

Topical: Development of New Algorithms for Space Biology

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Abstract

Advances in artificial intelligence (AI) algorithms provide the opportunity to both catalyze and be inspired by new space biological discoveries. Currently there is limited adaptation of emerging AI methods to address critical needs for NASA space biology research, and no spaceflight missions are dedicated to developing algorithms inspired by space biology and its needs. This white paper highlights established and emerging algorithms relevant to space biology and recommends investment in space biology inspired algorithm development in the coming decade.

Background

Machine learning (ML) is a type of computational modeling which ‘learns’ to predict an outcome of interest from sample data by iteratively improving the model to minimize prediction errors over training time. Deep learning (DL) is a type of machine learning that uses particularly large, often multi-layer models that can model particularly complex relationships. ML automates repetitive processes and when well-implemented, ML approaches can derive patterns from high-dimensional datasets without requiring significant manual input.

In life sciences knowledge discovery and research, classical ML techniques have a myriad of applications [1]. ‘Supervised’ learning creates a model trained on labeled datasets to predict the label of a new, unknown datapoint: classification predicts the category of a new data point (e.g. whether a biopsy is cancerous or healthy); regression or the problem of learning how to map input variables to continuous output variables (e.g., mapping the expression level of a gene to survival time). Unsupervised clustering is the problem of grouping similar data points in unsupervised mode (e.g., phylogenetic relationships between species). DL algorithms including neural networks are modeled after human neuronal signaling, and further improve such difficult tasks as image classification (e.g., diagnosis after training on retinal scans with and without retinopathy) [1].

However, ML implementation is constrained by data structure and sample number. The NASA Science Mission Directorate Strategic Data Management Working Group found that AI and ML methods are currently under-utilized in NASA science, due in part to the difficulty in adapting scientific datasets to be AI/ML analysis-ready [2]. These difficulties are compounded in the space biology field, where the cost per spaceflown sample is extremely high, so the sample numbers of each experiment are necessarily quite low by ML standards. Further, much space biological research data is now in the ‘omics space, leading to under-determined datasets with hundreds of thousands of features but tens of samples. In parallel, as we continue to explore the deep space environment, research datasets will necessarily harbor unfamiliar structure with no analogous Earth data and many unknown parameters, making it difficult to apply traditional ML models and assumptions.

Here, we highlight current ML methods with broad potential for space biological research applications, and recommend the development of novel, space biology inspired methods for the next decade of groundbreaking research. We identify algorithm development as a research area to advance knowledge in the effects of spaceflight on biological systems, with anticipated value to both human exploration and humans on Earth. Space biological data harbor many of the same constraints as data from rare disease populations (e.g. genetic diseases, childhood cancers) [3]. Development of tools and methods for knowledge discovery in small, heterogeneous datasets will benefit these populations on Earth.

Current Approaches

Class of Algorithm	Key Unique Features	Example Application	Relevancy to Space Biology	Select References
<i>Classification and Regression ML Models</i>	<ul style="list-style-type: none"> - Enables predictions on a subject level - Avoids generalization on a cohort that has high-variability in individual performance - Scalable, more features and measures can be added in the future 	Prediction of behavioral and physiological changes due to spaceflight stressors	Enables predicting how astronauts will react to space stressors before sending them on a mission	[4,5]
<i>Generative Models</i>	<ul style="list-style-type: none"> - Creates new data - Enables predictions based on theory - Pretrained models do not depend on large datasets 	<ul style="list-style-type: none"> - Generation of realistic synthetic datasets for ML benchmarking and pretraining - Generation of inferred data 	The need to generate larger, realistic datasets for training due to experimental sample number constraints.	[6]
<i>Knowledge Graphs</i>	Integrates many, diverse datasets by relationships between multiple attributes and meta-features	<ul style="list-style-type: none"> - Predicted physiological changes for human space travel by integration of spleen, liver and thymus gene expression data from mice flown in space 	Integration of Earth-based clinical knowledge with space biology data.	[7,8,9]
<i>Lifelong Learning</i>	Continually learns from new information	<ul style="list-style-type: none"> - A living lab on board spacecraft constantly iterating, developing and testing new hypotheses. - Biosensor monitoring that adapts with changes in the individual 	<ul style="list-style-type: none"> - Enables automated and hands-off knowledge gain. - Allows functions, such as anomaly detection, to be performed in areas that are dynamic and in flux, such as biological systems. 	[10,11]
<i>Network & Causal Inference</i>	Predicts mathematical causal relationships among many objects or samples	Identification of genes with causal relationship to a disease phenotype.	Causal features in space biological data, and future application to real-time health monitoring to enable preventative therapies.	[12]
<i>Neuromorphic Computing</i>	<ul style="list-style-type: none"> - Enables efficient edge computing - Uses analog circuitry instead of binary computing architectures to mimic the function of biological systems 	Real-time learning from data collected onboard spacecraft. Predicting neural synaptic plasticity. Support for AI learning capabilities in low-power, high radiation contexts.	Addresses limited compute power on spacecraft for the purpose of AI learning.	[13,14,15,16]
<i>Few-shot Learning</i>	<ul style="list-style-type: none"> - Learns from contextual information - Does not require replicates 	Extrapolation of drug performance based on similar molecular structure.	Significantly extends the utility of small, non-replicate space biology studies.	[17,18]

