intellegens

Applied machine learning

Introducing Intellegens

August 2024

About Us

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CSO

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Machine learning scientist

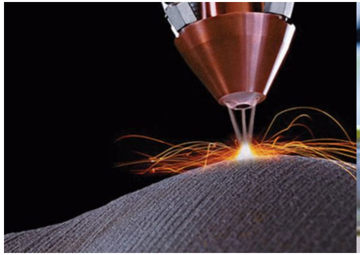
Agenda

10:00	Introductions
10:10	Machine learning, adaptive DOE, and Alchemite™
11:15	Break
11:30	Interactive demo
12.30	Lunch
Afternoon	Meetings about individual data sets

Introducing Intellegens

- Innovative method extracts value from sparse, noisy data to solve complex, high-dimensional problems
- Strong focus on ease-of-deployment for immediate ROI
- Key use cases: Chemicals, Materials, Life Sciences, Manufacturing Processes, Food & Beverage

UNIVERSITY OF CAMBRIDGE





Experimental design accelerated by machine learning

Data
Ingredients
Processes
Properties

Train

Machine learning model

Inform: find outliers, relationships, fill gaps

Get deep insights

Predict outcomes for new scenarios

Optimise system parameters for targets

Design better products and processes

Guide experiment: *what to test next?*

Do fewer experiments

Experiments

Customers, collaborations, and partnerships

Selected case study examples

Integration partners

Other selected customers

Fast-moving consumer goods corporation

Biotech

Plastics, paints & coatings maker

Global petrochemicals producers

Construction chemicals provider

Battery manufacturer

Major food & beverages corporation

Plant-based foods innovator

Leading steelmaker

Advanced materials organisation

Mining and cement company

Additive manufacturing specialist

intellegens

Applied machine learning

Training Slides

Machine Learning Enhanced Adaptive Experimental Design

Introduction to Machine Learning, Adaptive Design of Experiments, and Alchemite™

Training Agenda

In this session, we'll be discussing:

- An overview of typical R&D business challenges.
- A traditional and adaptive R&D workflow.
- A discussion on how machine learning can enhance adaptive experimental design to expedite product development, with relevant case studies.

Typical R&D Challenges

Typical R&D Business Challenges

"We have to innovate, fast, to beat the competition"

"Experimental programs cost $millions and take years"

"We must meet net zero targets *and* grow market share"

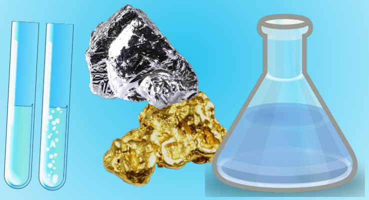
"Price, supply, and regulatory issues are very disruptive"

"We lose vital knowledge when people retire"

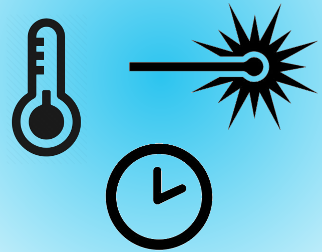
How to address these challenges while solving everyday R&D problems?

The trillion $ R&D problem

Ingredients



Processes



Properties

- → Mechanical properties
- → Cost
- → Viscosity
- → Density
- → Environmental impact
- → Stability...

For chemicals, alloys, pharmaceuticals, plastics, foods, paints, cosmetics… ***(worth $trillions!)***

- High dimensional problem space
- Sparse, noisy data
- Costly, time-consuming experimental programs

How is R&D typically performed?

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Try every possible experiment

Guaranteed to find the best result

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- May be infinitely many possibilities
- Budgets / timescales are finite

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Ask an expert

Uses knowledge from past projects

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Uses knowledge from past projects

- Expensive resource
- Limited time available

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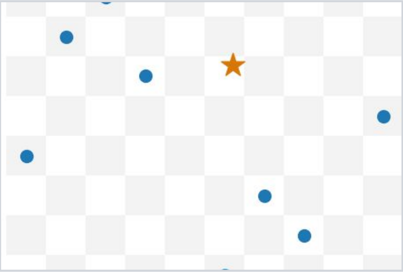

Structured design / DoE

Efficiently covers design space

How is R&D typically performed?

