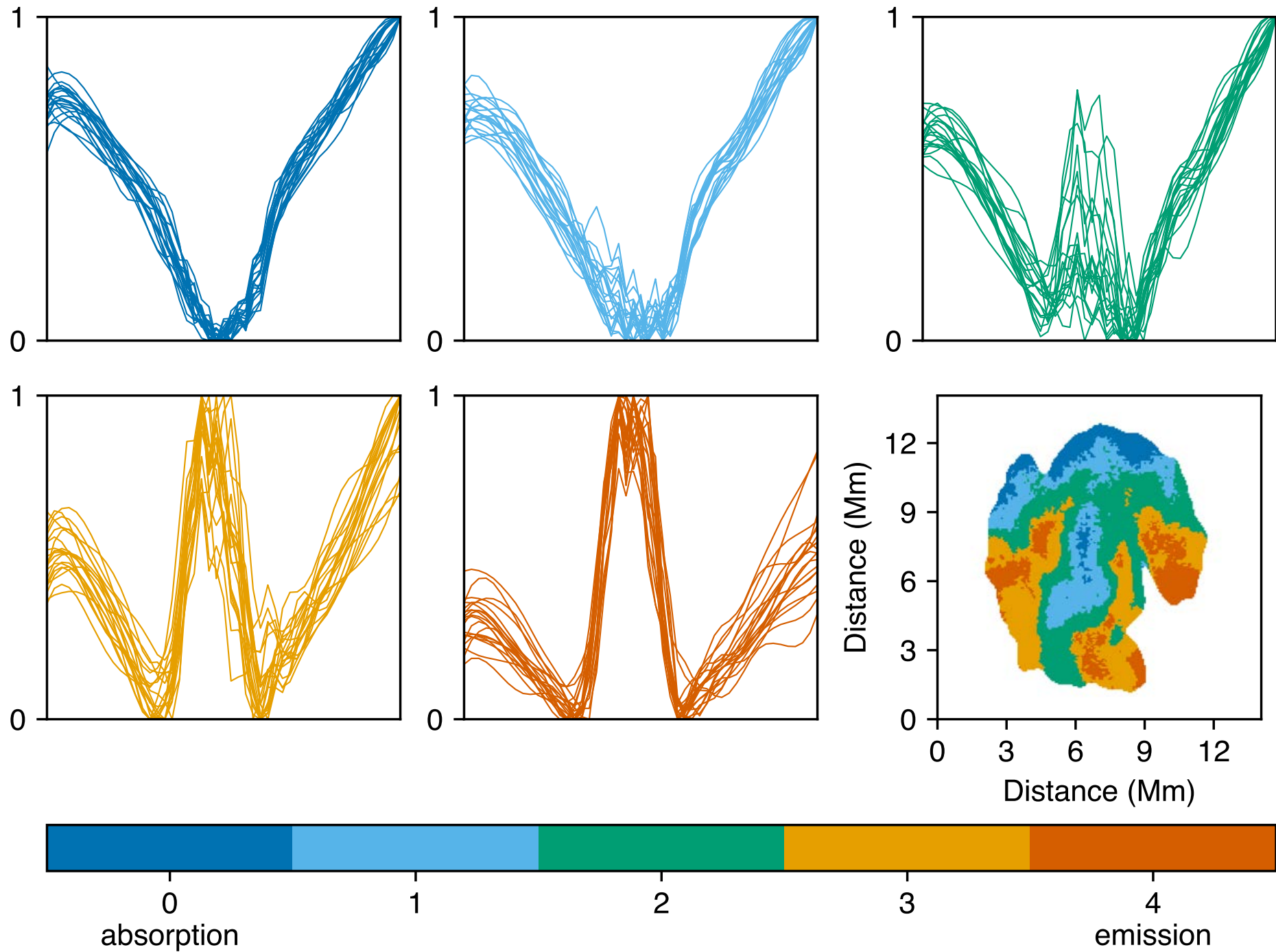
$$s = 49/25$$

Estimated degrees of freedom

$$\begin{aligned}\nu &= 4 \text{ (single Voigt)} \\ &= 8 \text{ (double Voigt)}\end{aligned}$$



