

# Investigation of possibilities and limitations for bulk automated analysis of big datasets of reflectance spectra of asteroids

Jakub Morawski

University of Coimbra

18<sup>th</sup> of January 2024

# Outline

Major components of the project:

# Outline

Major components of the project:

1. Downloading data

# Outline

Major components of the project:

1. Downloading data
2. Taxonomic classification (CANA)

# Outline

Major components of the project:

1. Downloading data
2. Taxonomic classification (CANA)
3. Automatic absorption band detection

# Outline

Major components of the project:

1. Downloading data
2. Taxonomic classification (CANA)
3. Automatic absorption band detection
4. Mineralogical content estimates based on empirical formulas

# Outline

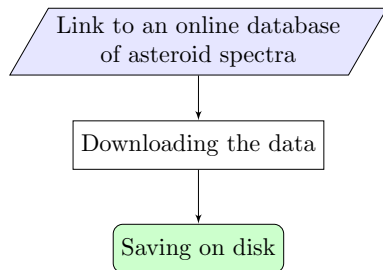
Major components of the project:

1. Downloading data
2. Taxonomic classification (CANA)
3. Automatic absorption band detection
4. Mineralogical content estimates based on empirical formulas
5. Visualisations with various plots

# Downloading data

Development stages:

## 1. Simple download

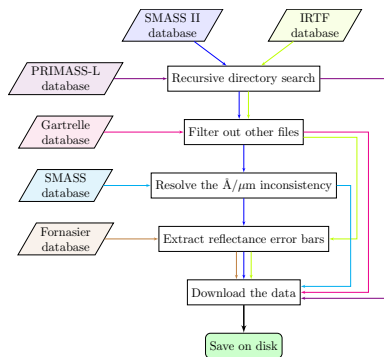




# Downloading data

Development stages:

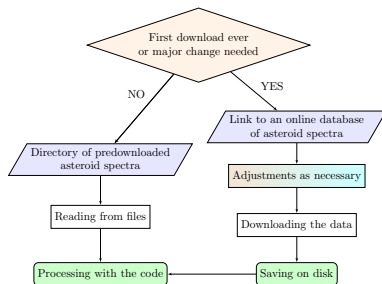
1. Simple download
2. **Unification between databases**



# Downloading data

Development stages:

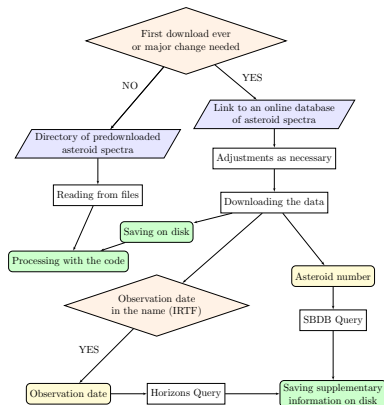
1. Simple download
2. Unification between databases
3. **Avoiding repeated downloads**



# Downloading data

Development stages:

1. Simple download
2. Unification between databases
3. Avoiding repeated downloads
4. **Extracting supplementary information from JPL databases**



## Small Body Database Lookup - not useful

**Small-Body Database Lookup**

Home / Tools / Small-Body Database Lookup

## Small-Body Database Lookup

Search...

**1 Ceres (A801 AA)**  
Classification: Main-belt Asteroid SPKID: 20000001 Related Links: Ephemeris

**Orbit Viewer** [show]

**Orbit Parameters** [hide]

Osculating Orbital Elements

Element	Value	Uncertainty (1-sigma)	Units
e	0.0789125317658808	4.7845E-12	
a	2.767254360873952	1.0197E-11	au
q	2.548863313217214	1.9207E-11	au
i	10.5668796009696	4.6112E-9	deg
node	80.25487772273573	6.19E-8	deg
peri	73.42179714001003	6.6129E-8	deg
M	60.0787728227207	6.5804E-9	deg
tp	2459919.898104763426 2022-Dec-06.39810476	3.1352E-8	TDB
period	1681.403889244621 4.603432961655362	9.2941E-9	d
n	0.2141067962025804	2.5446E-11	y
Q	2.58562540853009	1.1835E-12	deg/d
		1.1002E-11	au

Miscellaneous Details

solution date	2021-Apr-13 11:04:44
# obs. used (total)	1075
# delay obs. used	60
# Doppler obs. used	0
data-arc span	9520 days (26.06 years)
first obs. used	1995-01-05
last obs. used	2021-02-28
planetary ephem.	DE441
S-B pert. ephem.	SB441-N373
condition code	0
norm. resid. RMS	.43153
source	JPL
producer	Davide Farnocchia
Earth MOID	1.58322 au
Jupiter TMOID	2.09004 au
T_jup	3.310

**Physical Parameters** [hide]

Parameter	Value	Units	Sigma	Reference	Notes
[H] absolute magnitude	3.34			MPOT775928	
(g) magnitude slope	0.12			PDS3 (MPC 17257)	Fit
diameter	939.4	km	0.2	Nature vol. 537, pp515-51..	
extent	954.4 x 964.2 x 891.8	km	0.2 x 0.2 x 0.2	Nature vol. 537, pp515-51..	fit w.r.t. center of mass and in body-fll..
GM	62.6284	km <sup>3</sup> /s <sup>2</sup>	0.0009	Nature vol. 537, pp515-51..	
bulk density	2.162	g/cm <sup>3</sup>	0.008	Nature vol. 537, pp515-51..	