Try every possible experiment

Guaranteed to find the best result

- May be infinitely many possibilities
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Ask an expert

Uses knowledge from past projects

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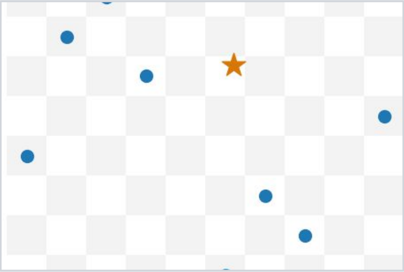


Structured design / DoE

Efficiently covers design space

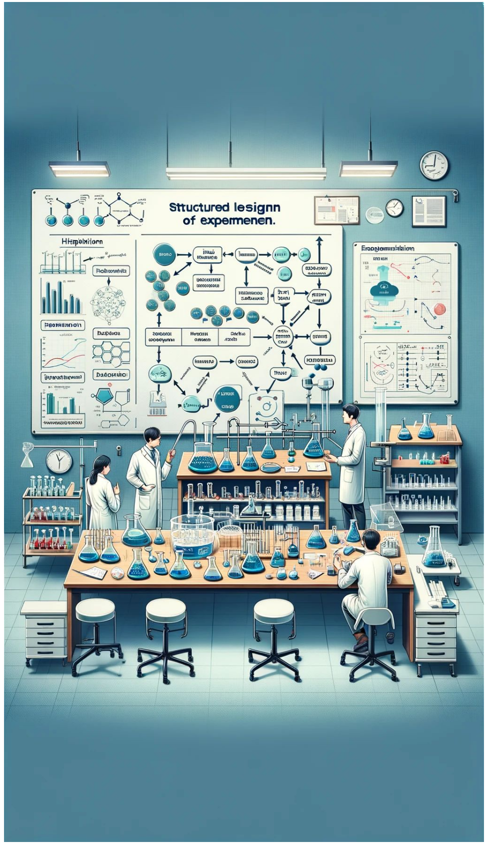
- May require a large number of experiments
- Requires statistical knowledge

Section 1 Questions

What is Structured Design of Experiments?

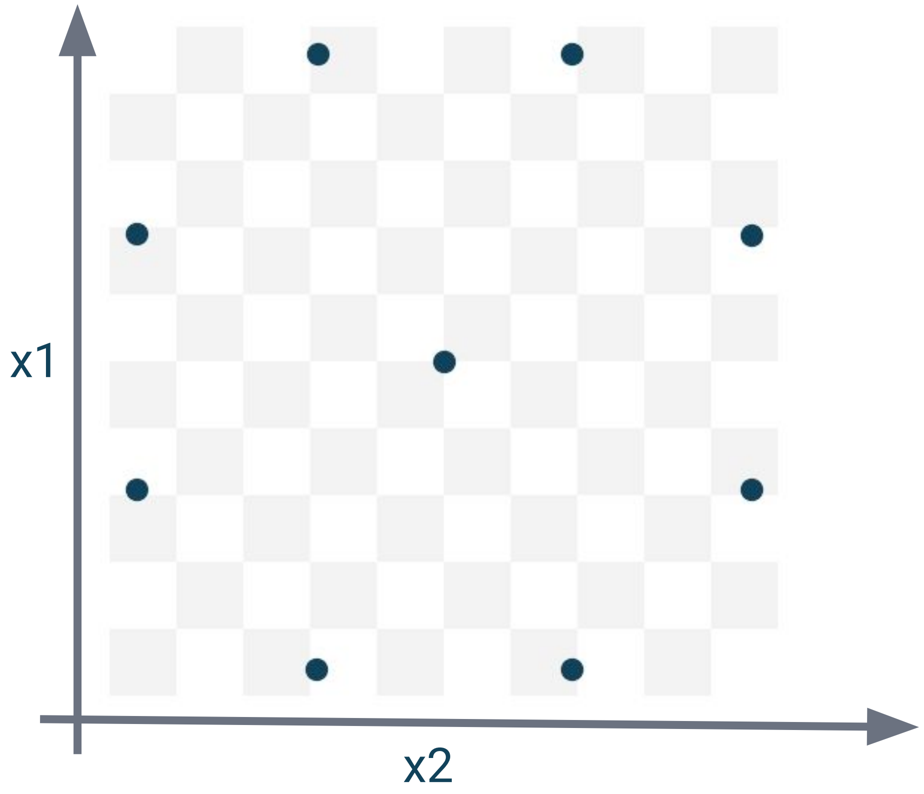
Structured Design of Experiments

- Structured DOE aims to cover design space as efficiently as possible
- Variety of structured designs available for different types of problem
- Requires advanced statistical knowledge to understand which design to use and interpret results