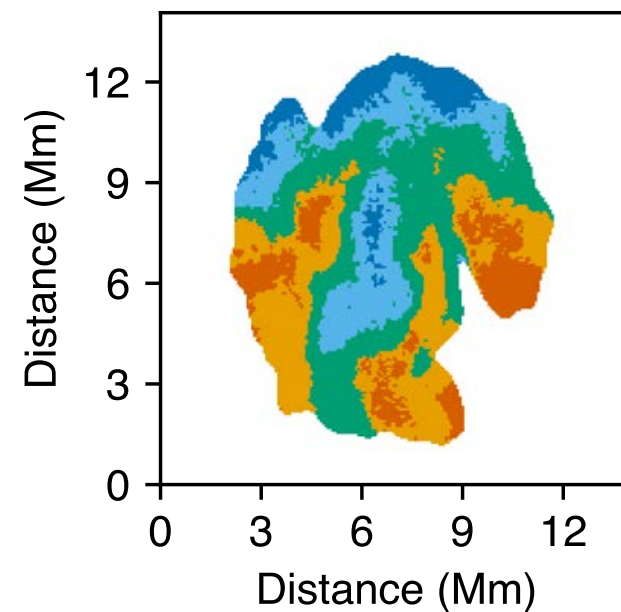
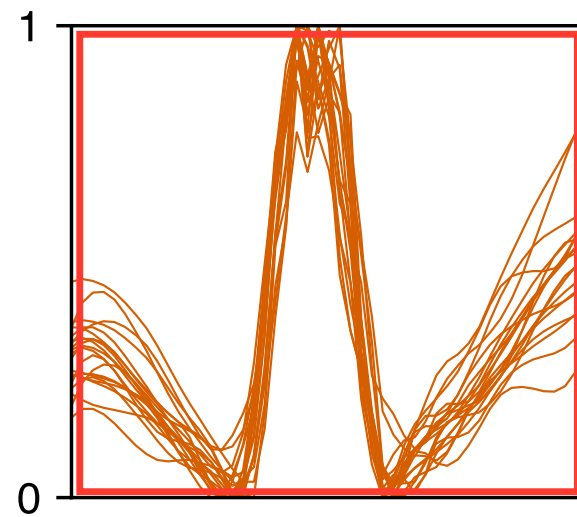
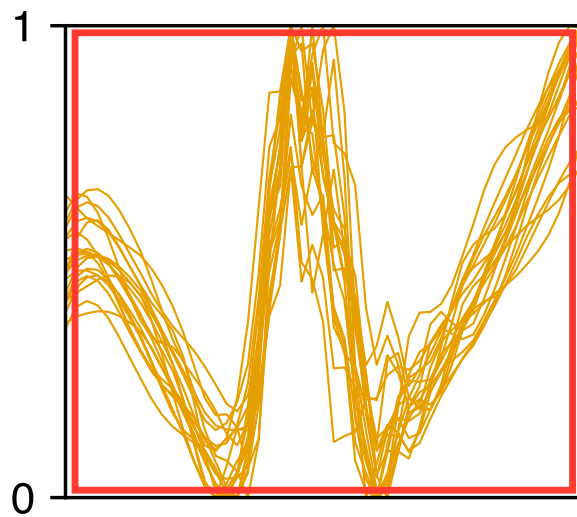
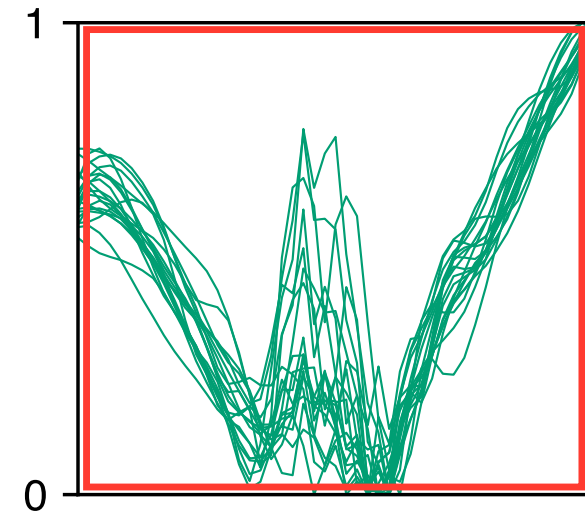
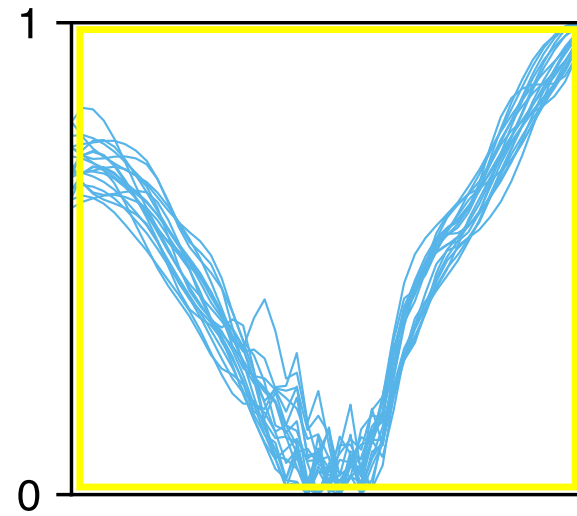
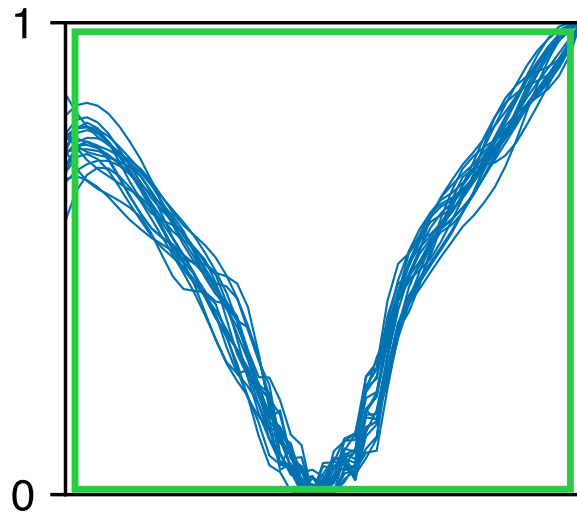
Neural network performance