# Supplementary information with APIs

Information	Query link
<b>SBDB Query:</b> name, a[AU], e, $i[^\circ]$ , diameter [km], synodic rotation period [h], albedo	<a href="https://ssd-api.jpl.nasa.gov/sbdb_query.api?fields=name,a,e,i,diameter,rot_per,albedo&amp;sb-cdata=%7B%20%22AND%22%20%3A%20%5B%20%22spkid%7CEQ%7C20000001%22%20%5D%20%7D%0A">https://ssd-api.jpl.nasa.gov/sbdb_query.api?fields=name,a,e,i,diameter,rot_per,albedo&amp;sb-cdata=%7B%20%22AND%22%20%3A%20%5B%20%22spkid%7CEQ%7C20000001%22%20%5D%20%7D%0A</a>
<b>Horizons Query:</b> observation phase angle	<a href="https://ssd.jpl.nasa.gov/api/horizons.api?format=text&amp;COMMAND=\" name='Itokawa\"&amp;OBJ_DATA=\"NO\"&amp;MAKE_EPHEM=\"YES\"&amp;EPHEM_TYPE=\"OBSERVER\"&amp;CENTER=\"geo\"&amp;TLIST=\"2001-03-28\"&amp;QUANTITIES=\"24\""'>https://ssd.jpl.nasa.gov/api/horizons.api?format=text&amp;COMMAND="Name=Itokawa"&amp;OBJ_DATA="NO"&amp;MAKE_EPHEM="YES"&amp;EPHEM_TYPE="OBSERVER"&amp;CENTER="geo"&amp;TLIST="2001-03-28"&amp;QUANTITIES="24"</a>
<b>Horizons Query:</b> $X, Y, Z$ coordinates $\Rightarrow$ $d[km] = \sqrt{X^2 + Y^2 + Z^2}$ heliocentric distance	<a href="https://ssd.jpl.nasa.gov/api/horizons.api?format=text&amp;COMMAND=\" name='Itokawa\"&amp;OBJ_DATA=\"NO\"&amp;MAKE_EPHEM=\"YES\"&amp;EPHEM_TYPE=\"VECTORS\"&amp;CENTER=\"@Sun\"&amp;TLIST=\"2001-03-28\"&amp;QUANTITIES=\"1\""'>https://ssd.jpl.nasa.gov/api/horizons.api?format=text&amp;COMMAND="Name=Itokawa"&amp;OBJ_DATA="NO"&amp;MAKE_EPHEM="YES"&amp;EPHEM_TYPE="VECTORS"&amp;CENTER="@Sun"&amp;TLIST="2001-03-28"&amp;QUANTITIES="1"</a>

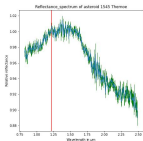
# Small Body Database information - example

number	name	$a$ [AU]	$e$	$[i^\circ]$	diameter [km]	rotation period [h]	albedo
110	Lydia	2.733	0.0797	5.96	86.09	10.927	0.1808
125	Liberatrix	2.743	0.0807	4.67	48.418	3.968	0.182
129	Antigone	2.867	0.2129	12.27	113.0	4.9572	0.151
132	Aethra	2.613	0.3871	24.97	42.87	5.1684	0.199
135	Hertha	2.429	0.2072	2.3	79.24	8.403	0.1436
16	Psyche	2.924	0.1342	3.1	226.0	4.196	0.1203
161	Athor	2.38	0.1368	9.06	40.992	7.28	0.23
201	Penelope	2.679	0.1791	5.76	85.877	3.7474	0.04
216	Kleopatra	2.793	0.251	13.12	122.0	5.385	0.1164
22	Kalliope	2.911	0.0987	13.7	167.536	4.1483	0.166
224	Oceana	2.645	0.045	5.85	58.236	9.401	0.166
250	Bettina	3.144	0.1363	12.82	120.995	5.0545	0.112
325	Heidelberga	3.216	0.1513	8.57	75.72	6.737	0.1068
338	Budrosa	2.912	0.0181	6.04	50.506	4.6084	0.276
347	Pariana	2.615	0.1638	11.69	48.615	4.0529	0.19
369	Aeria	2.649	0.0974	12.72	73.767	4.778	0.127
382	Dodona	3.122	0.1704	7.39	65.209	4.113	0.129
418	Alemannia	2.593	0.1188	6.82	40.33	4.671	0.201
441	Bathilde	2.806	0.0817	8.16	65.131	10.446	0.204
498	Tokio	2.652	0.2238	9.5	81.83	41.85	0.0694
516	Amherstia	2.677	0.2752	12.95	65.144	7.4842	0.202
55	Pandora	2.759	0.1444	7.18	84.794	4.804	0.204
558	Carmen	2.907	0.0383	8.37	54.811	11.387	0.131
69	Hesperia	2.976	0.17	8.59	138.13	5.655	0.1402
755	Quintilla	3.187	0.1355	3.24	41.21	4.552	0.124
785	Zwetana	2.572	0.2086	12.77	49.46	8.8882	0.12
849	Ara	3.144	0.201	19.54	80.756	4.116	0.186
860	Ursina	2.797	0.1084	13.29	34.561	9.386	0.116
872	Holda	2.732	0.0798	7.39	34.431	5.945	0.165
97	Klotho	2.668	0.2581	11.78	100.717	35.15	0.128

