

## 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

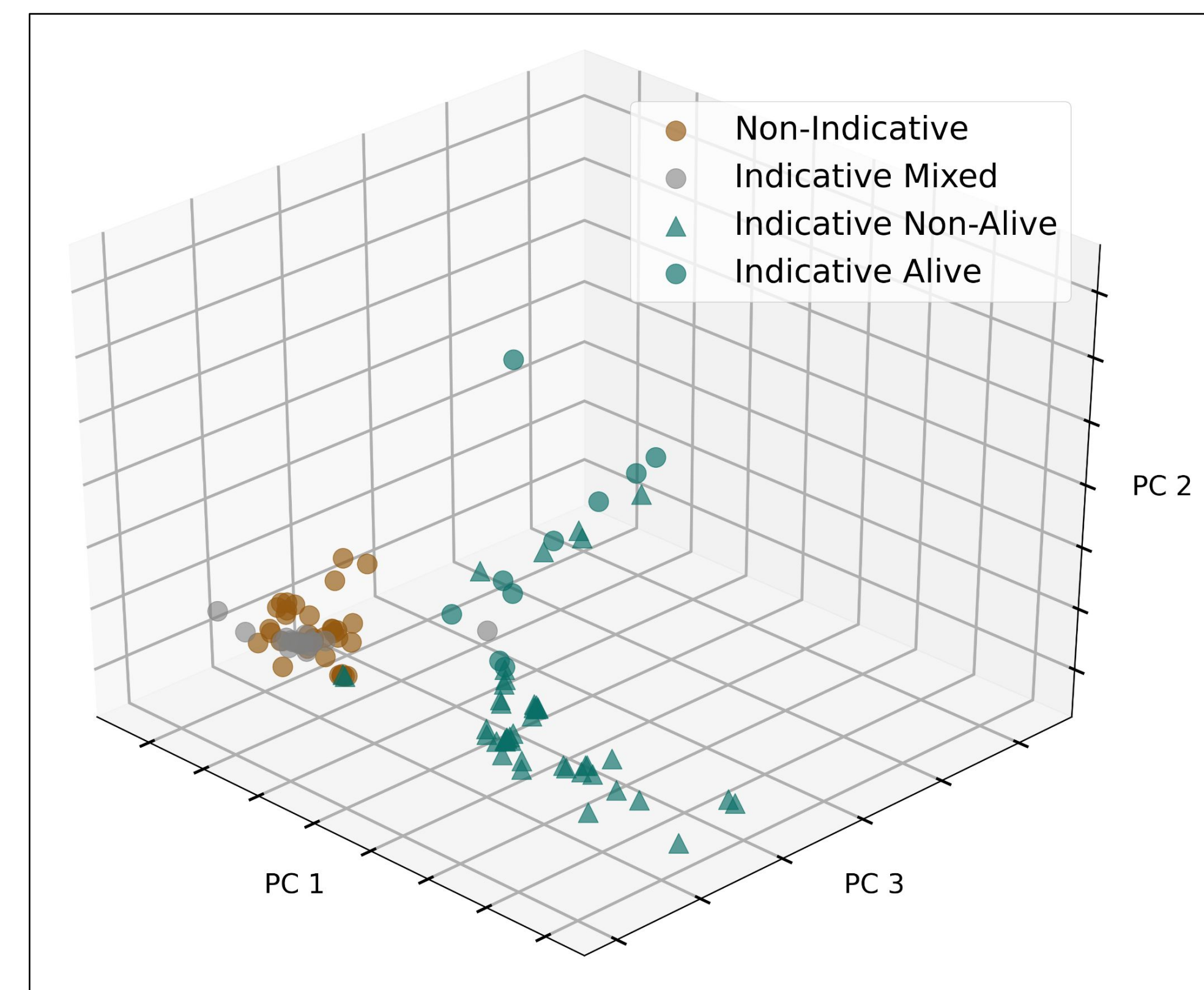
- We selected **elemental composition** due to its availability across diverse samples measured in published literature.
- Selected samples had to meet these criteria:
  1. Clearly **non-indicative** or **indicative** of life.
  2. Analogous to a theoretical mission sample.
  3. Completely characterized 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
<b>Non-indicative</b>	35	Lunar rock, basalt
<b>Indicative mixed</b>	19	Seawater, crop soil
<b>Indicative non-alive</b>	46	Coal, chalk, fossil
<b>Indicative alive</b>	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

