Interpretable machine learning models for autonomous characterization of analogue ocean world seawater chemistry and biosignature potential using isotope ratio data

Lily A. Clough[1,2], Brett A. McKinney[1], Bethany P. Theiling[3], Victoria Da Poian[3,6], Jonathan D. Major[4], Lauren M. Seyler[5]

[1]University of Tulsa, [2]Aurora Engineering, [3]NASA-Goddard Space Flight Center, [4]University of South Florida, [5]Stockton University, [6]Microtel LLC

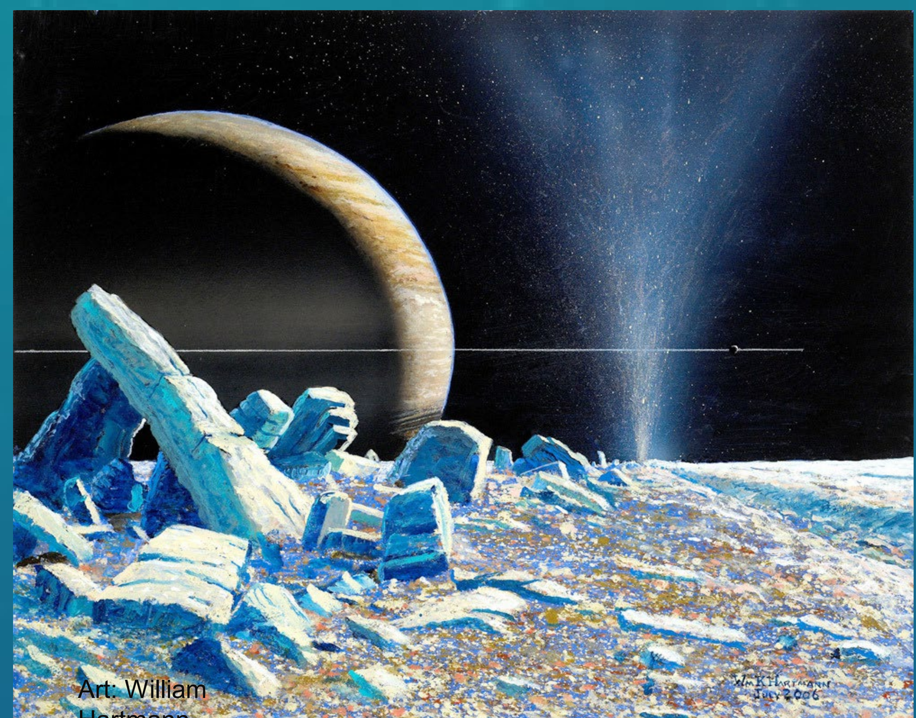
Introduction

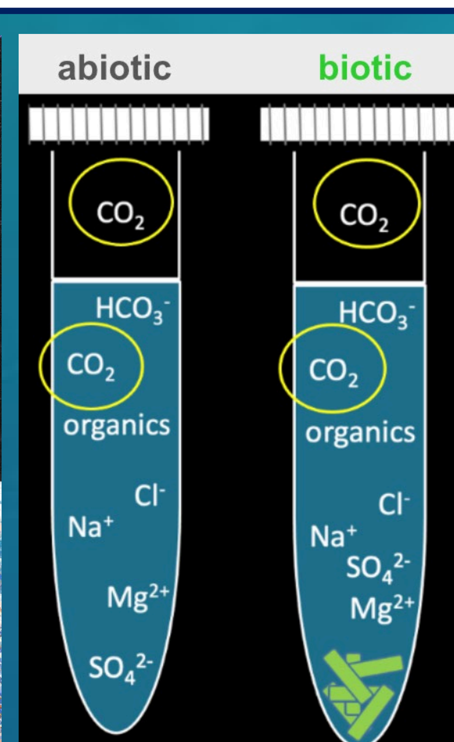
Isotope ratio mass spectrometry (IRMS) can be used to detect biosignatures[1] and seawater chemistry, but there can be overlap between fractionations caused by biotic and abiotic processes –there is potential for abiotic mimicry of biosignatures.