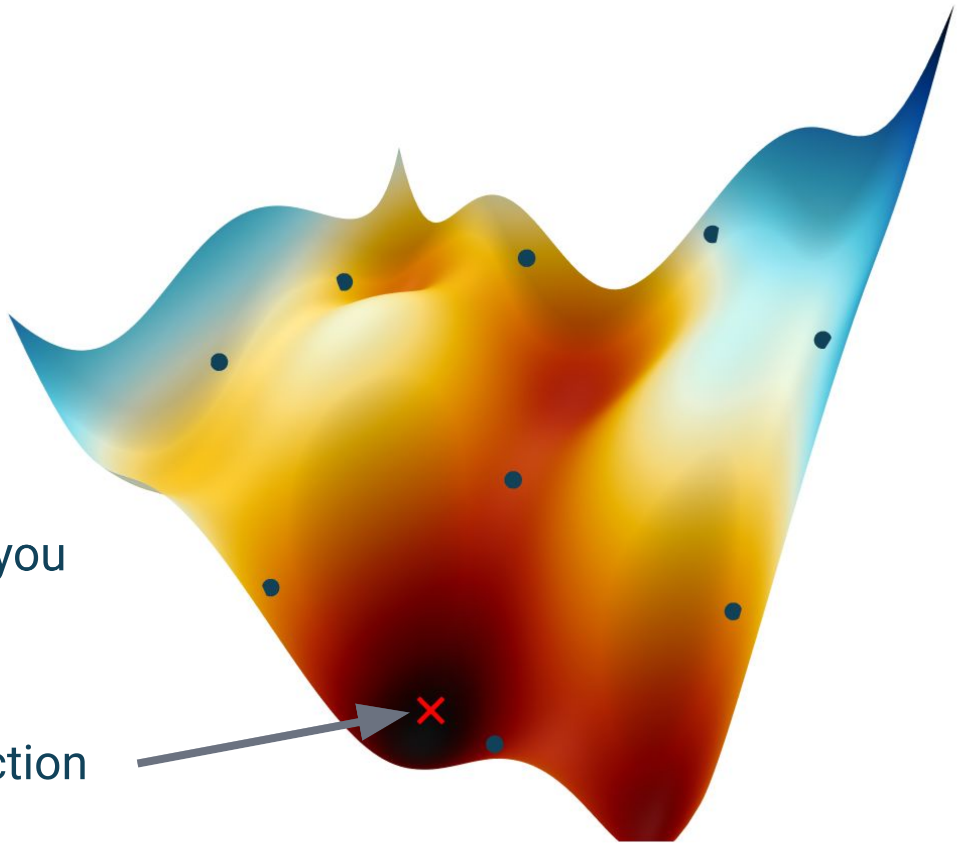
Example Design: Central Composite Design (CCD)

- Used for detecting second order effects (e.g. x1 * x2)
- Effective for modelling quadratic relationships
- Helps understand the curvature of the surface
- Assumes no strong nonlinearity in the response variable



Structured Design of Experiments

- But real science is rarely limited to second-order effects
- With structured DoE, you are stuck with what the design tells you
- If that does not achieve your goals you often need to start again



Minimum of the function

What is Adaptive Experimental Design?

What is adaptive experimental design?

Start with a Plan

- Scientists begin with an initial experimental design.

Adapt Based on Results

- Adjust the plan as new data is collected.
- Increases efficiency and saves time and resources.

No Computers Needed

- Simply review the data during the process.
- Modify the experimental plan as new information emerges.