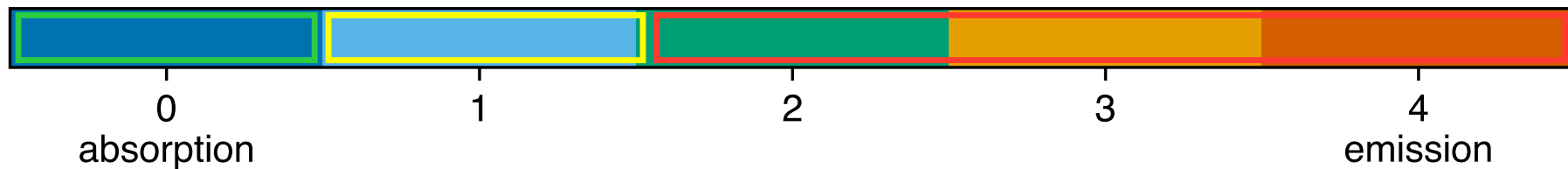
Neural network performance

Precision
91%

Recall
90%



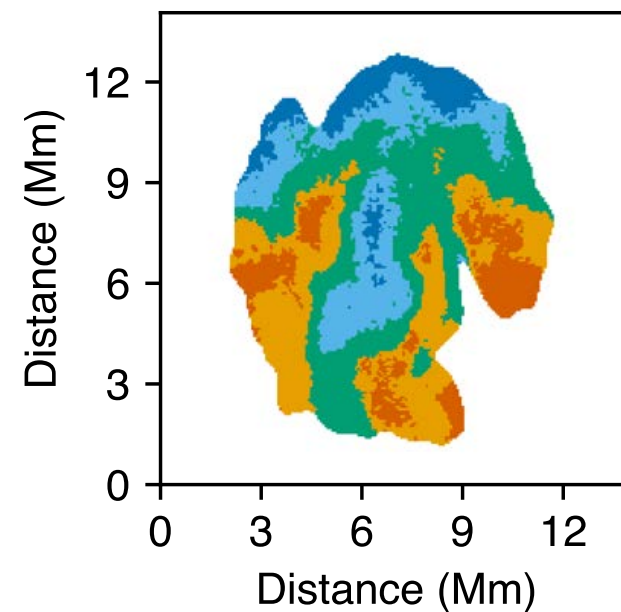
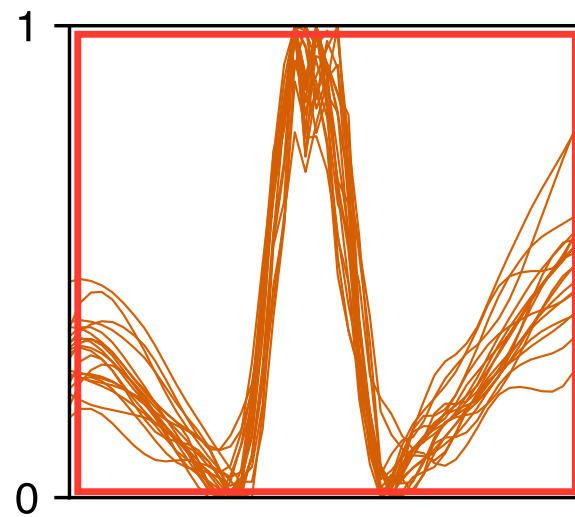
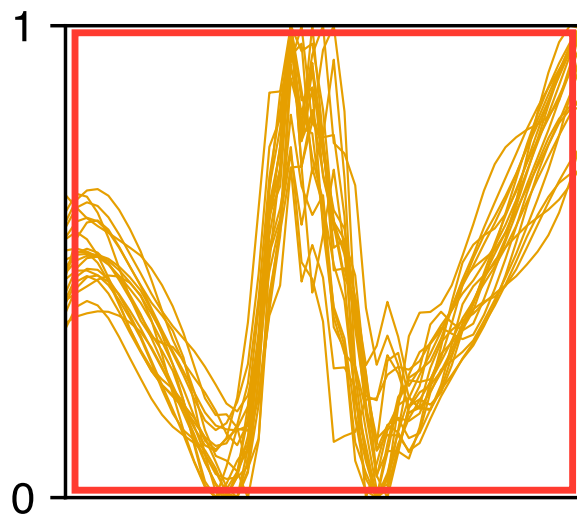
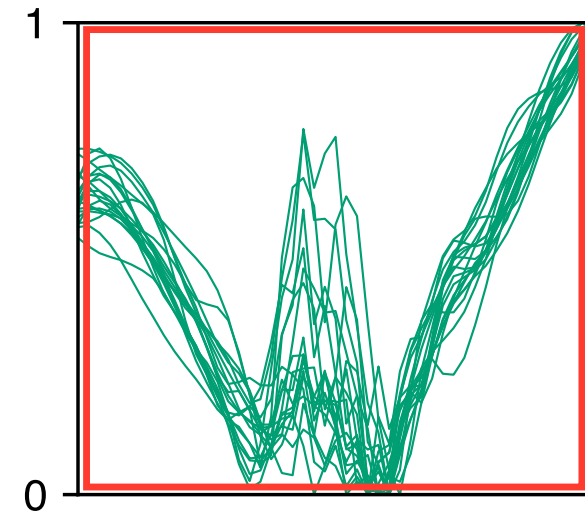
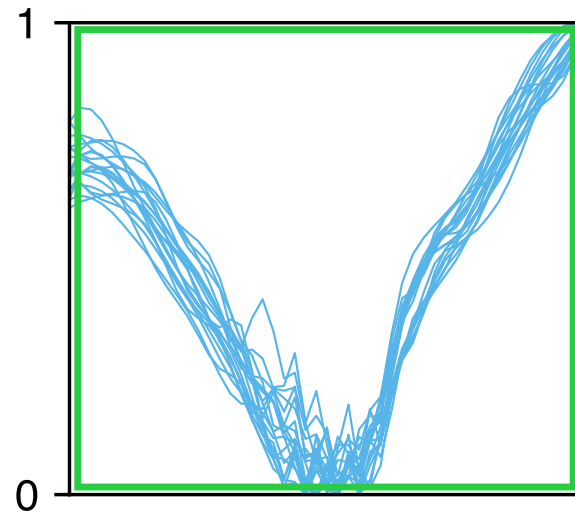
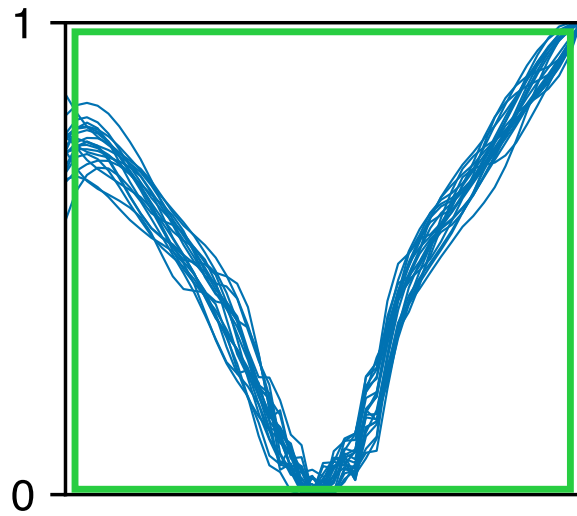
Precision Recall
 $\frac{tp}{tp + fp}$ $\frac{tp}{tp + fn}$
true/false positive/negative