Machine learning (ML) can use complex effects (multiple main effects and interactions) to disentangle abiotic mimicry and make accurate predictions.

ML predictions of extraterrestrial biosignatures require strong evidence and interpretable models with physically and mathematically meaningful feature spaces and false prediction diagnostics.

Isotope ratio measurements of volatile CO_2 can be used for ML detections of ocean world (OW) biosignatures and seawater chemistry





IRMS data for ML training are from volatile CO_2 in equilibrium with biotic and abiotic laboratory OW seawater analogues.

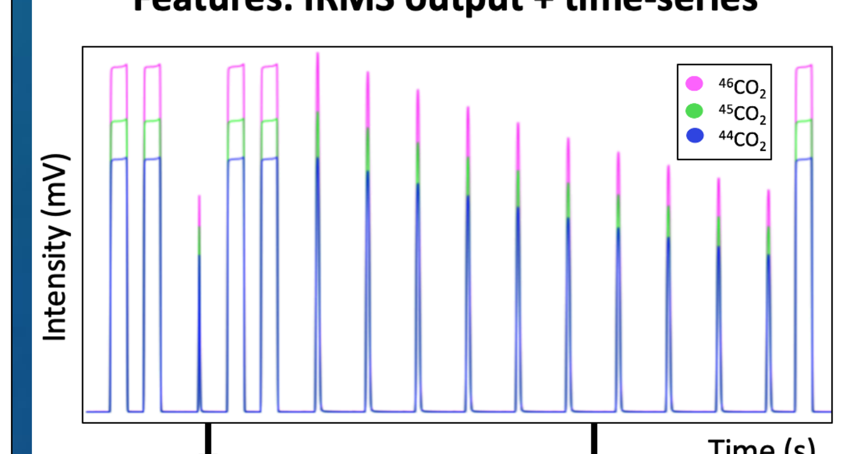
Automated Quality Control (QC), Data Processing, and Feature Construction

Features (variables) from IRMS measurements[2] are augmented with extracted time-series (TS) features[3].

Automated QC, data processing, and ML predictions prioritize data for transmission in support of science autonomy goals for ocean worlds missions[4,5].

Automated prioritization of data and ML detections of biosignatures and chemistry for future OW missions will enhance science return

Features: IRMS output + time-series



Time-series features
- Information entropies
- Autocorrelation
- Max shift in divergence /variance
- Time of max divergence/ variance
- Fluctuation

… (**48 TS features**)

IRMS-derived features
- Average $\delta^{18}O$
- Standard deviation $\delta^{18}O$
- Average $\delta^{13}C$
- Standard deviation $\delta^{13}C$
- Average peak area
- Standard deviation peak area
- Average peak intensity

… (**66 IRMS features**)