Adaptive Experimental Design

Adaptive Experimental Design

It's good practice to format data into a structured format with rows for experiments and columns for inputs and outputs.

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1			

Adaptive Experimental Design

Let’s say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1			

Adaptive Experimental Design - Round 1

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	

Try a formula

Adaptive Experimental Design - Round 1

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149

Measure property

Adaptive Experimental Design - Round 1

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149

Met requirements?

Adaptive Experimental Design - Round 1

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149

Met requirements?

Adaptive Experimental Design - Round 2

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	

Try a new formula

Adaptive Experimental Design - Round 2

Let’s say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	170

Measure property

Adaptive Experimental Design - Round 2

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	170

Met requirements?

Adaptive Experimental Design - Round 2

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	170

Met requirements?

Adaptive Experimental Design - Round 3

Let’s say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	170
Experiment 3	98.1	0.42	

Adaptive Experimental Design - Round 3

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
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Experiment 3	98.1	0.42	179

Adaptive Experimental Design - Round 3

Let's say we want a Yield of **> 185**

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Let's say we want a Yield of **> 185**

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Experiment 4	98.4	0.55	

Adaptive Experimental Design - Round 4

Let's say we want a Yield of **> 185**

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	Chemical 1	Chemical 2	Yield
Experiment 1	99.1	0.27	149
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Experiment 4	98.4	0.55	186

Adaptive Experimental Design - Round 4

Let's say we want a Yield of **> 185**

	INPUTS		PROPERTIES
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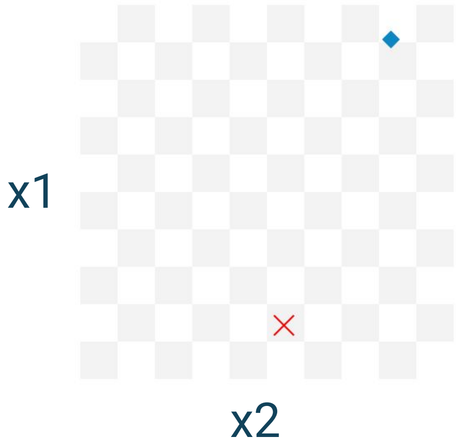
Experiment 1	99.1	0.27	149
Experiment 2	98.6	0.35	170
Experiment 3	98.1	0.42	179
Experiment 4	98.4	0.55	**186**

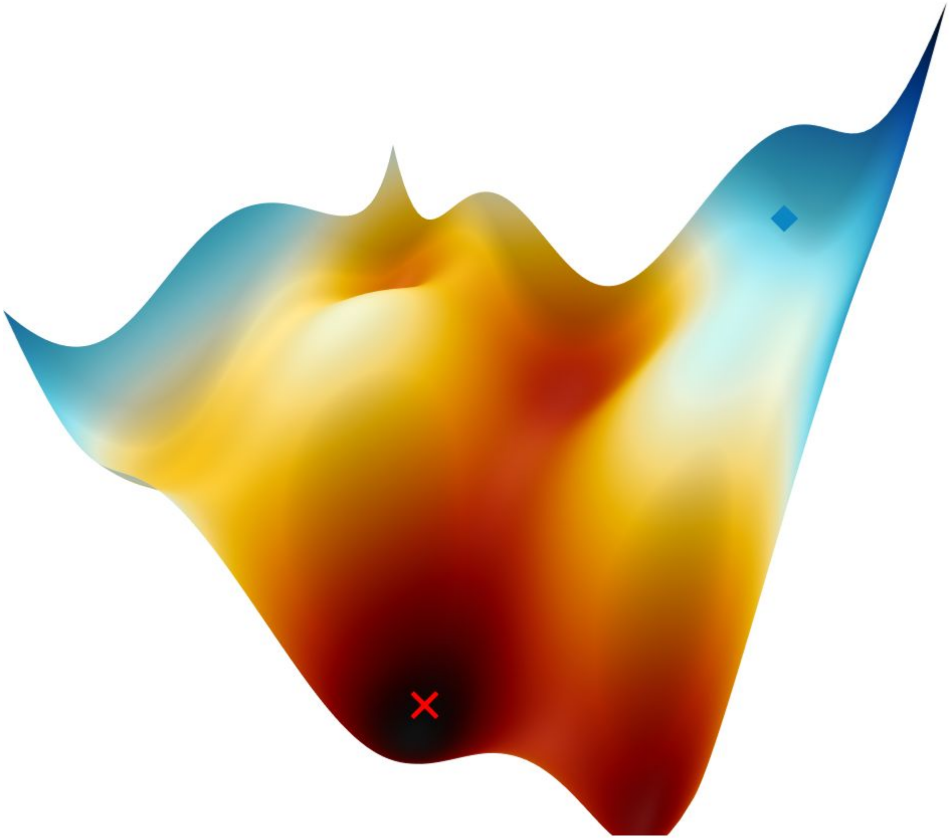
SUCCESS!