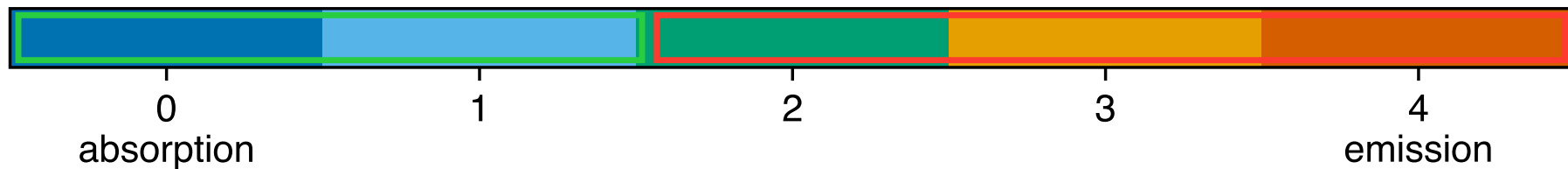
Neural network performance

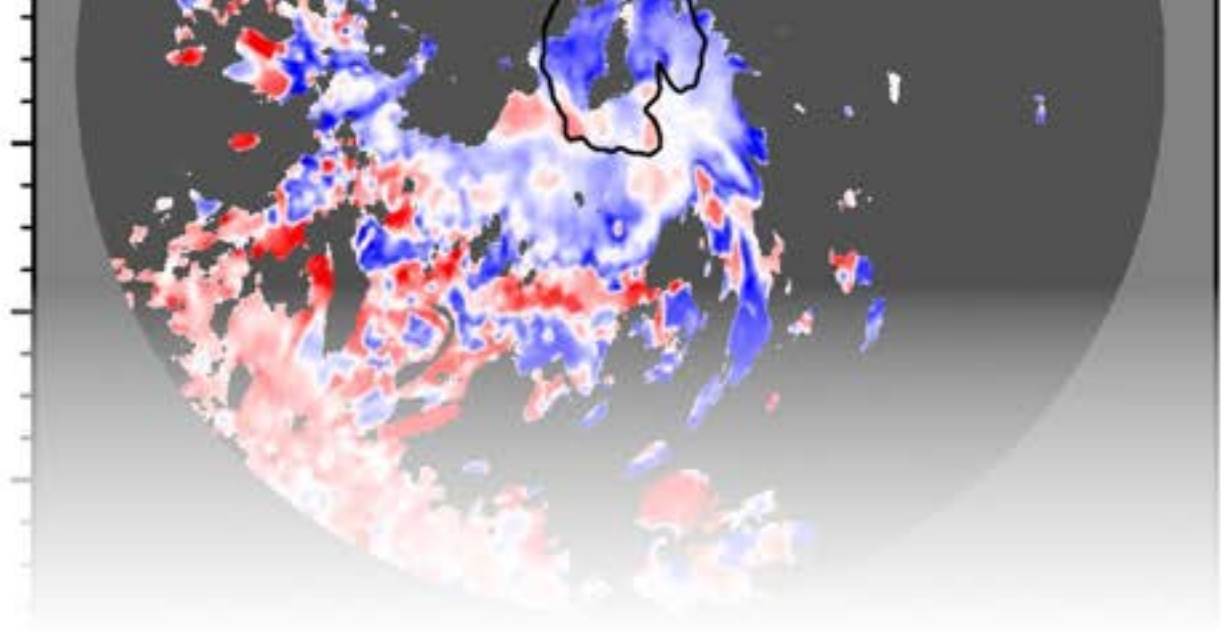
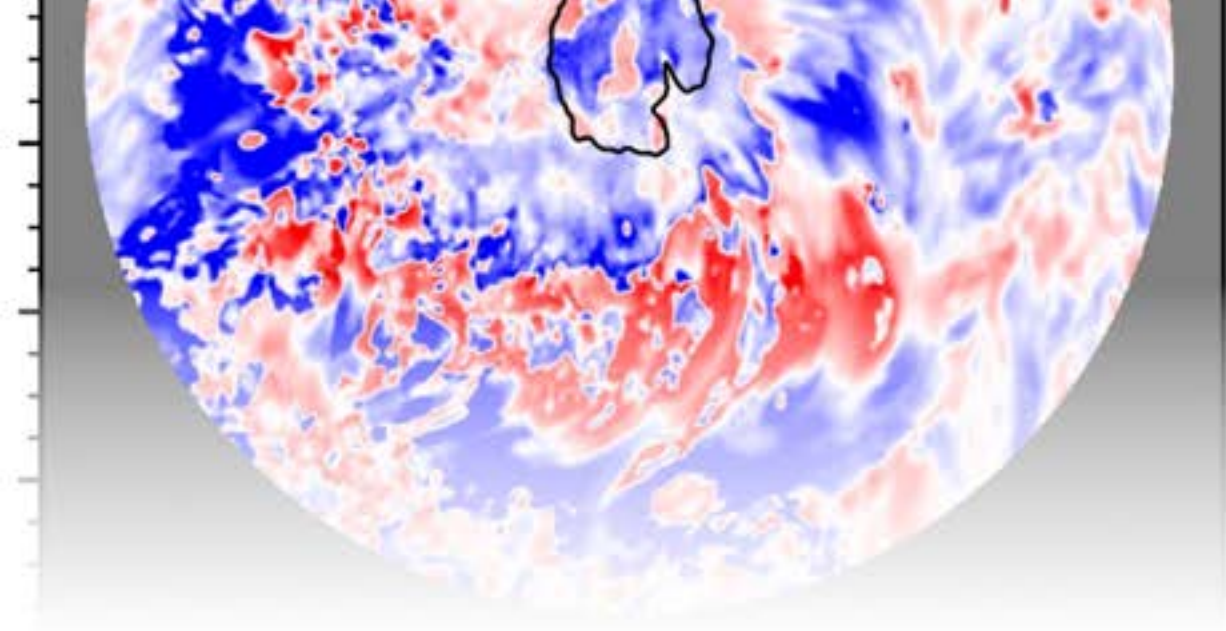
Precision
96%

Recall
95%



Precision Recall
 $\frac{tp}{tp + fp}$ $\frac{tp}{tp + fn}$
true/false positive/negative





API Overview

An overview of the methods and functions provided by MCALF

- **mcalf**

- mcalf.**models** — *classes for fitting spectra & storing results*
- mcalf.**profiles** — *functions that model spectra*
 - mcalf.profiles.**voigt**
 - mcalf.profiles.**gaussian**
- mcalf.**visualisation** — *functions to visualise results*
- mcalf.**utils**
 - mcalf.utils.**spec** — *functions for processing spectra*
 - mcalf.utils.**smooth** — *functions for smoothing n-dimensional arrays*
 - mcalf.utils.**mask** — *functions for masking the input data to limit the region computed*
 - mcalf.utils.**plot** — *functions for helping with plotting*
 - mcalf.utils.**misc** — *miscellaneous utility functions*

