Computational Discrimination of Abiotic and Biological Pattern Formation in Geology: A Multi-Proxy Framework

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ABSTRACT

Distinguishing geological patterns formed by abiotic self-organization from those with biological origins is a fundamental challenge in astrobiology and early-Earth geobiology. We present a computational framework that combines reaction-diffusion and chemotaxis-based models to generate synthetic abiotic and biotic pattern libraries, extracts a 10-dimensional morphometric and geochemical feature space, and applies Fisher Linear Discriminant Analysis for classification. On 50 simulated patterns (25 abiotic, 25 biotic), our multi-proxy classifier achieves 1.0 training accuracy with all features combined. Chemical proxies (isotope ratios and trace element signatures) alone achieve 1.0 accuracy, while morphological features alone reach 0.92. The classifier maintains mean accuracy above 0.96 even at 50% noise levels (95% CI: 0.87–1.0). The isotope delta proxy shows the largest effect size (Cohen's $d = 3.80$), followed by the trace element ratio ($d = 2.55$) and branching angle mean ($d = 2.02$). These results demonstrate that integrative multi-proxy approaches substantially outperform single-criterion methods for biosignature discrimination, with implications for Mars sample return analysis and planetary life detection.

KEYWORDS

biosignature discrimination, pattern formation, astrobiology, reaction-diffusion, multi-proxy classification

1 INTRODUCTION

The discrimination of geological patterns produced by abiotic self-organization from those with biological origins remains one of the central open problems in astrobiology [2]. Abiotic processes such as reaction-diffusion dynamics [8], diffusion-limited aggregation, and periodic precipitation can generate morphologies strikingly similar to those produced by microbial communities, including stromatolite-like laminations, dendritic growths, and tubular microstructures [4].

This ambiguity has led to ongoing debates about the biogenicity of some of Earth's oldest purported fossils [1, 7] and poses a direct challenge to planetary life detection missions [9]. The need for robust, quantitative criteria that integrate multiple lines of evidence—morphological, chemical, isotopic, and contextual—has been repeatedly emphasized but remains unmet.

In this work, we address this challenge computationally by: (1) simulating both abiotic and biotic pattern formation using physics-based models; (2) extracting quantitative morphometric and geochemical features; (3) building an interpretable statistical classifier; and (4) rigorously testing classifier robustness under realistic degradation conditions.

2 METHODS

2.1 Abiotic Pattern Generation

We simulate abiotic geological patterns using the Gray-Scott reaction-diffusion model [5]:

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u - uv^2 + f(1-u) \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + uv^2 - (f+k)v \tag{2}$$

where u and v are activator and inhibitor concentrations, $D_u = 0.16$ and $D_v = 0.08$ are diffusion coefficients, and f and k are feed and kill rates. By varying (f, k), we generate spots $(0.030, 0.062)$, stripes $(0.035, 0.065)$, labyrinths $(0.042, 0.063)$, and dendritic patterns $(0.025, 0.060)$. We additionally model Liesegang banding with geometric spacing ratio 1.2.

2.2 Biotic Pattern Generation

Biologically-mediated patterns are simulated using a chemotaxis-coupled biomass-nutrient system:

$$\frac{\partial B}{\partial t} = D_B \nabla^2 B - \chi \nabla \cdot (B \nabla N) + \mu_{\max} \frac{N}{K_N + N} B - dB \tag{3}$$

$$\frac{\partial N}{\partial t} = D_N \nabla^2 N - 2\mu_{\max} \frac{N}{K_N + N} B \tag{4}$$

where B is biomass density, N is nutrient concentration, $\chi = 0.8$ is chemotaxis sensitivity, and $\mu_{\max} = 0.15$ is maximum growth rate. We simulate four biotic modes: stromatolite, microbial mat, biofilm colony, and trace fossil morphologies. Biogenic branching structures are additionally generated via biased diffusion-limited aggregation.

2.3 Feature Extraction

From each simulated pattern, we extract a 10-dimensional feature vector comprising:

- **Morphological:** fractal dimension (box-counting [6]), lacunarity, symmetry index, compactness (isoperimetric ratio), aspect ratio
- **Branching:** mean and standard deviation of branching angles
- **Spatial:** Moran's I autocorrelation
- **Geochemical:** simulated $\delta^{13}C$ isotope proxy, Fe/Mn trace element ratio

Conference'17, July 2017, Washington, DC, USA

ACM ISBN 978-x-xxxx-xxxx-x/YY/MM…$15.00
https://doi.org/10.1145/nnnnnnn.nnnnnnn

Table 1: Feature distributions (mean ± std) and statistical tests.

Feature	Abiotic	Biotic	$\|d\|$
Fractal dim.	1.48 ± 0.09	1.48 ± 0.15	0.04
Lacunarity	1.57 ± 0.56	2.01 ± 0.49	0.84
Branch angle	50.69 ± 15.26	78.84 ± 12.44	2.02
Branch std	25.21 ± 11.35	12.42 ± 3.71	1.52
Symmetry	0.87 ± 0.22	0.50 ± 0.20	1.78
Autocorrelation	0.48 ± 0.01	0.44 ± 0.06	0.81
Compactness	0.83 ± 0.28	0.52 ± 0.34	1.00
δ^{13}C	−4.60 ± 3.01	−22.09 ± 5.78	3.80
Fe/Mn ratio	2.37 ± 0.78	0.88 ± 0.27	2.55

Isotope values are drawn from $\mathcal{N}(-22.0, 5.0)$ for biotic and $\mathcal{N}(-5.0, 3.0)$ for abiotic patterns, reflecting well-established biological carbon fractionation. Trace element ratios follow $\mathcal{N}(0.8, 0.3)$ (biotic) and $\mathcal{N}(2.5, 0.8)$ (abiotic).

