

On Finding Good Experiments (in astronomy)

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Abstract

One of the key choices we have as scientists is to design informative experiments. Using examples from astronomy, we discuss a machine learning perspective of the scientific method. With AI promising accurate predictions, we revisit the question of adaptively designing new measurements that take previous data into account. Following this scientific method framing, we illustrate some recent ideas on using machine learning to recommend experiments in genomics. The goal of this talk is to start a conversation about what it means to recommend experiments in astronomy.

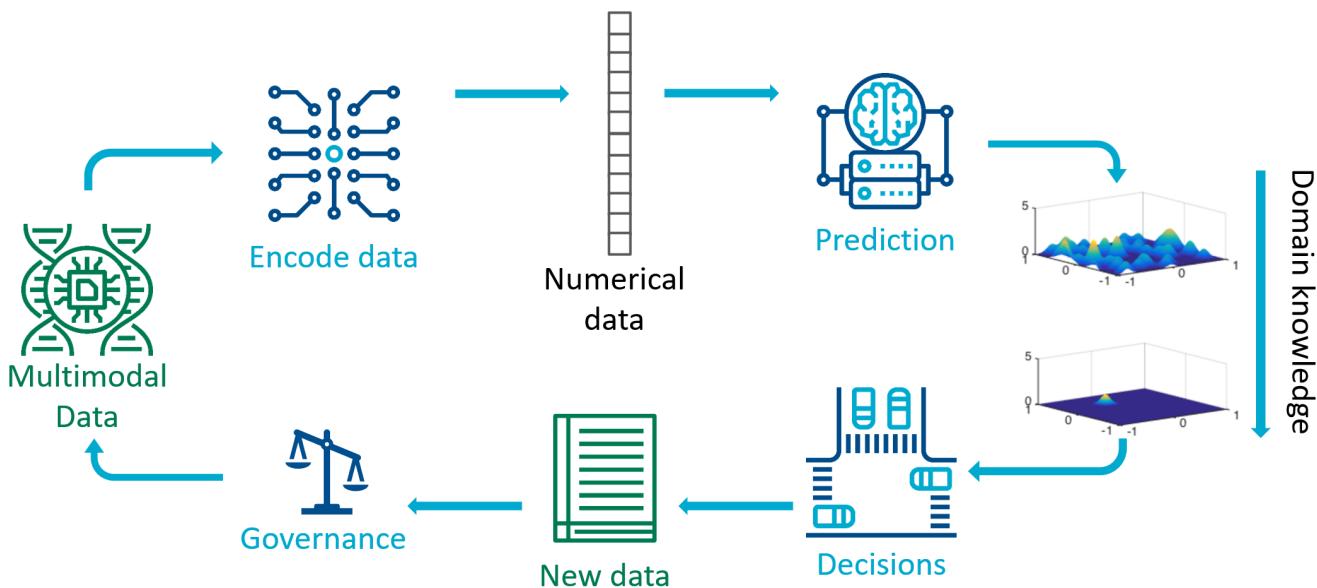


Figure 1: Machine Learning for Scientific Discovery

What is an experiment?

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- **Cross identification** Alger, M. J., Banfield, J. K., Ong, C. S., Rudnick, L., Wong, O. I., Wolf, C., Andernach, H., Norris, R. P., & Shabala, S. S.; Radio Galaxy Zoo: machine learning for radio source host galaxy cross-identification. MNRAS 2018
<https://academic.oup.com/mnras/article/478/4/5547/4999919>
- **Estimate uncertainty** Yong, Ong, Uncertainty quantification of the virial black hole mass with conformal prediction, MNRAS 2023.
<https://academic.oup.com/mnras/article/524/2/3116/7224601>
- **Train with physics simulations** Nguyen, Tang, Alger, Marchal, Muller, Ong, McClure-Griffiths; TPCNet: representation learning for HI mapping; MNRAS 2025
<https://academic.oup.com/mnras/article/536/1/962/7908519>
- **Photometric classification** Tran, Ong, Wolf, PeerJ Comp. Sci. 2018; Combining active learning suggestions
<https://peerj.com/articles/cs-157/>

How do we find them?