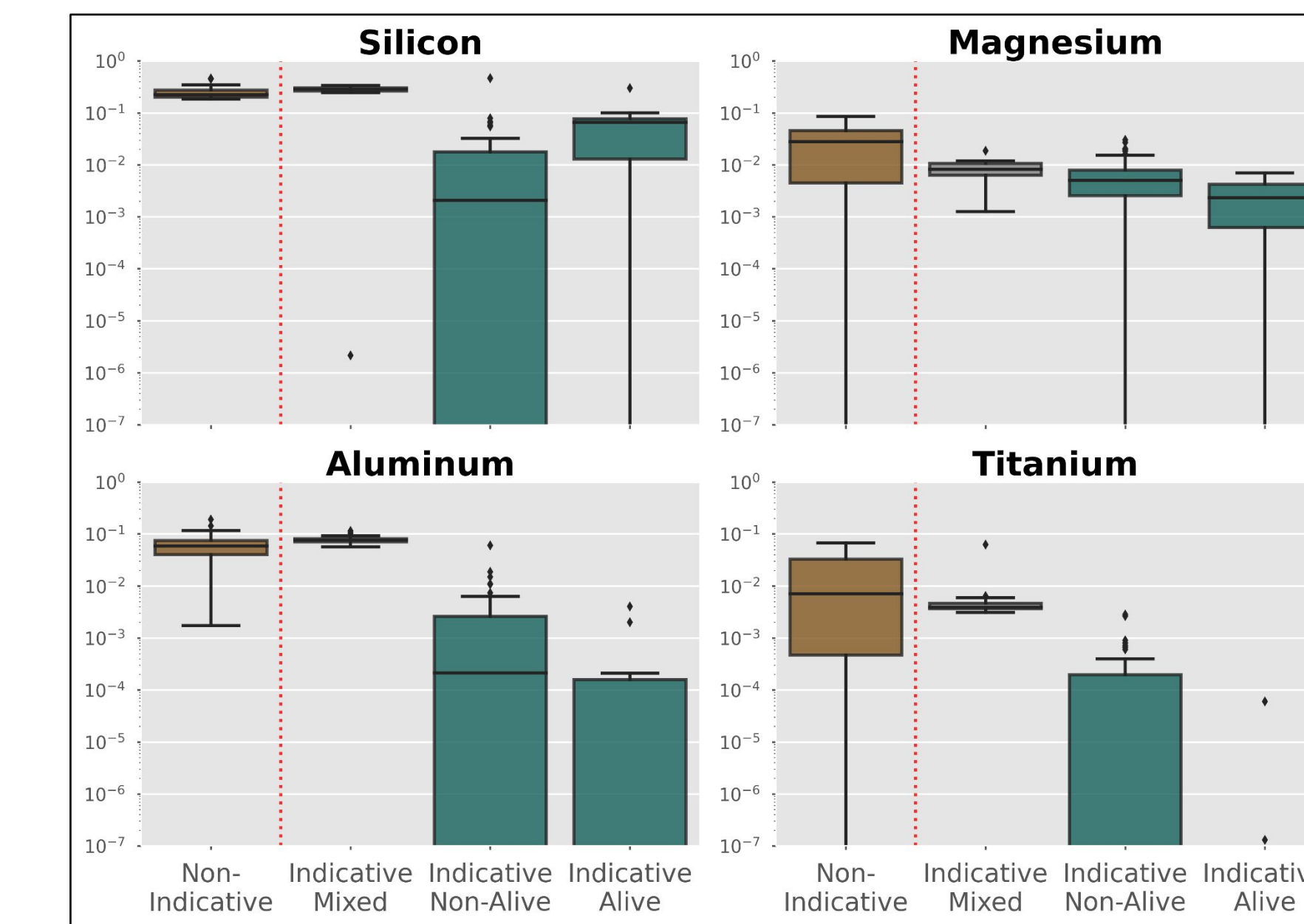
These four classification algorithms offer different ways of making predictions.