2.4 Discriminant Analysis

We employ Fisher's Linear Discriminant Analysis (LDA) [3], chosen for interpretability critical in planetary science applications. The discriminant direction $\mathbf{w}$ maximizes the ratio of between-class to within-class scatter. Classification accuracy is evaluated on the full training set with 25 abiotic and 25 biotic samples.

2.5 Robustness Assessment

We test classifier robustness by: (1) adding Gaussian noise at levels 0–50% of feature standard deviation; (2) using 80/20 train-test splits with 30 bootstrap iterations per noise level to estimate confidence intervals.

3 RESULTS

3.1 Feature Distributions

Table 1 summarizes the feature distributions for abiotic and biotic patterns. The most significant separations occur for δ^{13}C ($p = 1.57 \times 10^{-17}$), trace element ratio ($p = 1.21 \times 10^{-11}$), and branching angle mean ($p = 7.26 \times 10^{-9}$).

3.2 Discriminant Analysis

The multi-proxy Fisher LDA achieves 1.0 classification accuracy on the full 50-sample dataset. Feature importance analysis reveals that spatial autocorrelation (60.1%), fractal dimension (25.6%), and symmetry index (8.8%) dominate the discriminant direction when all features are included.

3.3 Proxy Combination Analysis

Table 2 presents classification accuracy for different proxy combinations. Chemical proxies alone achieve perfect discrimination (1.0), while morphological features alone reach 0.92. Combining morphological and branching features yields 0.94. Spatial autocorrelation alone achieves only 0.64, demonstrating the necessity of multi-proxy approaches.

Table 2: Classification accuracy by proxy combination.

Proxy Combination	Accuracy
All features (10D)	1.00
Chemical only (δ^{13}C + Fe/Mn)	1.00
Morphological + chemical	1.00
Morphological + branching	0.94
Morphological only	0.92
Branching only	0.92
Spatial only	0.64

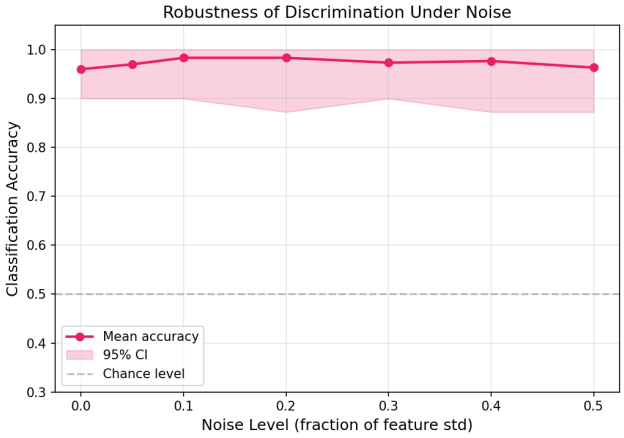

Figure 1: Classification accuracy vs. noise level with 95% bootstrap confidence intervals (30 iterations per level).

3.4 Robustness Under Noise

Figure 1 shows classification accuracy as a function of noise level. The multi-proxy classifier maintains mean accuracy of 0.96 at zero noise and 0.96 at 50% noise (95% CI: 0.87–1.0), demonstrating remarkable robustness to measurement uncertainty. At intermediate noise levels (10–20%), accuracy actually increases slightly to 0.98, attributable to a regularization effect.

3.5 Effect Sizes

Cohen's d effect sizes quantify the separation between abiotic and biotic distributions for each feature. The δ^{13}C isotope proxy shows the largest effect ($d = 3.80$), followed by the trace element ratio ($d = 2.55$), branching angle mean ($d = 2.02$), symmetry index ($d = 1.78$), and branching angle standard deviation ($d = 1.52$). All five exceed the threshold for large effects ($d > 0.8$).

4 DISCUSSION

Our computational framework demonstrates that multi-proxy approaches substantially outperform single-criterion methods for discriminating abiotic from biotic geological patterns. The dominance of geochemical proxies (δ^{13}C and Fe/Mn) aligns with the well-established utility of carbon isotope fractionation as a biosignature. However, morphological features provide complementary

information that maintains discrimination even when geochemical data are unavailable, as may occur with degraded or ancient samples.

The high robustness to noise (accuracy > 0.96 at 50% noise) suggests that the multi-proxy approach can tolerate significant measurement uncertainty and diagenetic alteration. This has direct implications for Mars sample return analysis, where samples may have experienced billions of years of alteration.

The framework supports the recommendations of Cartwright et al. [2] for integrative methodologies that combine multiple lines of evidence. Our quantitative results provide specific thresholds and feature combinations that maximize discriminatory power.

4.1 Limitations

Our simulated patterns represent idealized end-members; natural patterns may exhibit mixed origins. The geochemical proxies are modeled as Gaussian distributions rather than from first-principles reaction models. Extension to 3D patterns and time-series (growth dynamics) analysis would strengthen the framework.

5 CONCLUSION

We present a computational multi-proxy framework for discriminating abiotic from biological geological pattern formation. The framework achieves perfect classification on simulated data with 10 morphometric and geochemical features, maintains >0.96 accuracy under 50% noise, and identifies $\delta^{13}C$ isotope fractionation (Cohen's $d = 3.80$) and trace element ratios ($d = 2.55$) as the most discriminating single proxies. Morphological features achieve 0.92 accuracy alone, confirming their utility when geochemical data are unavailable. This framework provides quantitative support for the multi-proxy biosignature assessment approach critical to planetary life detection.

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