mcalf.**models**: Using a model

```
model = mcalf.models.IBIS8542Model(...)
```

1. ***initialise** model*

```
model.load_array(...)
```

2. ***load** spectra*

```
model.train(...)  
model.test(...)
```

3. ***train** classifier*

```
result_list = model.fit(...)
```

4. ***fit** spectra*

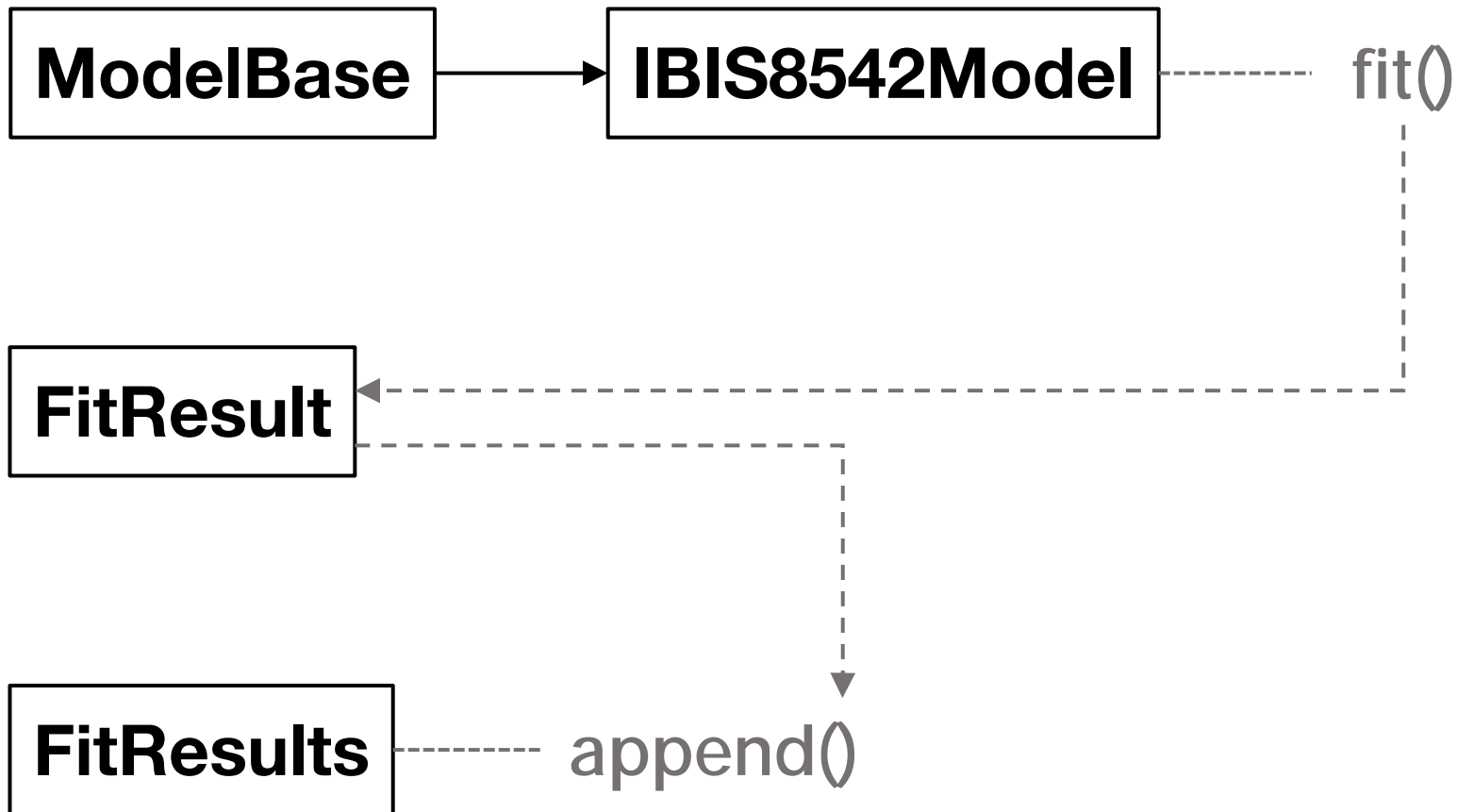
```
results = mcalf.models.FitResults(...)  
for fit in result_list:  
    results.append(fit)
```

5. ***merge** results*

```
results.save(...)
```

6. ***save** results*

mcalf.**models**: Class inheritance



mcalf.**models**: Basic model subclass

```
from mcalf.models import ModelBase, FitResult
```

```
class Model(ModelBase):
```

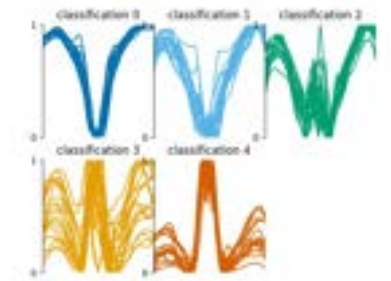
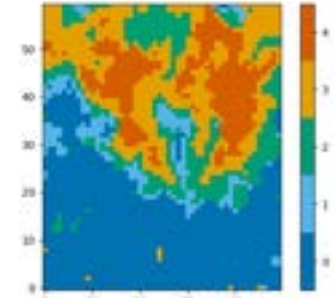
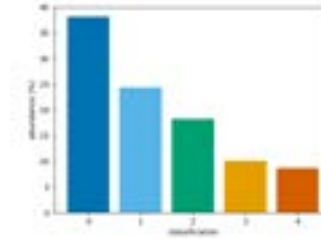
```
    def _fit(self, spectrum, classification=None, spectrum_index=None):
        # Use `classification` to define fitting method
        # Apply fitting method to `spectrum`
        fitted_params = ...
        fit_info = {
            'classification': classification, 'index': spectrum_index,
            'success': ..., 'profile': ..., 'chi2': ...,
        }
        return FitResult(fitted_params, fit_info)
```

```
    def plot(self, ...):
        pass
```

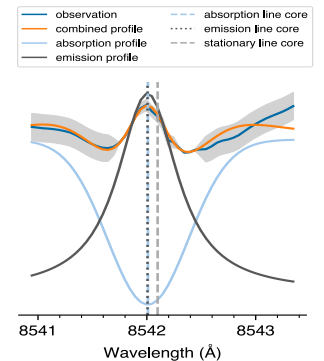
} optional

mcalf.visualisation

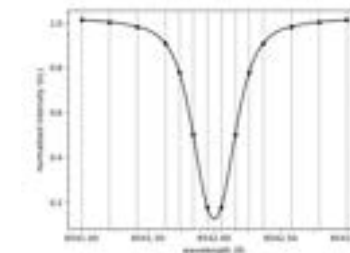
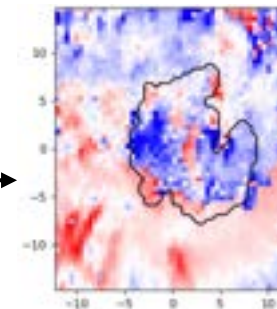
- mcalf.visualisation.**bar(...)** — *bar chart of classification abundances*
- mcalf.visualisation.**plot_class_map(...)** — *2D map of classifications*
- mcalf.visualisation.**plot_classifications(...)** — *spectra grouped by classification*
- mcalf.visualisation.**init_class_data(...)** — *precompute classification plotting data*