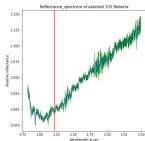
# Taxonomic classification - theory

## C-complex classes (carbonaceous chondrite like)

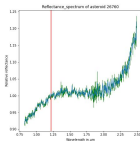
► B



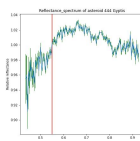
► C



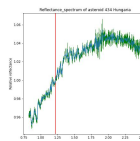
► Cb



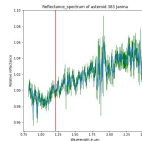
► Cg(\*)



► Cgh

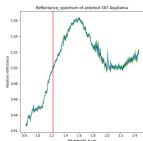


► Ch

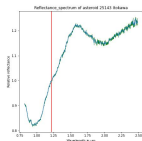


## S-complex classes (Si, olivine/pyroxene, ordinary chondrites)

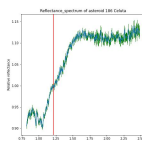
► S



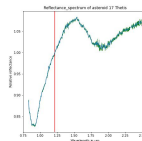
► Sa



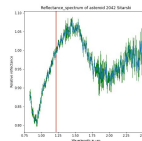
► Sq



► Sr



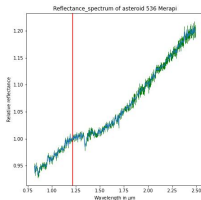
► Sv



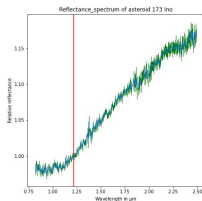
# Taxonomic classification - theory

## X-complex classes (few features, compositionally degenerate)

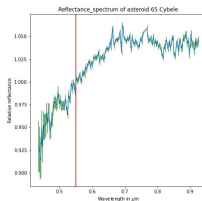
► X



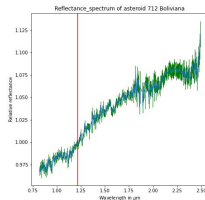
►  $X_c(@)$



►  $X_e(*)$



►  $X_k$

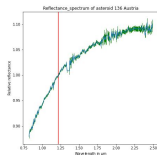




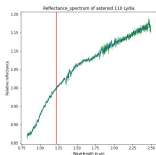
# Taxonomic classification - theory

## End member classes (extreme or distinct characteristics)

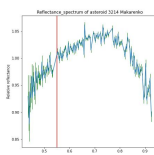
► T



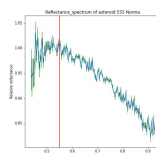
► D



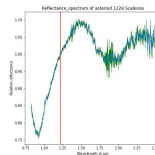
► Q(\*)



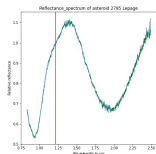
► O(\*)



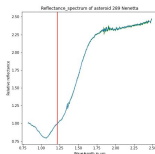
► R



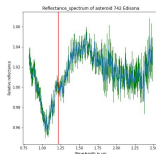
► V



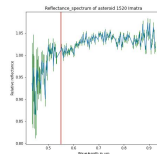
► A



► L

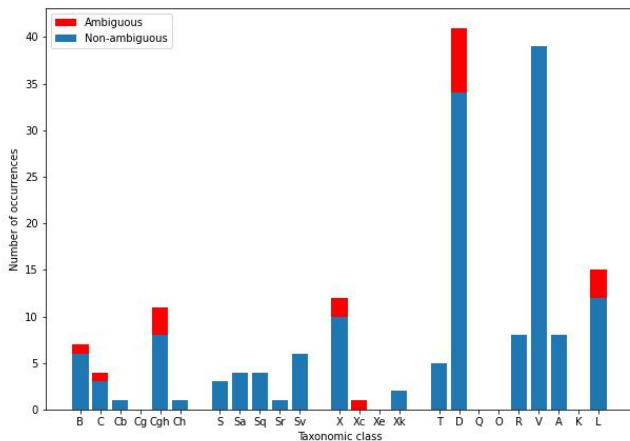


► K



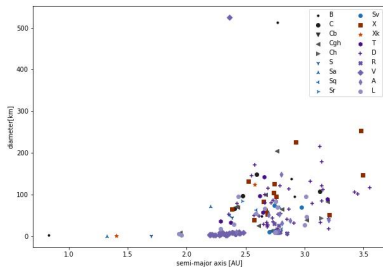
# Taxonomic classification of the IRTF dataset

Taxonomic classification of asteroid spectra from the IRTF database with possible ambiguities

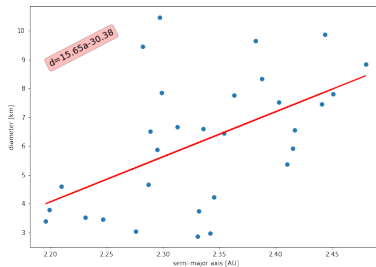


# Parameter space representation

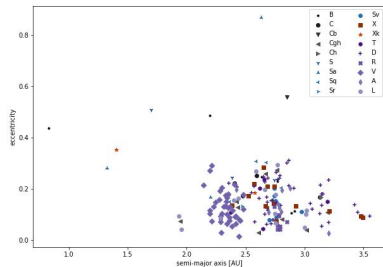
Taxonomic classification of asteroid spectra from the IRTF database, in the parameter space of semi-major axis [AU] and diameter[km]