<i>Simulations & Digital Twins</i>	Mimics relationships of a living organism or otherwise complex object	Characterize and predict responses to space-relevant perturbations using a realistic mouse digital twin.	Enables experimentation and modeling of extreme space environments that are difficult to access and research.	[19,20]
<i>Transfer Learning</i>	Maps models and data from one system to predict relationships of another system	Mapping single cell RNA sequencing cell types from mouse data to human.	Extrapolate from model organisms to the effects of space in humans	[21,22]

Table 1. Overview of Select Current Methods Relevant to Space Biology

Table 1 highlights a selection of promising ML and DL methods, and ways they are and can be applied to space biology. As one recent example, knowledge graphs containing data from over 30 human biomedical databases (including omics, symptoms, drug interactions, and chemical structures) integrated with gene expression data from spaceflown mouse spleen, liver and thymus predicted human physiological changes occurring in space [9]. In another recent work, researchers utilized ionized radiation dose, along with pre-irradiation cognitive behavioral test scores, and trained ML models accompanied by traditional statistical analyses to predict cognitive test scores post-irradiation on a subject-based level [4,5]. There have been critical advances in model development relevant across many fields but particularly space biology where small sample sizes often are a limiting factor. For example, novel few-shot learning approaches and graphical AI algorithms can eliminate the need to have copious data (or even any replicates) while still enabling robust predictions [17,18].

A class of methods particularly applicable to space biology is transfer learning, where models trained on a source domain (e.g., a system or organism of interest) can be extrapolated to a different target domain. Two potential applications of transfer learning are immediately obvious in the space biology research field. First, the majority of space biology research data uses model organisms (mouse, rat, fruit fly, etc.) but the ultimate application is human astronaut health, where currently very few data points are available and which harbor key differences from model organisms. Transfer learning has been used successfully in terrestrial research for mapping single cell RNA sequencing cell types from mouse data to human [22]. Second, as spaceflight biological research advances from low earth orbit flight to Lunar or Mars missions over the next decade, the timely downlink of experiment data to Earth for analysis will become increasingly more challenging. Rather, key real-time insights could be gained by uplinking weights from terrestrial models pre-trained on relevant experimental or biomedical data, to generate predictions based on *in-situ* data. Few-shot and one-shot learning also fall under extreme transfer-based and meta-transfer approaches [23], where contextual or prior information from a small sample size classifies novel information.

Other emerging approaches, like the human brain-inspired neuromorphic computing, enable the use of energy-efficient physical hardware (e.g., memristors) that can solve AI problems with minimal compute constraints [14]. Neuromorphic computing devices can significantly reduce power consumption (e.g., a few mW/cm² vs. 50-100 W/cm²) compared to traditional central processing units relying on silicon complementary metal oxide semiconductors [24]. These energy savings are particularly critical in resource and compute limited situations like in space travel. One example of a space biology application of neuromorphic computing would be to enable real-time analysis of on-board sensors and *in situ* computing on a space station (e.g., to efficiently control

the environmental conditions for incubated mammalian cell culture systems in space, or to give immediate health feedback to astronauts from biosensors).

Opportunities for New Algorithms for Space Biology

Building on key early milestones in applying ML to space biology data [4,5,9] and the untapped potential of existing AI methods (Table 1), we propose that additional research is warranted to best apply ML and DL methods to space biology datasets. Among the challenges that existing methods can address to advance space biology are the following:

- **Data structures:** There is a growing, unmet need for flexible data-structures that themselves evolve and learn to optimize handling of space data in a well-organized form, especially if semantic in nature [25,26].
- **Predictive algorithms:** Relationships within available space datasets need to be modeled to enable predictions to plan for new missions.
- **Classification techniques:** Discriminating between different biological states, such as whether or not a disease exists, has typically relied on a limited number of features which were often assessed using simple threshold rules. There is a need to enhance these algorithms to use subtle patterns buried within hundreds or even thousands of features in order to perform more nuanced classification.
- **Benchmark datasets:** Benchmark space biology datasets which represent all key factors of space biological data (e.g., small, heterogeneous, sparse data, unevenly sampled datasets with biases) need to be produced to test new AI algorithms.