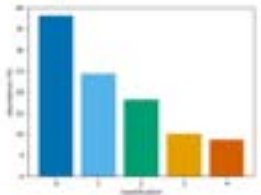
- mcalf.visualisation.**plot_ibis8542(...)** — *IBIS8542Model.plot(...)*
- mcalf.visualisation.**plot_spectrum(...)** — *spectrum with wavelength grid*



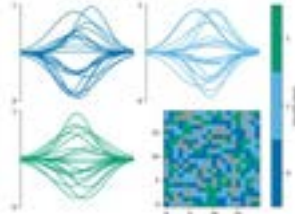
- mcalf.visualisation.**plot_map(...)** — *2D velocity map*



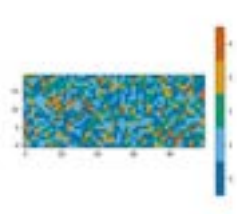
mcalf. **visualisation:** Example Gallery



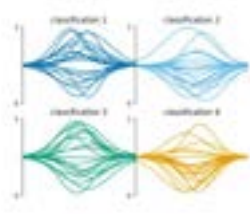
Plot a bar chart of classifications



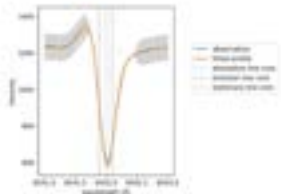
Combine multiple classification plots



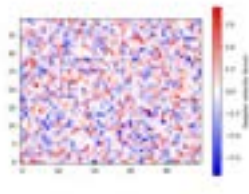
Plot a map of classifications



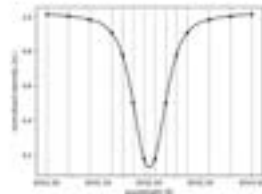
Plot a grid of spectra grouped by classification



Plot a fitted spectrum



Plot a map of velocities



Plot a spectrum

<https://mcalf.macbride.me/en/stable/gallery/>

MCALF Publications

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A | JUL 2020

Accurately constraining velocity information from spectral imaging observations using machine learning techniques

MacBride, CD; Jess, DB; Grant, SDT; Khomenko, E; Keys, PH; Stangalini, M

JOURNAL OF OPEN SOURCE SOFTWARE | MAY 2021

MCALF: Multi-Component Atmospheric Line Fitting

MacBride, CD; Jess, DB

PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A | JUL 2020

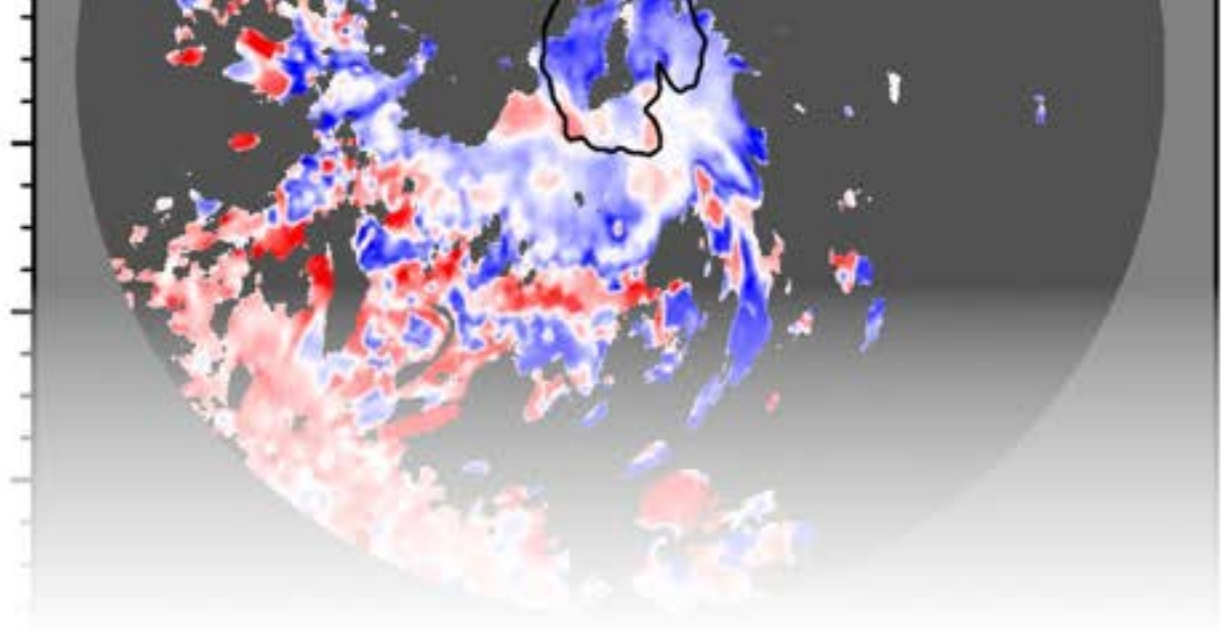
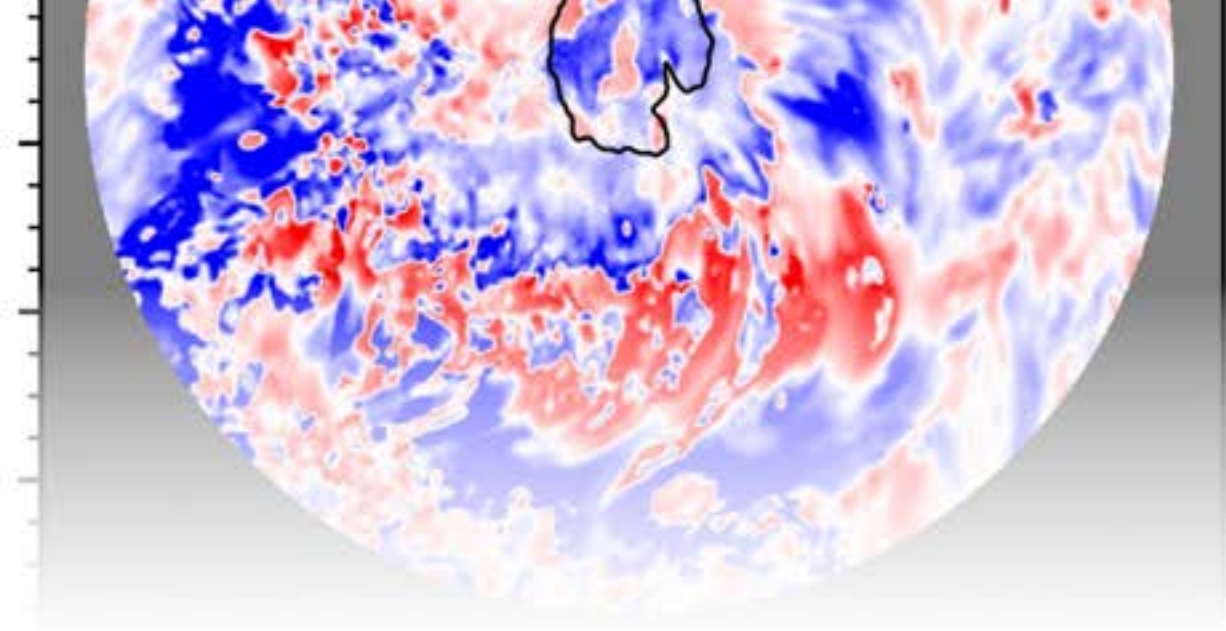
Accurately constraining velocity information from spectral imaging observations using machine learning techniques