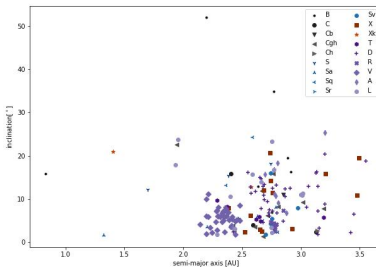
Closeup look on the small V class asteroid cluster



Taxonomic classification of asteroid spectra from the IRTF database, in the parameter space of semi-major axis [AU] and eccentricity



Taxonomic classification of asteroid spectra from the IRTF database, in the parameter space of semi-major axis [AU] and inclination[°]



# Absorption band detection - definitions

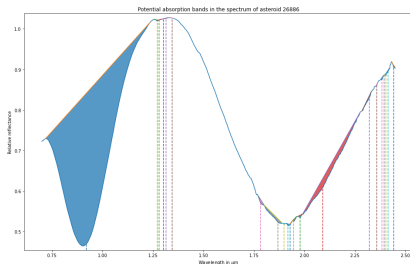
Continuum line:

$$cont(w) = r(w_{\min}) + \frac{w - w_{\min}}{w_{\max} - w_{\min}} \cdot (r(w_{\max}) - r(w_{\min}))$$

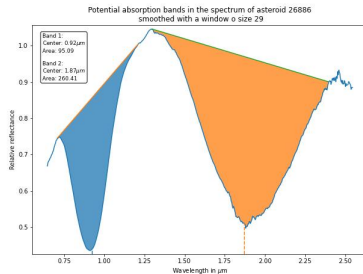
Band criterion:

$$V(w_{\min}, w_{\max}) = \begin{cases} 1 & \text{if } \forall w \in (w_{\min}, w_{\max}) r(w) < cont(w) \\ 0 & \text{otherwise} \end{cases}$$

Old algorithm



New algorithm



# Absorption band detection - smoothing

Formula from the report  
(wrong):

$$\tilde{r}(w_i) = \frac{\sum_{j=\max(-\lfloor \frac{n}{2} \rfloor, 1-i)}^{\min(-\lfloor \frac{n}{2} \rfloor + n - 1, N-i)} r(w_{i+j})}{n}$$

Correct formula:

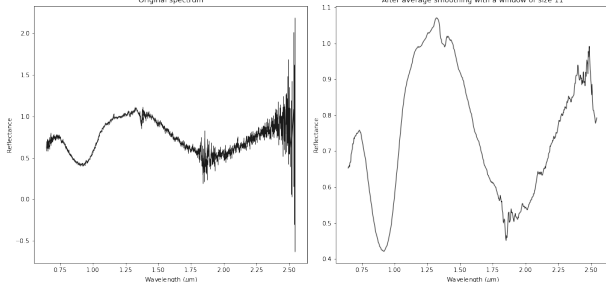
$$\tilde{r}(w_i) = \frac{\sum_{j=j_1}^{j_2} r(w_{i+j})}{j_2 - j_1 + 1}$$

where:

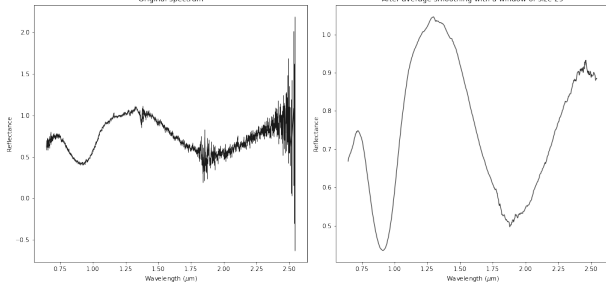
$$j_1 = \max\left(-\lfloor \frac{n}{2} \rfloor, 1-i\right)$$

$$j_2 = \min\left(-\lfloor \frac{n}{2} \rfloor + n - 1, N-i\right)$$

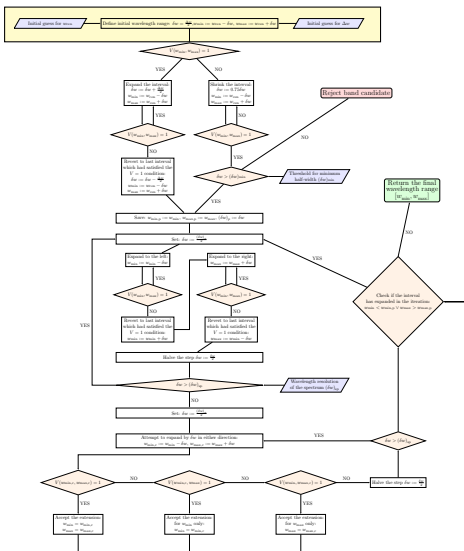
Results of applying the operation of average smoothing with a window of size 11 on the asteroid 26886 spectrum



Results of applying the operation of average smoothing with a window of size 29 on the asteroid 26886 spectrum