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

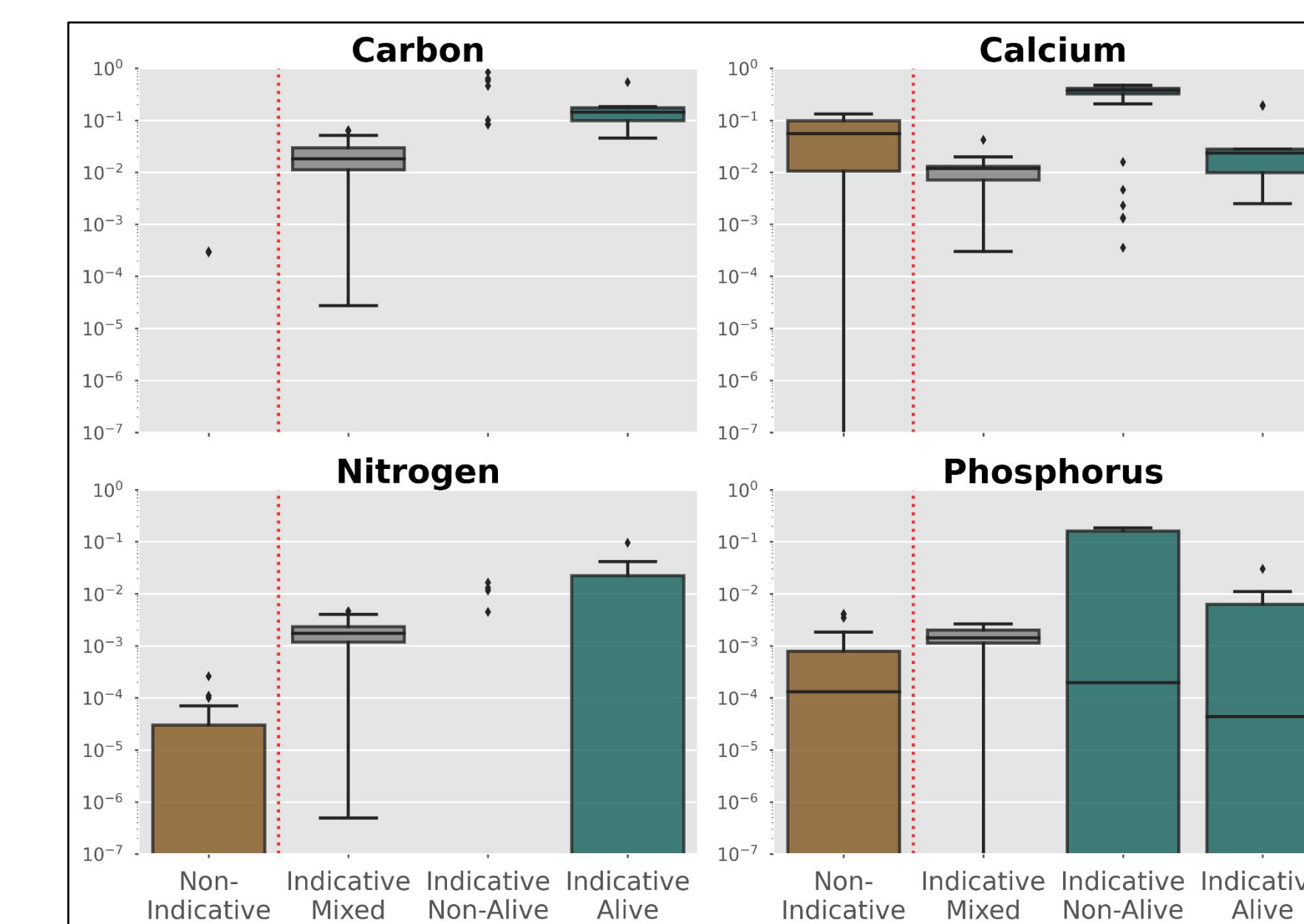
### Model training and testing

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