Now visualised

Adaptive Experimental Design - Round 1

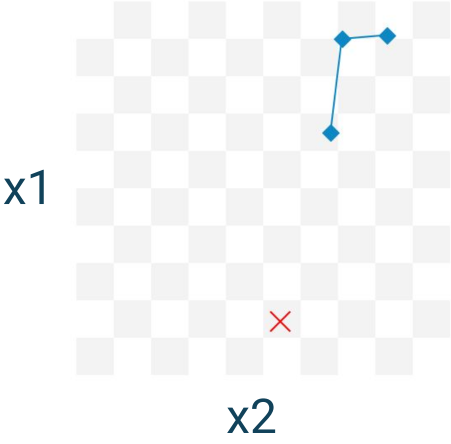
- Adaptive experimental design uses existing data to guide the best route to the goal

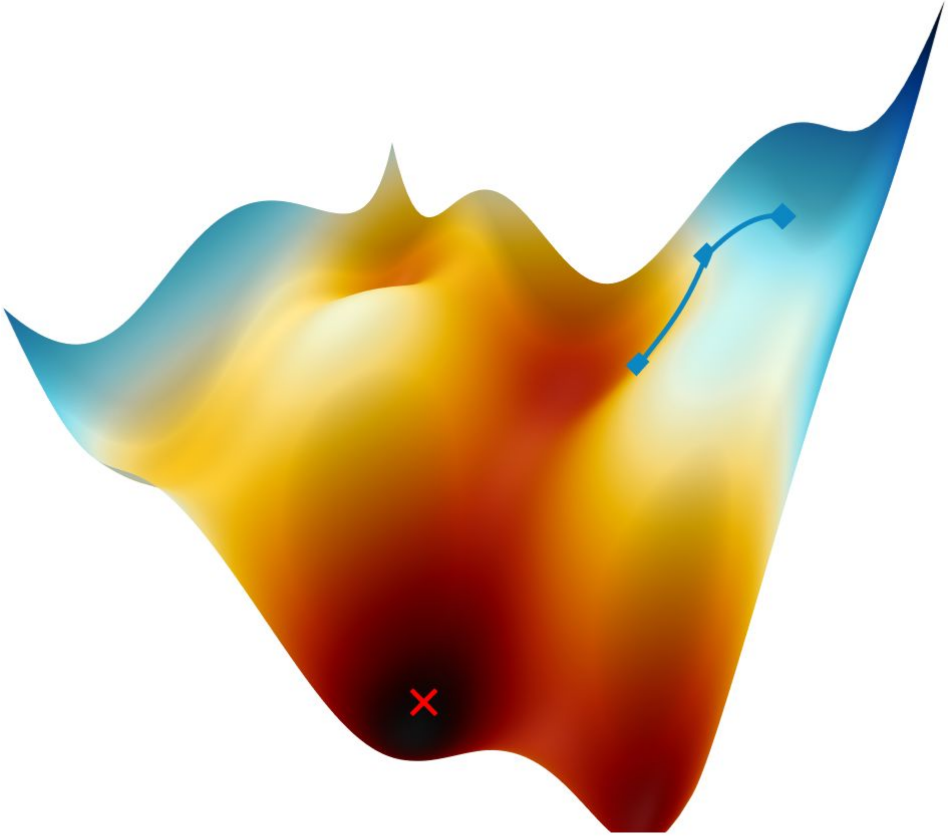




Adaptive Experimental Design - Round 2

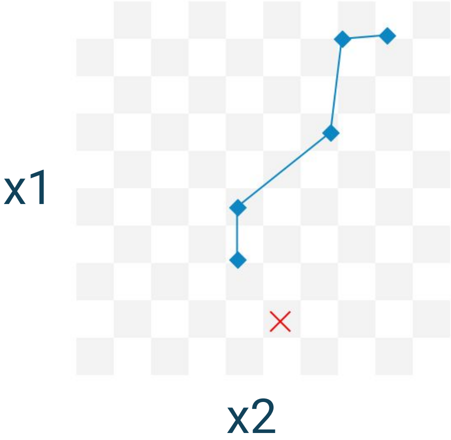
