Introduction

Introduction to Automated Science

SLAS 2024

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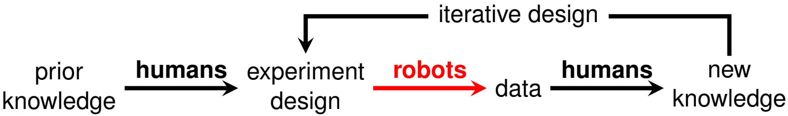
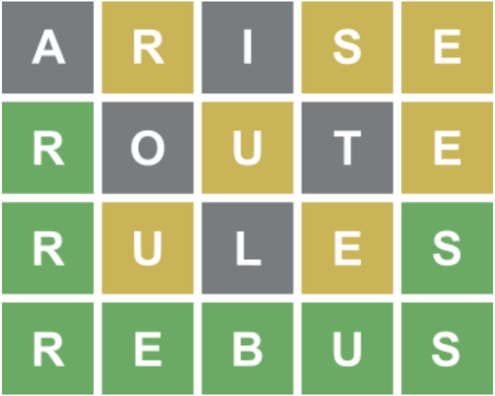
Automated Science can use **laboratory automation** to run the experiments it designs; however, we consider experiments designed by AI and executed by humans to be "automated science".

Laboratory Automation vs. Automated Science

Laboratory Automation vs. Automated Science



Why sequential experiments?



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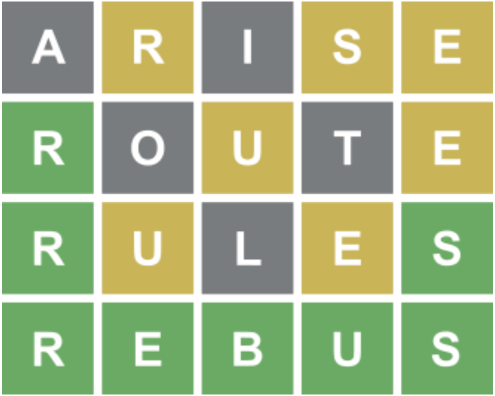
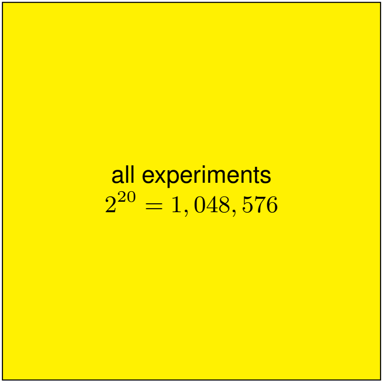


How many guesses would you need if all the guesses were checked in a single batch?

Why sequential experiments? Searching amino acid combinations

Before any experiments.



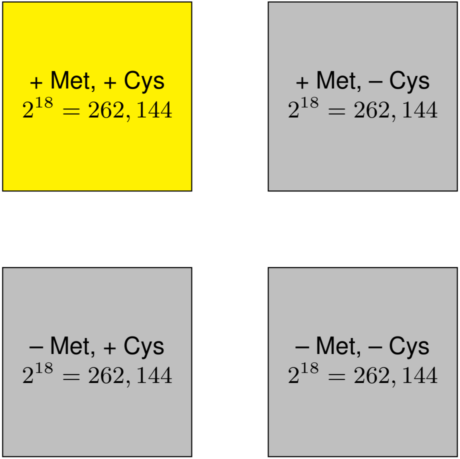
Why sequential experiments? Searching amino acid combinations

After learning Met is essential.

+ Met	– Met
$2^{19} = 524,288$	$2^{19} = 524,288$

Why sequential experiments? Searching amino acid combinations

After learning Met and Cys are essential.



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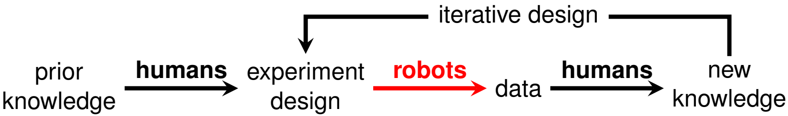

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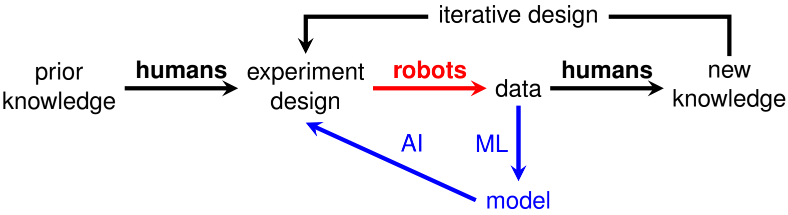

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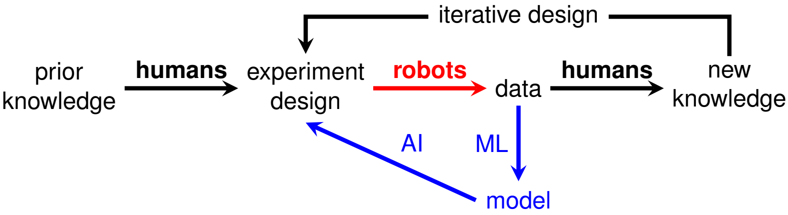
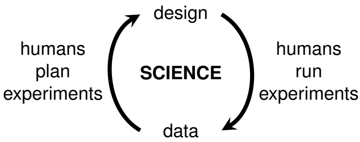


Designing experiments to improve a model
is easier than
designing experiments to create knowledge.