Full variable space = 104 features

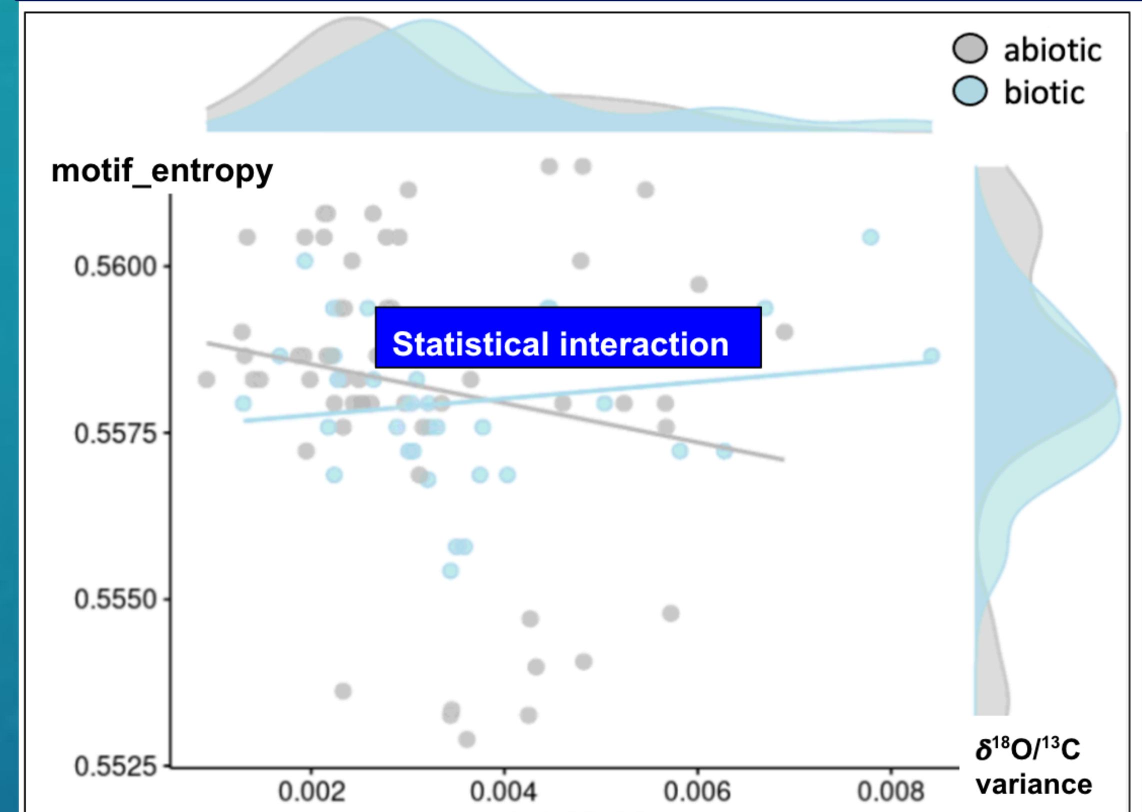
Feature selection = **reduced** feature space

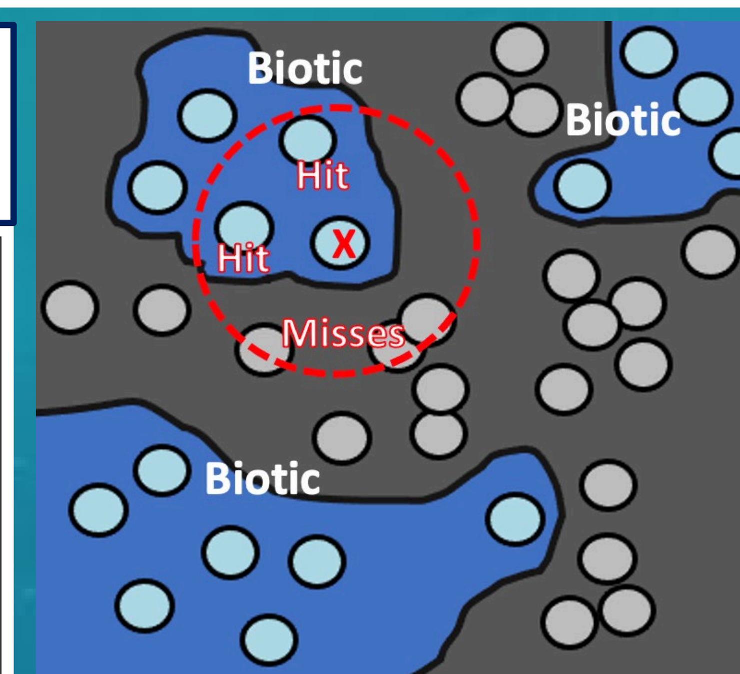
Machine Learning Feature Selection

How can we determine the important predictors for biosignatures and salt detection?

NPDR-LURF feature selection = **LASSO**-penalized[6] **Nearest-Neighbors Projected Distance Regression (NPDR[7])** using **Unsupervised Random Forest[8] (URF)** proximity distance

Statistical interactions between variables = changes in correlation based on class





NPDR feature selection finds interactions by using nearest-neighbors (hits/misses) in a high dimensional feature (variable) space.