- Adaptive experimental design uses existing data to guide the best route to the goal

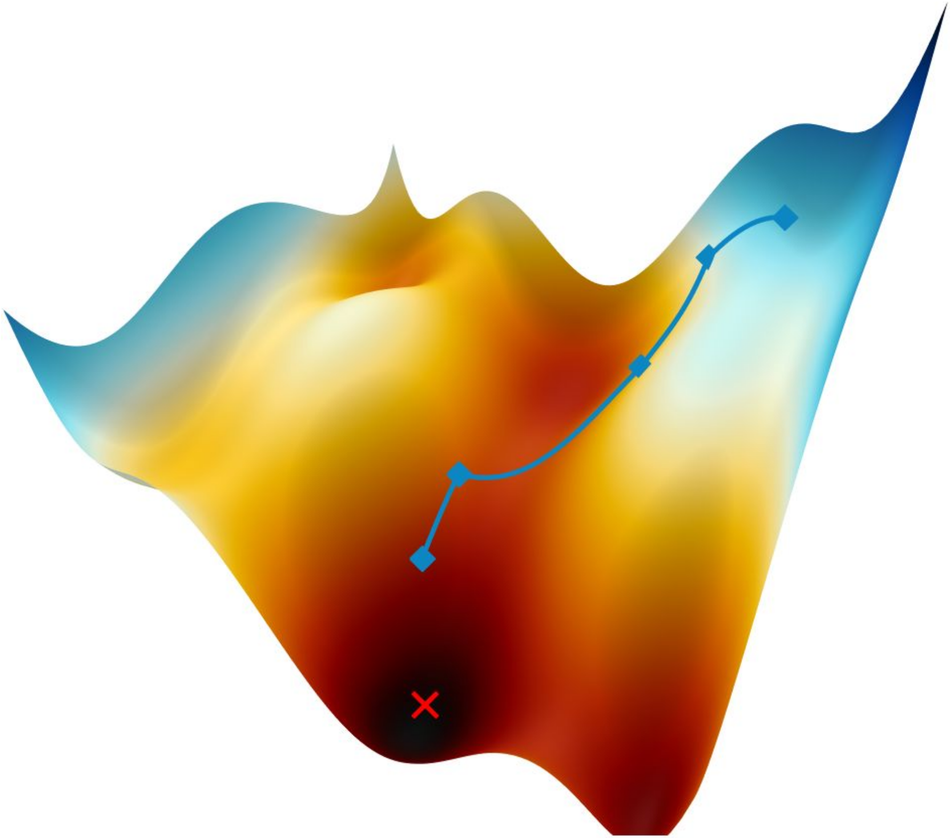




Adaptive Experimental Design- Round 3

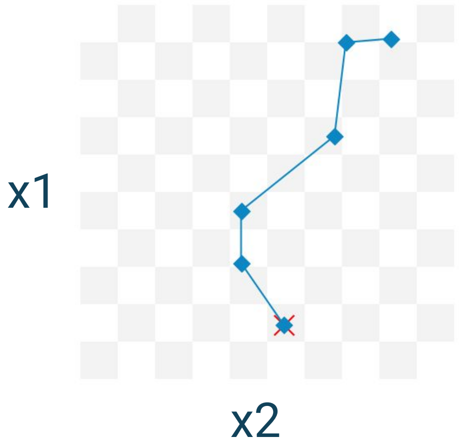
- Adaptive experimental design uses existing data to guide the best route to the goal