Automated Science does not require robots



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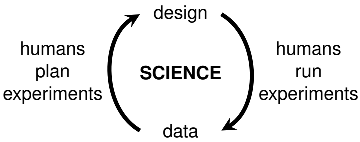

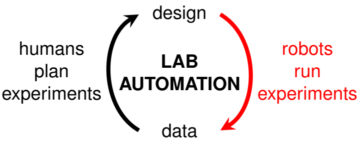

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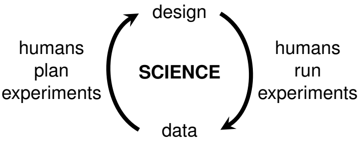

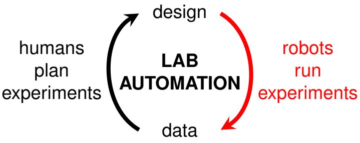

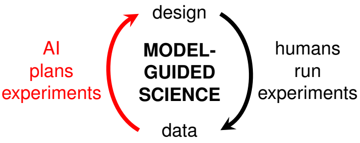

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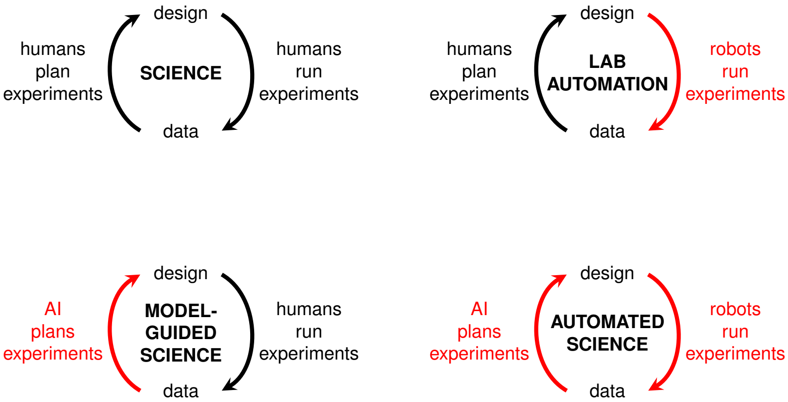

The language of Automated Science

AI agents design experiments by varying **factors**.

- **Discrete factors** belong to a fixed set of values (e.g. cell lines, reagent supplier, drug A or drug B).
- **Continuous factors** can take any value inside a range (e.g. concentration, time, temperature).

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cell line 1 + 0.1 μM drug A + 45 minute incubation

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- **replicated** to capture the variation in the experimental system (i.e. biological replicates).
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The **response** is a quantitative output of the systems that will be learned or optimized.

The goals of Automated Science

Automated Science can use either of two objectives.

- **Optimization** seeks the treatment with the maximum (or minimum) response.
- **Characterization** seeks the most informative treatments for learning the response.

We'll see later that optimization and characterization are related by the *exploration/exploitation tradeoff*.

Optimization ("engineering")

Optimization seeks a treatment that maximizes, minimizes, or moves the response closest to a goal.

Optimization can be *constrained* or *unconstrained*.

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Examples

- Find enzymes expression levels in a pathway that maximize lipid titers in a fermenter.
- Find reactions conditions that maximize yield of a chemical synthesis.
- Find drug combinations that return phosphorylation to normal levels.
- Find gene deletions that minimize production of a byproduct *while maintaining a threshold level of primary production.*

Characterization (“science”)

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Complete characterization learns both the main effects of the factors and their interactions. The complexity of the interactions depends on both the model and the experiments.

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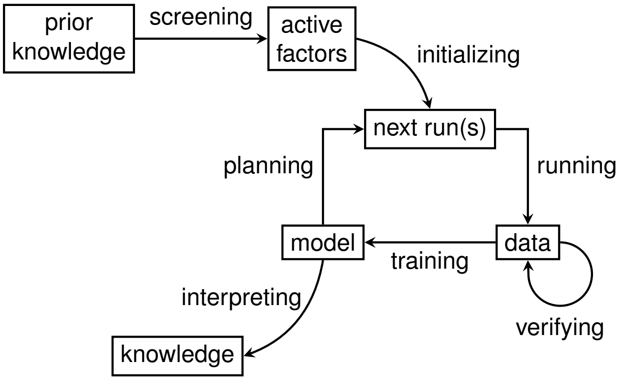
Examples

- Learn how media factors affect expression of a target gene.
- Learn how reagent concentrations affect absorbance of a nanocrystal.
- Learn how drug combinations affect protein phosphorylation.

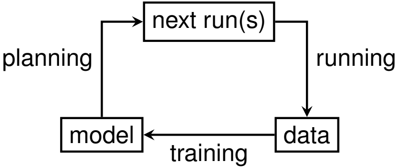
The Automated Science Cycle



Case Studies

Outline

This course focuses on the core of the Automated Science cycle:



We will discuss

- Planning experiments with a trained model.
- Selecting an appropriate Bayesian model.
- Challenges when performing AI-planned experiments.

The course emphasizes your role as an *integrator* between modelers, automation engineers, and scientists.