Prediction of Biosignatures and Seawater Chemistry

Random Forest classification and regression are used to predict the presence of biosignatures, $MgSO_4$, $NaHCO_3$, pH and ionic strength using NPDR-LURF selected features.

High accuracy (>88%) salt + biosignature models

RF Classification: $NaHCO_3$/no_$NaHCO_3$

Train data	$NaHCO_3$	no_$NaHCO_3$
Samples	89	51

Train data	$NaHCO_3$	no_$NaHCO_3$
Samples	22	12

Test accuracy = 97.2%	$NaHCO_3$	no_$NaHCO_3$
$NaHCO_3$	33	0
no_$NaHCO_3$	2	36

true (rows) / predicted (columns)

RF Classification: $MgSO_4$/no_$MgSO_4$

Train data	$MgSO_4$	no_$MgSO_4$
Samples	81	209

Test data	$MgSO_4$	no_$MgSO_4$
Samples	18	53

Test accuracy = 98.6%	$MgSO_4$	no_$MgSO_4$
Abiotic	17	1
Biotic	0	53

true (rows) / predicted (columns)

RF Classification: biotic/abiotic

Train data	abiotic	biotic
Samples	89	51

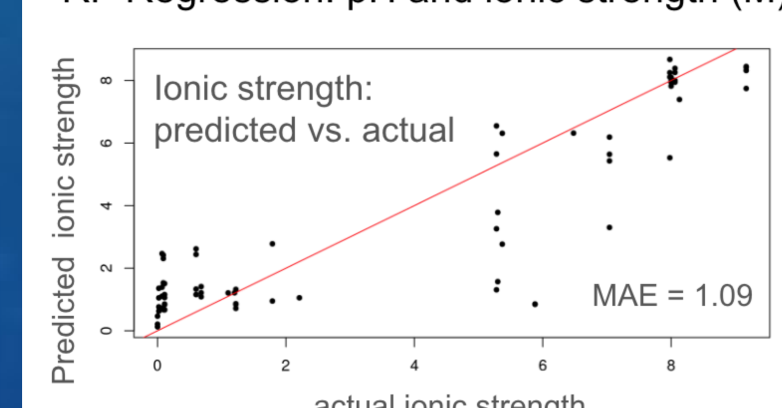
Train data	abiotic	biotic
Samples	22	12

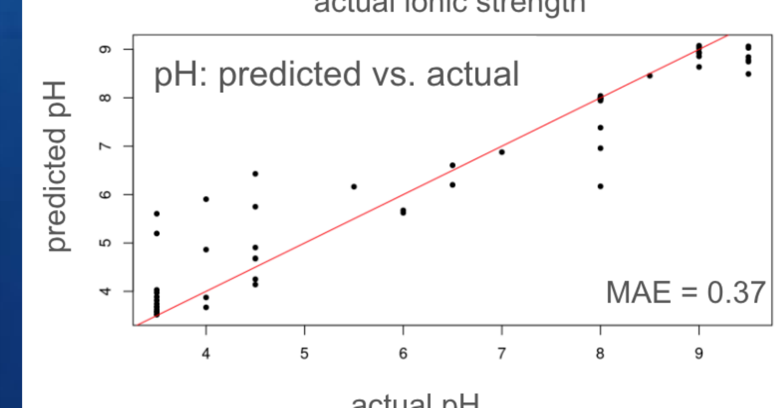
Test accuracy = 88.2%	Abiotic	Biotic
Abiotic	20	2
Biotic	2	10

true (rows) / predicted (columns)

Feasible pH + ionic strength prediction using NPDR selected features

RF Regression: pH and ionic strength (M)