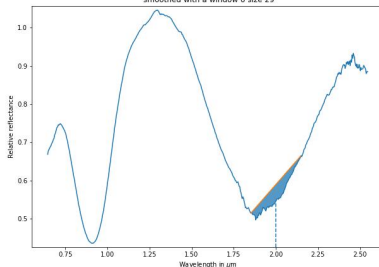
# Absorption band detection - algorithm



Initial guess

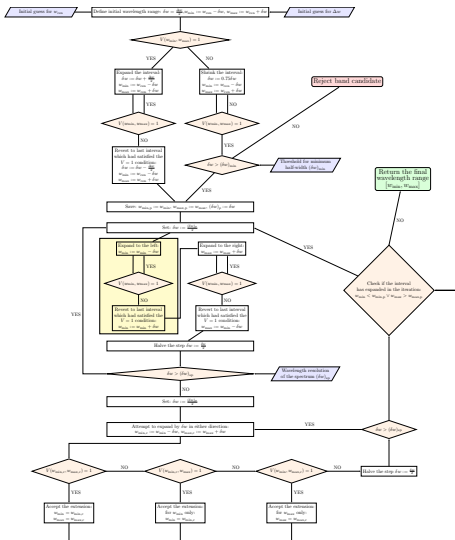
$$w_{\max} - w_{\min} = 0.3 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29





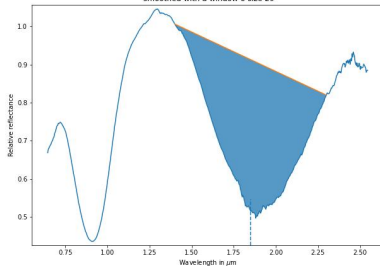
## Absorption band detection - algorithm



Moving left

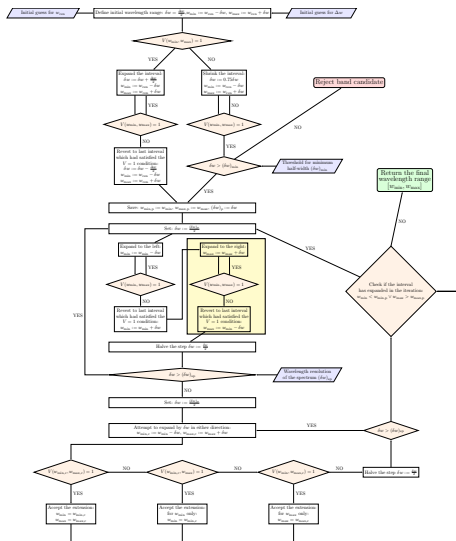
$$W_{\max} - W_{\min} = 0.9 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29





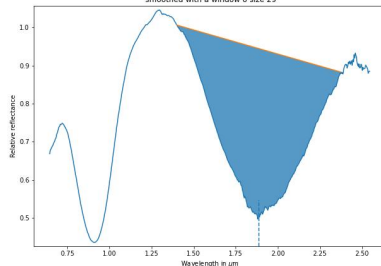
# Absorption band detection - algorithm



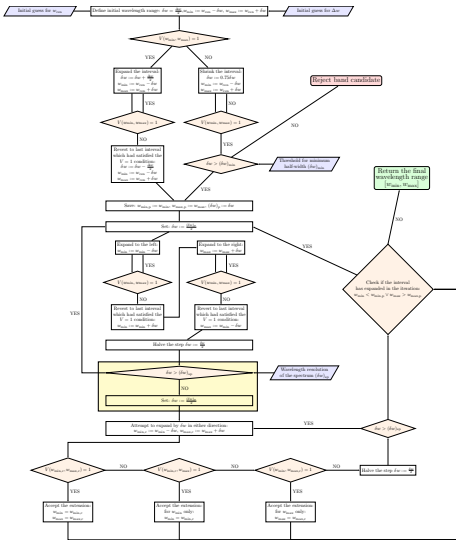
Moving right

$$w_{\max} - w_{\min} = 0.975 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29



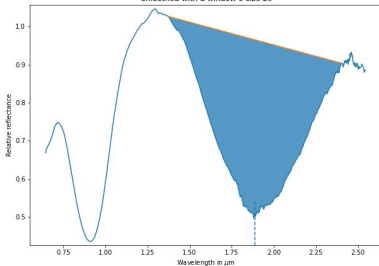
## Absorption band detection - algorithm



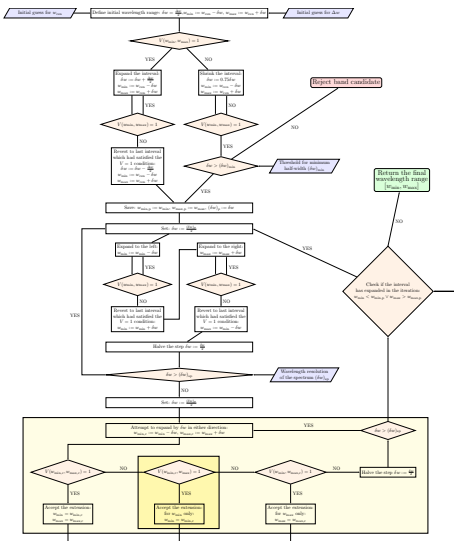
## After the first loop

$$w_{\max} - w_{\min} = 1.031 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window o size 29