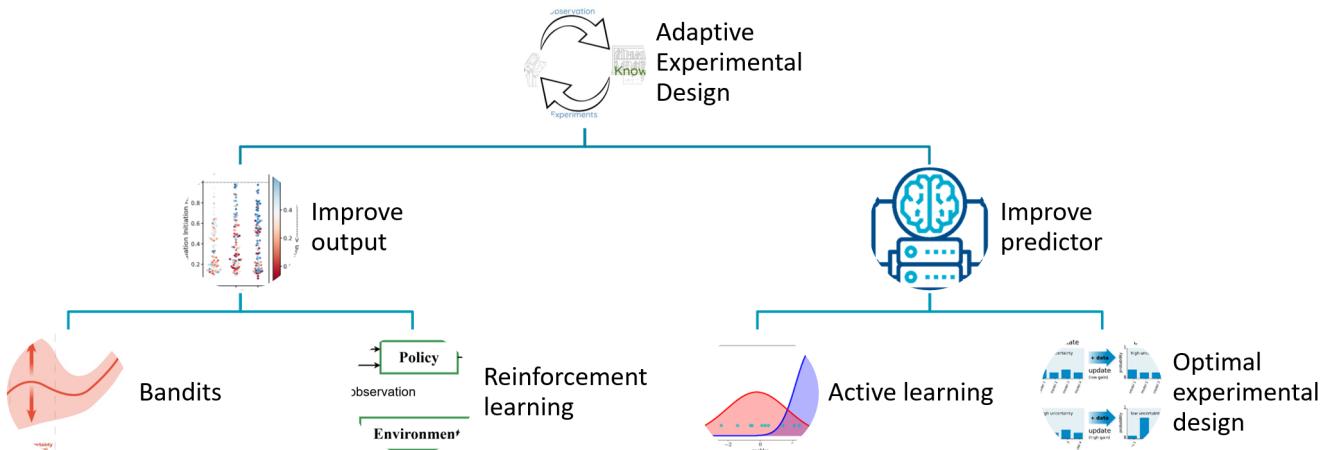


Figure 2: Adaptive experimental design

- **Layperson view** Adaptive experiments: Machine learning can help scientific discovery
<https://researchoutreach.org/articles/adaptive-experiments-machine-learning-help-scientific-discovery/>
- **Overview of learning cycle** Blau, Chades, Ong, Machine Learning for Biological Design, Synthetic Biology, 2024
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- **Ribosome binding site** Zhang, Holowko, Zumpe, Ong; Machine Learning Guided Batched Design of a Bacterial Ribosome Binding Site; ACS Syn Bio, 2022
<https://pubs.acs.org/doi/10.1021/acssynbio.2c00015>
- **Islands of Fitness, generative model** Steinberg, Oliveira, Ong, Bonilla; Variational Search Distributions, ICLR 2025
https://proceedings.iclr.cc/paper_files/paper/2025/hash/055fc19a3ce780b96cff15ffe738c1f1-Abstract-Conference.html
- **Multiobjective generative model** Steinberg, Wijesinghe, Oliveira, Koniusz, Ong, Bonilla; Amortized Active Generation of Pareto Sets, NeurIPS 2025
<https://neurips.cc/virtual/2025/poster/116473>

What does good mean?

- When accurate prediction models yield harmful self-fulfilling prophecies, Patterns, 2025
<https://doi.org/10.1016/j.patter.2025.101229>
- **ML and biology** Zhang, Ong; Opportunities and Challenges in Designing Genomic Sequences, 2021
https://mengyanz.github.io/files/wcb_main.pdf
- **ML and social science** Chades, McGrath, Bohensky, Carter, Coates, Harwood, Islam, Kandanaarachchi, Ong, Reeson, Stone-Jovicich, Paris, Scowell, Wissing, Douglas; Four Compelling Reasons to Urgently Integrate AI Development with Humanities, Social and Economic Sciences; IEEE Trans on Tech and Society, 2025
<https://ieeexplore.ieee.org/document/10960694/>
- **Need domain expertise** Hartman, Ong, Powles, Kuhnert; Position: We need responsible, application-driven (RAD) AI research, ICML 2025
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