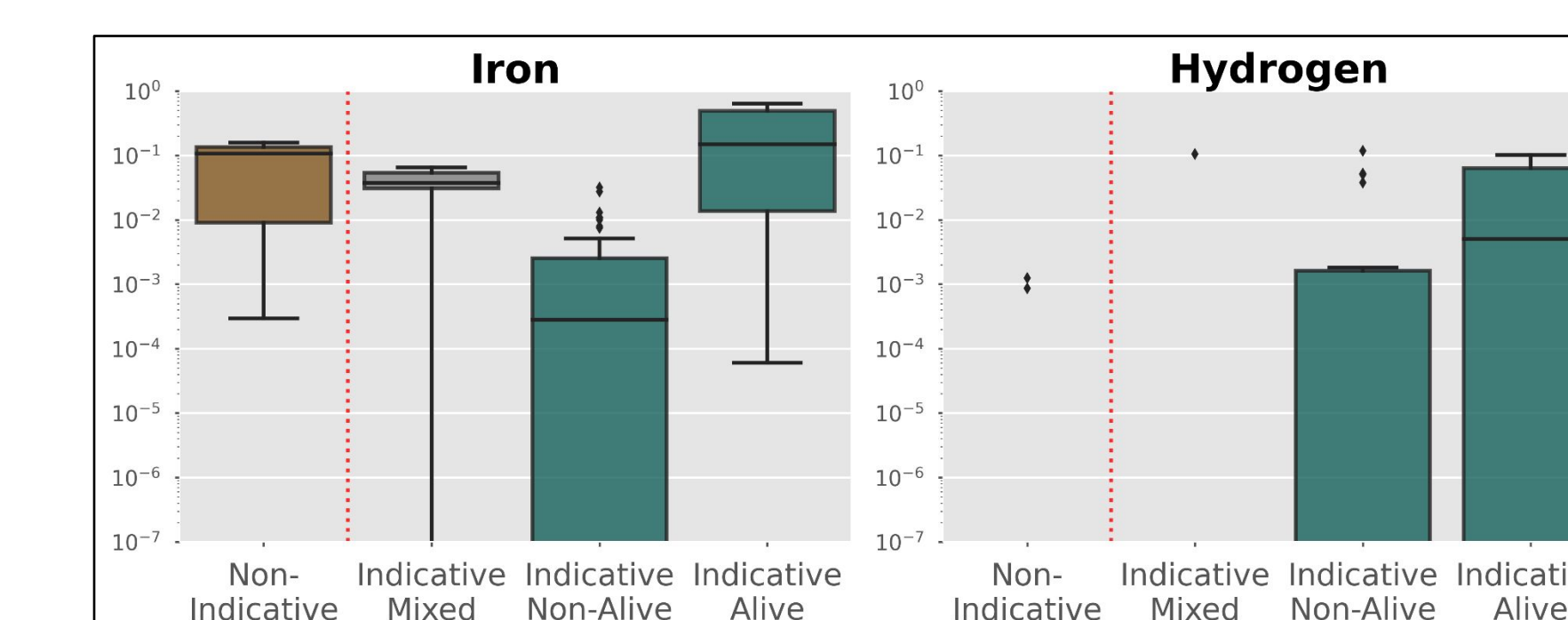
**Figure 2:** Boxplots showing the abundance of elements in the four sample types.