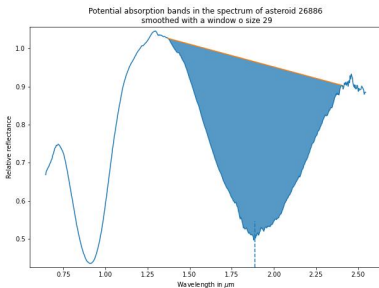


## Absorption band detection - algorithm

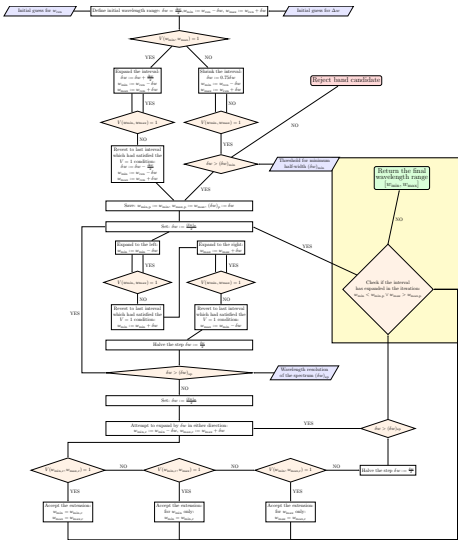


## Halving a step until extended

$$w_{\max} - w_{\min} = 1.031 \mu\text{m}$$

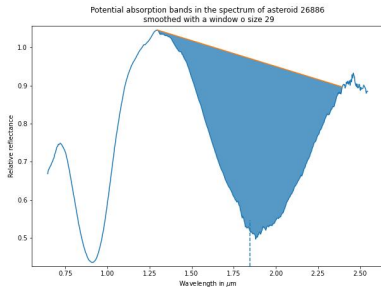


## Absorption band detection - algorithm



## Completed

$$w_{\max} - w_{\min} = 1.097 \mu\text{m}$$

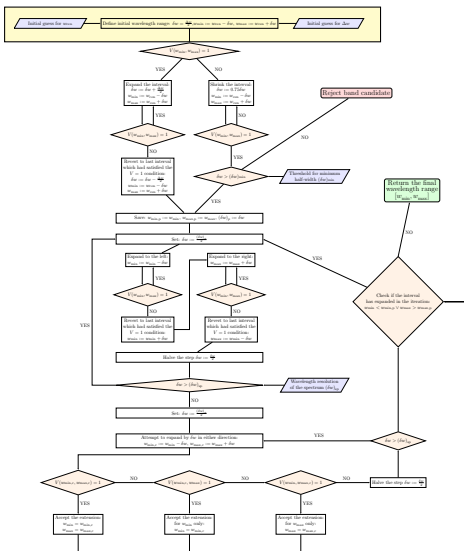
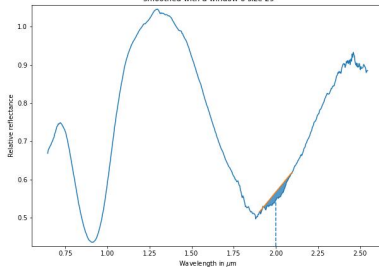


# Absorption band detection - algorithm

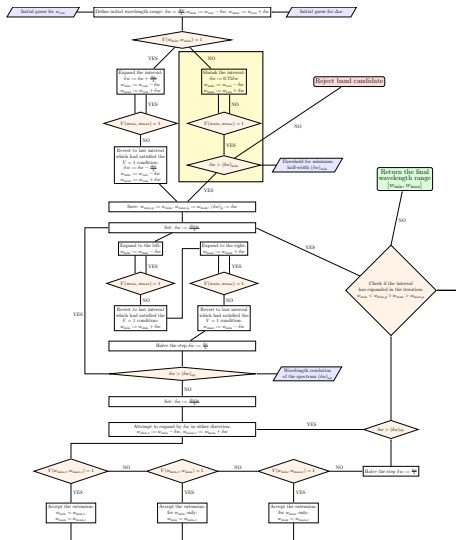
## Initial guess

$$w_{\max} - w_{\min} = 0.2 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29



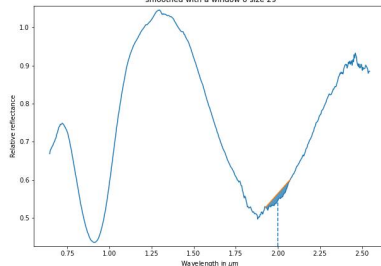
# Absorption band detection - algorithm



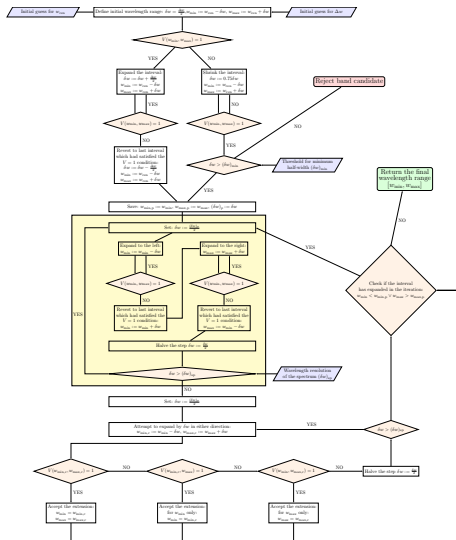
Shrinking

$$w_{\max} - w_{\min} = 0.15 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29