From the *Example Gallery*:

Working with IBIS data

This example shows how to initialise the `mcalf.models.IBIS8542Model` class with real IBIS data, and train a neural network classifier. We then proceed to fit the array of spectra and visualise the results.

https://mcalf.macbride.me/en/stable/gallery/models/plot_ibis8542data.html



Infrastructure

An overview of MCALF's DevOps methods and services

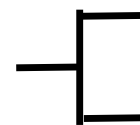
Testing

OpenAstronomy / [azure-pipelines-templates](#)

<div><div>✓ Basic Tests</div><div>1 job completed1m 31s</div><div>100% tests passed</div></div> <div><div>✓ py38 [linux]1m 26s</div></div>	<div><div>✓ Pre-release Tests</div><div>12 jobs completed8m 58s</div><div>100% tests passed</div></div> <div><div>✓ py36 [macos]2m 47s</div><div>✓ py37 [macos]2m 14s</div><div>✓ py36 [windows]4m 18s</div><div>✓ py37 [windows]4m 8s</div><div>✓ py36-oldestdeps [lin...1m 5...</div><div>✓ py37-oldestdeps [lin...1m 2...</div><div>✓ py36-oldestdeps [m...3m ...</div><div>✓ py37-oldestdeps [ma...6m ...</div><div>✓ py38-oldestdeps [ma...6m ...</div><div>✓ py36-oldestdeps [wl...4m ...</div><div>✓ py37-oldestdeps [win...2m ...</div><div>✓ py38-oldestdeps [win...3m ...</div></div>	<div><div>✓ Figure Tests</div><div>3 jobs completed5m 25s</div><div>100% tests passed</div></div> <div><div>✓ py38-figure [linux]1m 11s</div><div>✓ py38-figure [macos]5m 0s</div><div>✓ py38-figure [windows]2m 51s</div></div>
<div><div>✓ Detailed Tests</div><div>5 jobs completed6m 33s</div><div>100% tests passed</div></div> <div><div>✓ py36 [linux]1m 30s</div><div>✓ py37 [linux]1m 16s</div><div>✓ py38 [macos]6m 23s</div><div>✓ py38 [windows]2m 17s</div><div>✓ py38-oldestdeps [lin...1m 2...</div></div>	<div><div>✓ Release</div><div>5 jobs completed13m 31s</div><div>4 artifacts</div></div> <div><div>✓ sdist1m 13s</div><div>✓ wheels_cp3[6-8]-mac...11...</div><div>✓ wheels_cp3[6-8]-ma...7m ...</div><div>✓ wheels_cp3[6-8]-win...7m...</div><div>✓ publish1m 9s</div></div>	