**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

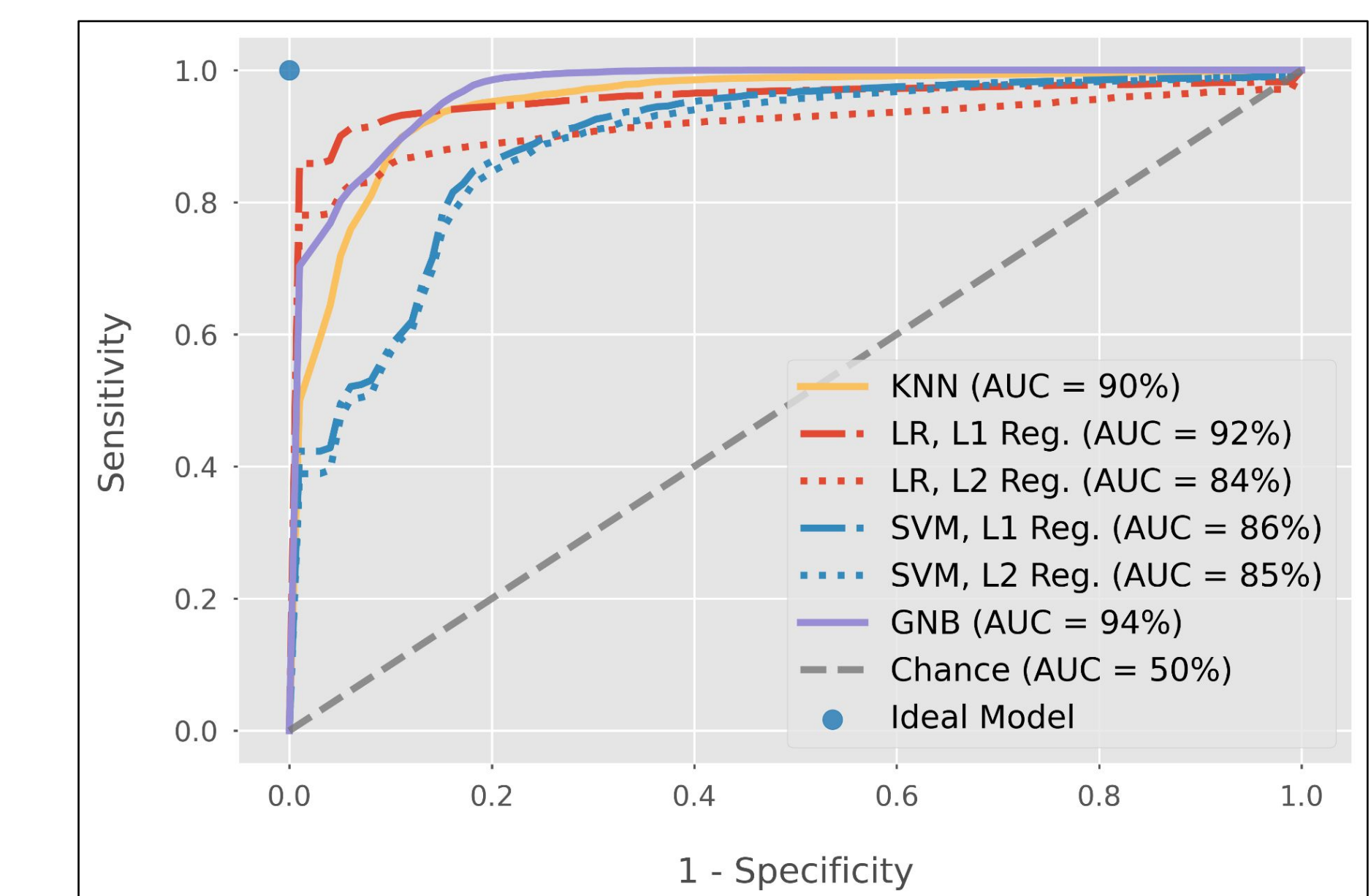
- All models found C and Ca as strong, and Cl as moderate.
- Most models found N, K, and P as moderate.

### 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  $88\% \pm 4\%$ .
- 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.

## Acknowledgements

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