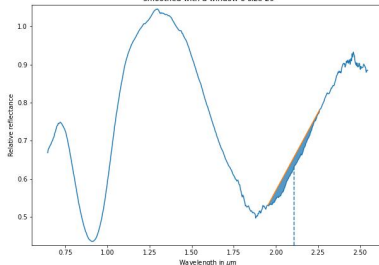
# Absorption band detection - algorithm



After the first loop

$$w_{\max} - w_{\min} = 0.309 \mu\text{m}$$

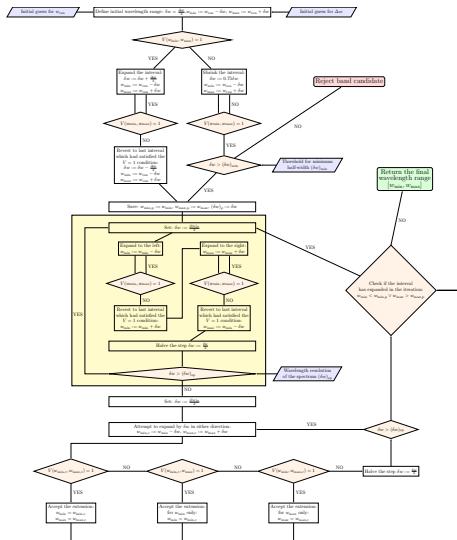
Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29







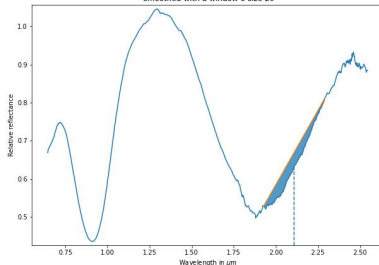
# Absorption band detection - algorithm



## Another iteration

$$w_{\max} - w_{\min} = 0.366 \mu\text{m}$$

Potential absorption bands in the spectrum of asteroid 26886 smoothed with a window of size 29



## Empirical formulas - corrections

Temperature:

$$T = \sqrt[4]{\frac{(1 - A)L_{\odot}}{16\epsilon\sigma d^2}}$$

$$\Delta\text{BAR} = 0.00075 T - 0.23$$

## Empirical formulas - corrections

Temperature:

$$T = \sqrt[4]{\frac{(1 - A)L_{\odot}}{16\epsilon\sigma d^2}}$$

$$\Delta\text{BAR} = 0.00075 T - 0.23$$

Ordinary chondrites (S-complex?)

$$\Delta\text{BII} = 0.06 - 0.0002 T$$

Howardites and eucrites (V class)

$$\Delta\text{BI} = 0.01656 - 0.0000552 T$$

$$\Delta\text{BII} = 0.05067 - 0.00017 T$$

## Empirical formulas - corrections

Temperature:

$$T = \sqrt[4]{\frac{(1-A)L_{\odot}}{16\epsilon\sigma d^2}}$$

$$\Delta\text{BAR} = 0.00075 T - 0.23$$

Ordinary chondrites (S-complex?)

$$\Delta\text{BII} = 0.06 - 0.0002 T$$

Howardites and eucrites (V class)

$$\Delta\text{BI} = 0.01656 - 0.0000552 T$$

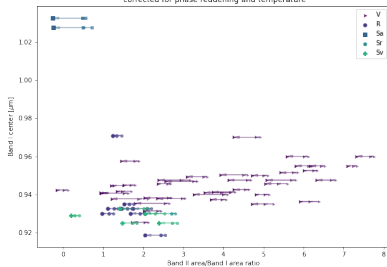
$$\Delta\text{BII} = 0.05067 - 0.00017 T$$

Phase angle:

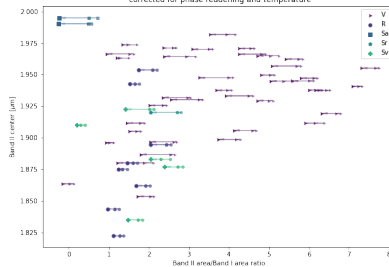
$$\Delta\text{BAR} = -0.0292 \cdot \alpha$$

# Corrections in practice

Band I center vs band area ratio for asteroids in the IRTF database  
based on spectra smoothed with a window of size 11  
corrected for phase reddening and temperature



Band II center vs band area ratio for asteroids in the IRTF database  
based on spectra smoothed with a window of size 11  
corrected for phase reddening and temperature



# Empirical formulas - mineralogy

Ordinary chondrites (S-complex?)

$$\frac{\text{opx}}{\text{opx} + \text{ol}} = 0.242 \cdot \text{BAR} + 0.272, \quad \frac{\text{ol}}{\text{opx} + \text{ol}} = -0.242 \cdot \text{BAR} + 0.728$$

# Empirical formulas - mineralogy

Ordinary chondrites (S-complex?)

$$\frac{\text{opx}}{\text{opx} + \text{ol}} = 0.242 \cdot \text{BAR} + 0.272, \quad \frac{\text{ol}}{\text{opx} + \text{ol}} = -0.242 \cdot \text{BAR} + 0.728$$

$$\frac{\text{fa}}{\text{ol}} = -12.849 \cdot (\text{BI})^2 + 26.565 \cdot \text{BI} - 13.423$$

$$\frac{\text{fs}}{\text{px}} = -8.791 \cdot (\text{BI})^2 + 18.249 \cdot \text{BI} - 9.217$$

