National Aeronautics and Space Administration

Algorithmic Detection of Elemental Biosignatures

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Introduction

Machine learning models that classify a planetary exploration sample as **non-indicative** or **indicative** of life can **play an important role in planning life-detection missions:**

1. They are based on clearly defined and consistent algorithms, regardless of sample type or origin.
2. They can reveal distinguishing features of life and suggest important measurements in a future mission.
3. They can be used to understand how combinations of different biosignatures affect overall confidence.

The need for this last capability was identified as a key gap in The Ladder of Life Detection (Neveu 2018).

Data Collection

- We selected **elemental composition** due to is availability across diverse samples measured in published literature.
- Selected samples had to meet these criteria:
    1. Clearly **non-indicative** or **indicative** of life.
    2. Analogous to a theoretical mission sample.
    3. Completely characterized by the elemental data.
- X-ray diffraction, mass spectrometry, etc. measurements were standardized to a simulated limit of detection.
- **Four clusters of samples** emerged in the principal component analysis (PCA) (**Fig. 1**) and boxplots (**Fig. 2**).

Sample Type	Number	Examples
Non-indicative	35	Lunar rock, basalt
Indicative mixed	19	Seawater, crop soil
Indicative non-alive	46	Coal, chalk, fossil
Indicative alive	10	Biofilm, bacteria

Modeling

Approach

- Classify a sample as **non-indicative** or **indicative** of life from its elemental composition.
- Apply a variety of common statistical models, as consensus among the models lends confidence.
- Use the Python scikit-learn software.

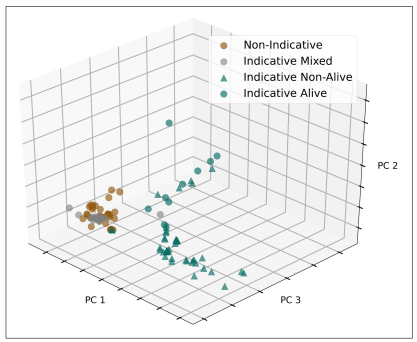

Figure 1: *PCA (reduces multi-dimensional elemental composition data into the most variable components), used for* ***KNN****.*

Model selection

These four classification algorithms offer different ways of making predictions.

- K-nearest neighbors (**KNN**)
- Logistic regression (**LR**)
- Linear support vector machines (**SVM**)
- Gaussian naïve Bayes (**GNB**)

Model training and testing

- The models were **trained** and **tested** on random splits of the data (40:60 splits, 1,000 each).

Figure 2: *Boxplots showing the abundance of elements in the four sample types.*

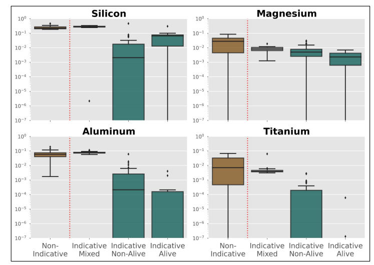

Figure 2a: *Elements found to be predictive of a* ***non-indicative of life*** *sample*

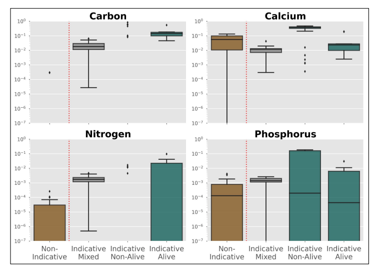

Figure 2b: *Some elements found to be predictive of an* ***indicative of life*** *sample.*

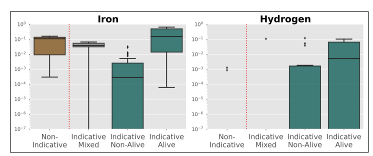

Figure 2c: *Some elements with varied predictions.*

Results

Elements predictive of a non-indicative of life sample

- All models found Si abundance to be a strong predictor.
- Most models found Mg, Al, and Ti as moderate predictors.

Elements predictive of an indicative of life sample

- All models found C and Ca as strong, and Cl as moderate.
- Most models found N, K, and P as moderate.

Elements with varied prediction directions

- Fe (slightly non-indicative), H (slightly indicative), O (varied widely), Na, Mn, and S.
- Some of these elements were not present in enough samples to be important predictors.

Model Performance

- Mean accuracy scores were similar, averaging 88% ± 4%.
- More false positives than false negatives (preferred tradeoff).

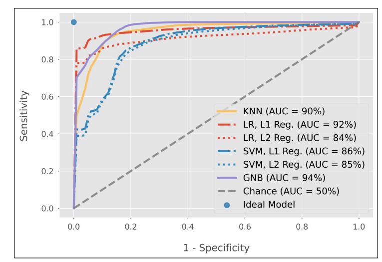

Figure 3: *Receiver Operator Characteristics (**LR** and **GNB** are shown to be the best performing models).*

Future Work

- Expand data to include other types of data, e.g. isotope fractionation, free energy, spectral information, etc.
- Implement non-linear models, e.g. neural networks.

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