We propose that the added complexity and difficulty of research in extreme space environments necessitates the organized and concerted development of novel, next-generation ML algorithms and models specifically for space biology datasets. This category of algorithms and computational paradigms encompasses methods inspired (1) by the structure of space-related data, (2) by the features of extremophiles on Earth, and/or (3) by newly identified biological information about potential species on extraterrestrial bodies.

Domain-specific knowledge, data structures and discovery have catalyzed new algorithms and computational paradigms in other fields. Examples include the application of machine learning force fields in material science [27], and life-long learning AI approaches that learn continually from the incorporation of new data applied to modeling human neurogenesis or the growth of new neurons [10,11]. Beyond capitalizing on the classical and contemporary ML methods highlighted (Table 1), we propose concerted research efforts into the development of next-generation, novel algorithms to enable discovery in space biology. These new methods would need to be particularly well-suited to the challenges of learning on datasets gathered in unfamiliar environments with limited Earth-based contextual comparisons. These methods will necessarily be more eliminative than affirmative in nature due to the unfamiliarity of the scenarios and examples. We envision that development and utilization of these algorithms will propel space biological research toward a comprehensive, predictive profile of life under a variety of extraterrestrial conditions. Full realization, deployment and productivity of these models in space will depend on deep space computing clouds [28], and widespread in-space data fusion and storage onboard spacecraft, as detailed in a Planetary Science and Astrobiology topical white paper by Mahabal *et al.* [29].

A related tangible opportunity is in space-biology inspired (SBI) algorithms. While neuromorphic computing is inspired by the neural cognitive function of humans, an entirely new suite of algorithms can be informed by the compute systems of Earth-based organisms found in

extreme or harsh environments and those predicted in extraterrestrial settings. Developing algorithms that mimic neural cognitive systems beyond that of humans is one example of how out-of-the-box model and algorithm design may enable better performance on biological data in general – which is currently less amenable to classical DL model architectures [30] – and may be more adaptive to very out-of-distribution contexts encountered during space travel. For example, immortal jellyfish (hydra) found in low oxygen or even anoxic environments in the deep ocean have the ability to continually self-regenerate [31], and hydra’s ability to complete common behavioral tasks with varying numbers of neurons and dynamic neural circuits is informing how we study redundancy, robustness, and efficiency in computational tasks. From these and other extremophiles, we can develop SBI algorithms with features that optimize for robustness to noise and/or to extreme variation while performing computing tasks. In turn, these SBI algorithms can help characterize the biosystems and organisms that may be dwelling in a variety of environments beyond Earth. Analogously, an emerging area of AI research centers on biocomputing, using genetic materials (e.g., DNA, RNA) and/or other biochemical reactions to perform computing tasks [32]. As we identify new biology from extremophiles on Earth and in space, the scope of building blocks for transferring information will expand, offering new avenues for biocomputing.

To capitalize on these opportunities and catalyze discoveries, we propose developing SBI methods specifically for datasets collected in settings beyond low earth orbit. Classification of diverse computing features of discovered biological systems can form the basis to predict new organisms or design synthetic organisms with increasingly sophisticated intellectual/computing capabilities [32,33]. As space exploration continues, biological data will be collected in extreme and unfamiliar environments, without analogous settings on Earth. Further, understanding and developing SBI and other novel methods now will aid in unbiased understanding of the function of extraterrestrial organisms.

Summary

We believe that investing in AI algorithms applied to and inspired by space biology will benefit the scientific community in two distinct ways. First, we believe widespread incorporation of ML methods will generate novel insights and vastly improve the reproducibility of biological results through expediting knowledge discovery and reducing human bias through automating analysis, which we anticipate will have significant value for the next decade of human space exploration. It should be noted that in all cases, care must be taken to avoid introducing bias as much as possible. Second, efforts to develop novel algorithms to address the challenges of space biological research (extreme, unknown environments; small dataset size; model organism to human translation) will have direct value for humans on Earth, who will benefit from application of these models to similarly difficult biomedical questions such as rare diseases with small sample sizes, or research and clinical environments with limited access.

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