# Empirical formulas - mineralogy

Ordinary chondrites (S-complex?)

$$\frac{\text{opx}}{\text{opx} + \text{ol}} = 0.242 \cdot \text{BAR} + 0.272, \quad \frac{\text{ol}}{\text{opx} + \text{ol}} = -0.242 \cdot \text{BAR} + 0.728$$

$$\frac{\text{fa}}{\text{ol}} = -12.849 \cdot (\text{BI})^2 + 26.565 \cdot \text{BI} - 13.423$$

$$\frac{\text{fs}}{\text{px}} = -8.791 \cdot (\text{BI})^2 + 18.249 \cdot \text{BI} - 9.217$$

Howardites and eucrites (V class)

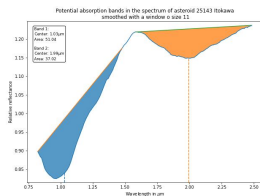
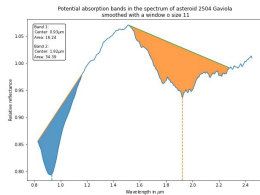
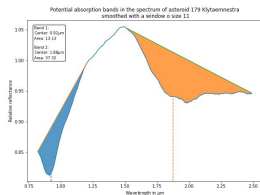
$$\frac{\text{fs}}{\text{px}} = 10.234 \cdot \text{BI} - 9.1382$$

$$\frac{\text{wo}}{\text{px}} = 3.961 \cdot \text{BI} - 3.6055$$



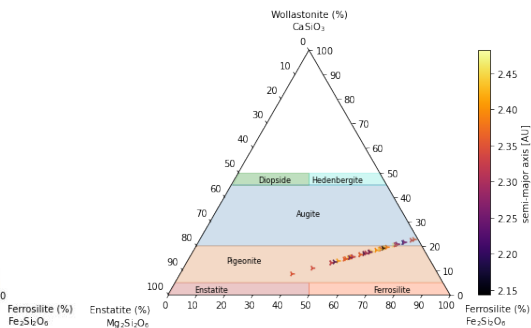
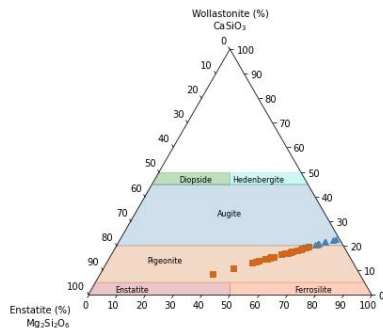
# IRTF S-complex asteroids

Asteroid	$\frac{\text{opx}}{\text{opx}+\text{ol}}$	$\frac{\text{fa}}{\text{ol}}$	$\frac{\text{fs}}{\text{px}}$
Sv class			
1662 Hoffmann	<b>63.0%</b>	17.8%	15.7%
179 Klytaemnestra	85.0%	17.8%	15.7%
1858 Lobachevskij	32.0%	18.7%	16.4%
2042 Sitarski	76.5%	21.0%	18.0%
2504 Gaviola	<b>61.3%</b>	19.5%	16.9%
Sr class			
17 Thetis	76.6%	18.8%	16.5%
Sa class			
25143 Itokawa	21.5%	30.6%	25.3%
43 Ariadne	21.1%	30.7%	25.4%



# IRTF V class asteroids

$$\frac{fs}{px} = 10.234 \cdot BI - 9.1382, \quad \frac{wo}{px} = 3.961 \cdot BI - 3.6055$$



# Conclusions

- ▶ It is possible to access bulk spectroscopic data on asteroids and supplementary information about their orbital and physical parameters

# Conclusions

- ▶ It is possible to access bulk spectroscopic data on asteroids and supplementary information about their orbital and physical parameters
- ▶ Observation date is an important parameter which should always be provided for the sake of phase angle corrections

# Conclusions

- ▶ It is possible to access bulk spectroscopic data on asteroids and supplementary information about their orbital and physical parameters
- ▶ Observation date is an important parameter which should always be provided for the sake of phase angle corrections
- ▶ Empirical formulas have limited ranges of applicability, researchers should design experiments and observations to improve them

# Conclusions

- ▶ It is possible to access bulk spectroscopic data on asteroids and supplementary information about their orbital and physical parameters
- ▶ Observation date is an important parameter which should always be provided for the sake of phase angle corrections
- ▶ Empirical formulas have limited ranges of applicability, researchers should design experiments and observations to improve them
- ▶ While a bulk approach can help highlight interesting cases from a larger group, they should still be verified individually, especially when making mineralogical statements

# Conclusions

- ▶ It is possible to access bulk spectroscopic data on asteroids and supplementary information about their orbital and physical parameters
- ▶ Observation date is an important parameter which should always be provided for the sake of phase angle corrections
- ▶ Empirical formulas have limited ranges of applicability, researchers should design experiments and observations to improve them
- ▶ While a bulk approach can help highlight interesting cases from a larger group, they should still be verified individually, especially when making mineralogical statements
- ▶ Including Modified Gaussian Model and Shkuratov model in the code could help support the statements made and discover further insights into the data