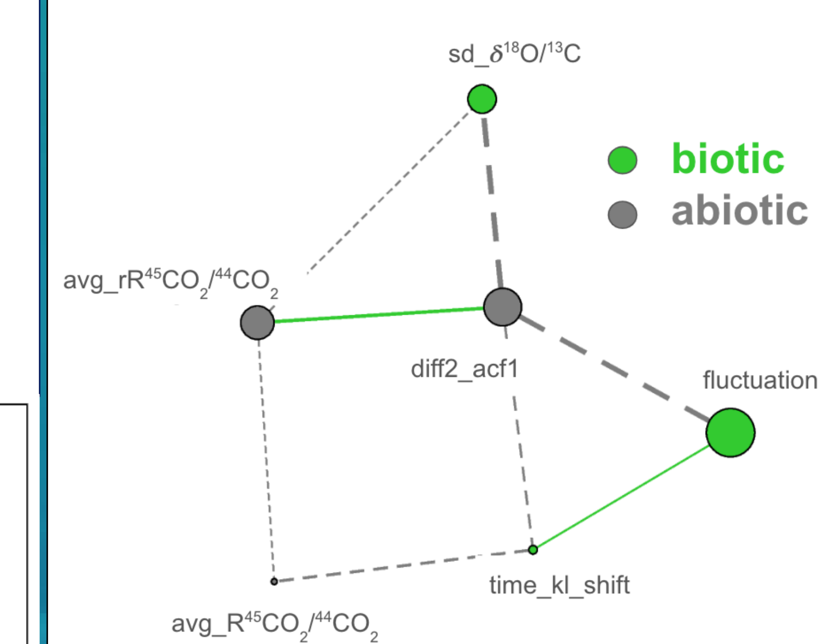
MAE = mean absolute error
Red line = 45 degree line showing ideal prediction

Networks for Model Interpretation

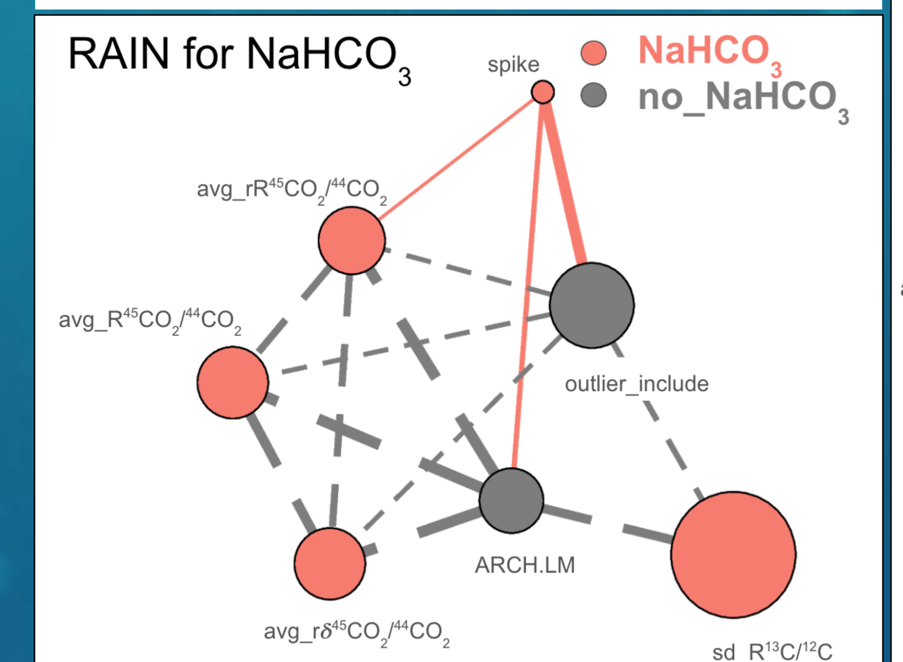
RAINs (Regression Association-Interaction Networks) visualize main effects and interactions between features

- **Node size** = main effect magnitude
- **Edge thickness** = interaction magnitude
- **Color** = effect increases probability of class

