

# Machine Learning approaches for detection and classification of astrochemical spectra (P2.2)



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#### INTRODUCTION

- A couple of interesting problems:
  - Detection of regions of interesting emission in Astronomical Data Cubes.

• Manual classification of astrochemical spectra can be a complicated task, several factors affect the characteristics of a spectral line on their way towards us.

## DETECTION OF REGIONS OF INTEREST (ROI)

DBSCAN: Unsupervised clustering algorithm, ideal for irregular shapes, has some pros and cons. Executed over Moment-0 of a data cube. Works for high emission cubes.





## Training Species

Species	Chemical Name	Ordered Freq (GHz) (rest frame)	Resolved QNs
COv=0	Carbon Monoxide	115.2712	1-0
COv=0	Carbon Monoxide	230.538	2-1
COv=0	Carbon Monoxide	345.796	3-2
COv=0	Carbon Monoxide	461.0408	4-3
COv=0	Carbon Monoxide	576.2679	5-4
COv=0	Carbon Monoxide	691.4731	6-5
HCO+v=0	Formylium	356.7342	4-3
cis-CH2OHCHO v=0	Glycolaldehyde	220.2041	11( 4,7)- 10(3,8)
cis-CH2OHCHO v=0	Glycolaldehyde	220.1967	7(6,2)- 6(5,1)
cis-CH2OHCHO v=0	Glycolaldehyde	220.1969	7(6,1)- 6(5,2)
SO2v2=1	Sulfur dioxide	345.80717	80(7,73)-81(6,76)
CH3C4H	Methyl diacetylene	345.78207	85(5)-84(5)
SO2v=0	Sulfur dioxide	356.75518	10(4,6)-10(3,7)
CH3OCHOv=1	Methyl Formate	345.79385	29(13,16)-29(12,17)
CH3OCHOv=1	Methyl Formate	345.79392	29(13,17)-29(12,18)A
C-H13CCCH	Cyclopropenylidene	345 79652	8(2 6)-7(2 5)

## MACHINE LEARNING APPROACHES

Artificial Neural Networks and Support Vector Machines, both are very popular supervised classification methods, they have several properties that allow good generalization

#### TRAINING DATA

Modified ADMIT code to generate synthetic training examples Initial physical parameters: Frequency and Intensity, more to come