— **tox** —



pytest-dev / **pytest-cov**

matplotlib / **pytest-mpl**



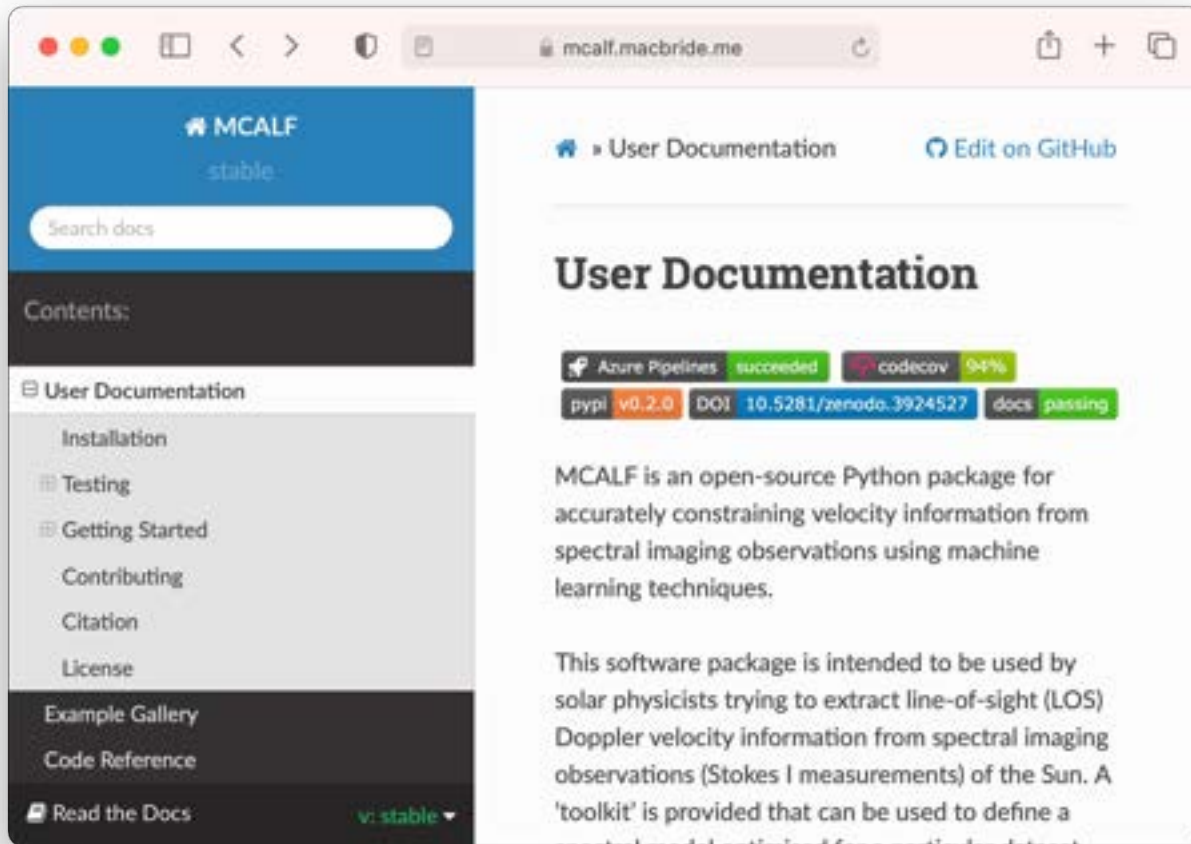
Publishing



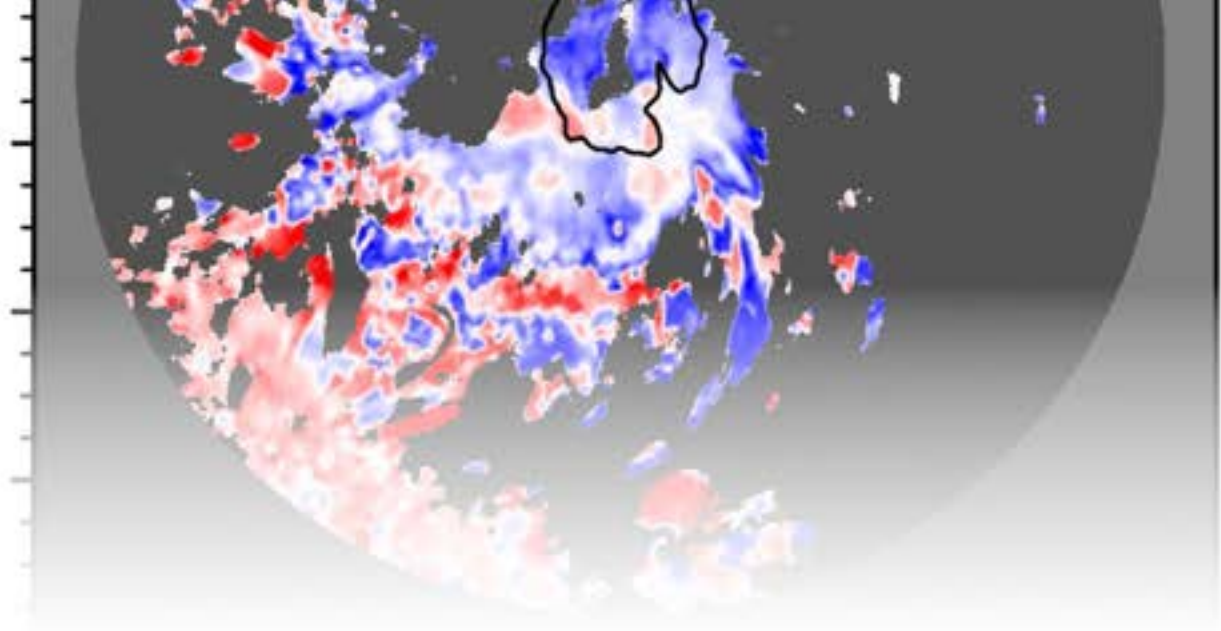
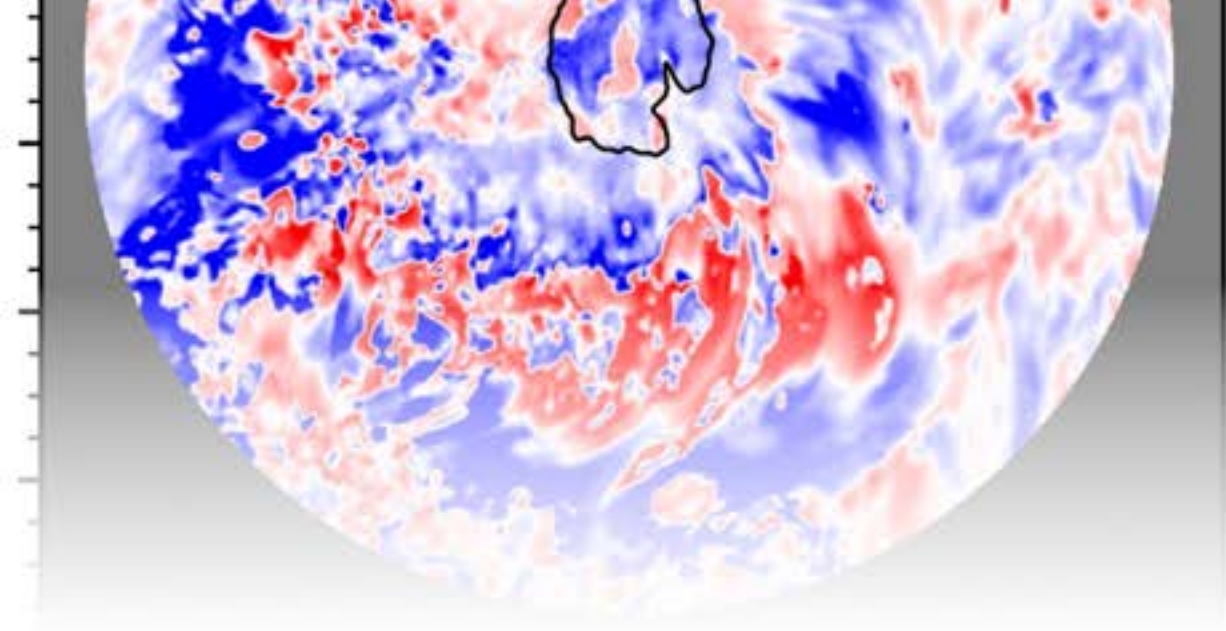
OpenAstronomy / **azure-pipelines-templates**

zenodo

Documentation



- Read the Docs
- Sphinx
 - Sphinx-Gallery
 - astropy / **sphinx-automodapi**



Future

How MCALF can be improved and developed

MCALF: Multi-Component Atmospheric Line Fitting

MCALF is an open-source Python package for accurately constraining velocity information from spectral imaging observations using machine learning techniques.



Conor MacBride

PhD Student, Queen's University Belfast

GitHub

github.com/ConorMacBride/mcalf

Documentation

mcalf.macbride.me



David Jess

Reader, Queen's University Belfast

Install

`pip install mcalf`

`conda install mcalf`

✉ cmacbride01@qub.ac.uk | conor@macbride.me

🌐 macbride.me

🐙 [ConorMacBride](https://github.com/ConorMacBride)