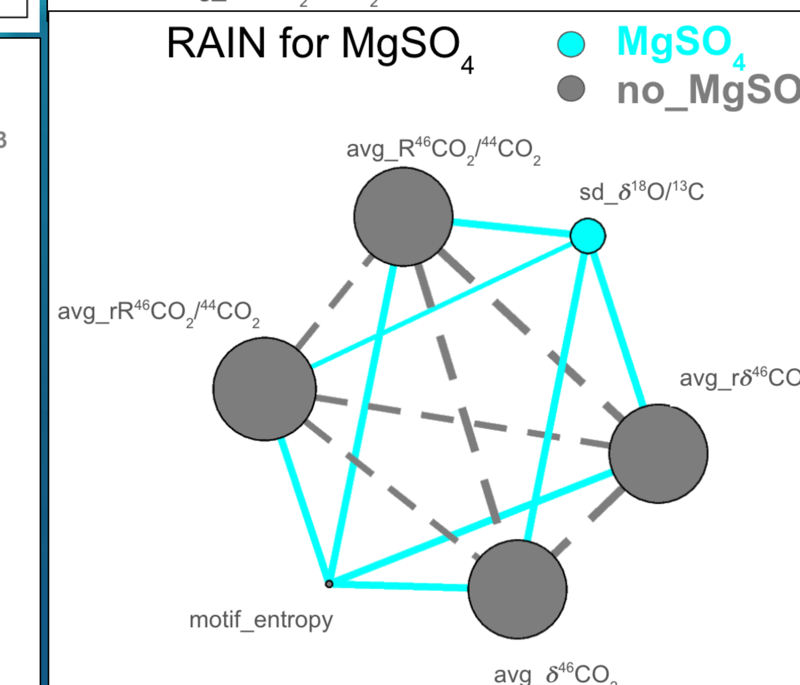
RAIN for biosignatures - 0.3% CO_2



RAIN for $NaHCO_3$



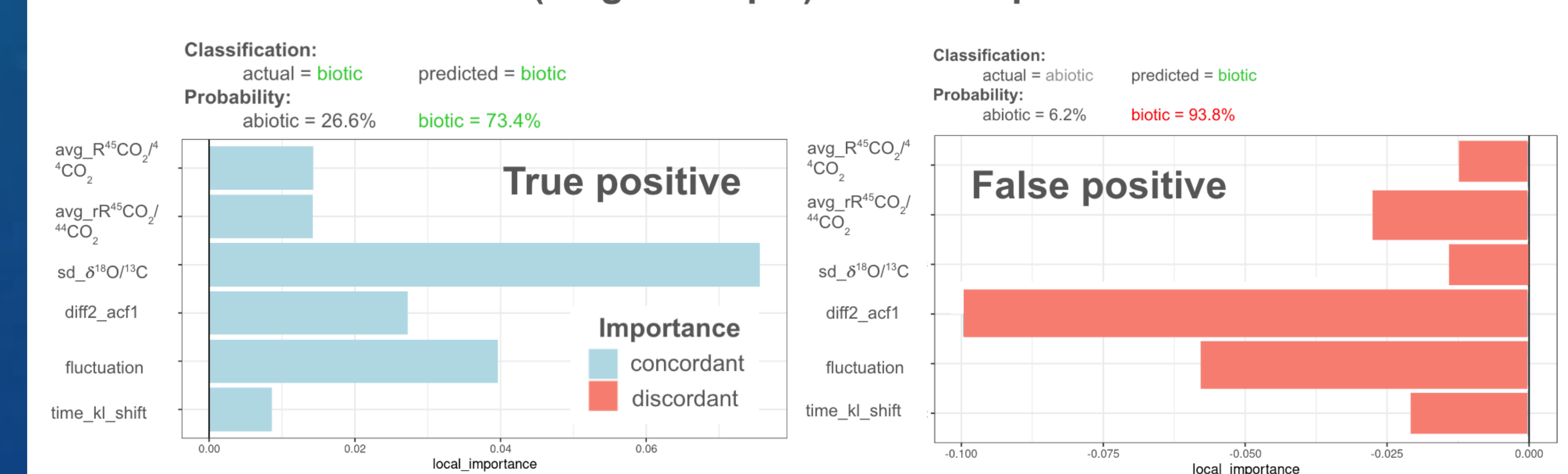
RAIN for $MgSO_4$



Diagnosing False Positives and Negatives

Local variable importance scores of globally-important variables (selected from all samples) are discordant in false prediction samples.

Local (single-sample) feature importance



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