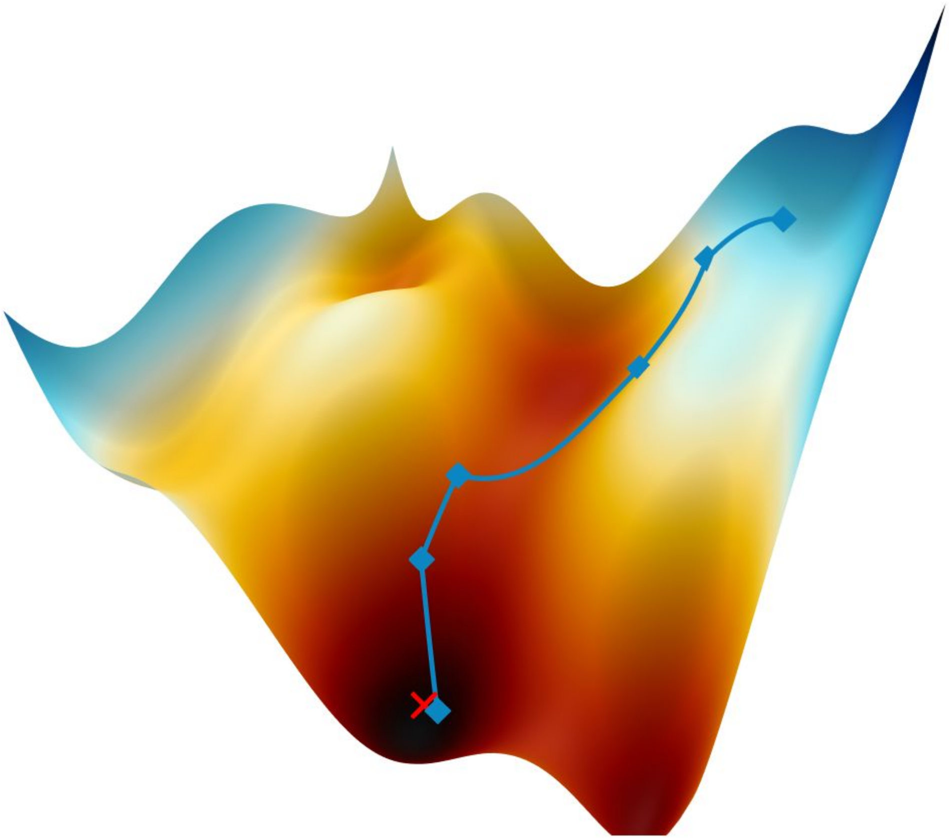




Adaptive Experimental Design - Round 4

- Adaptive experimental design uses existing data to guide the best route to the goal





Sounds easy so what's the catch?

How data actually is in R&D

How data actually is in R&D

INPUTS

COMPOSITION			PROCESS
Iron	Carbon	Mn	Temp (C)

How data actually is in R&D

INPUTS

OUTPUTS

COMPOSITION			PROCESS	PROPERTIES		
Iron	Carbon	Mn	Temp (C)	TS	YS	HBW

How data actually is in R&D

	INPUTS				OUTPUTS		
	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149

How data actually is in R&D

	INPUTS				OUTPUTS		
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	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149
Experiment 2	98.6		0.9			80	170

How data actually is in R&D

Tens of properties

Thousands of materials

	INPUTS				OUTPUTS		
	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149
Experiment 2	98.6		0.9			80	170
Experiment 3		0.42		1100			179
Experiment 4	98.4	0.55	0.8		118	70	

How data actually is in R&D

This noisy, sparse, and high dimensional data is challenging for scientists to understand

Tens of properties

Thousands of materials

	INPUTS				OUTPUTS		
	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149
Experiment 2	98.6		0.9			80	170
Experiment 3		0.42		1100			179
Experiment 4	98.4	0.55	0.8		118	70	

Problems with Classical Adaptive Experimental Design

Complex Inputs

- Problems often involve a lot more than a couple of input variables.

Multiple Targets

- Aim to optimize one output without compromising others.

Data Issues

- Data is often complicated, noisy, sparse, and high-dimensional.

Section 2 Questions

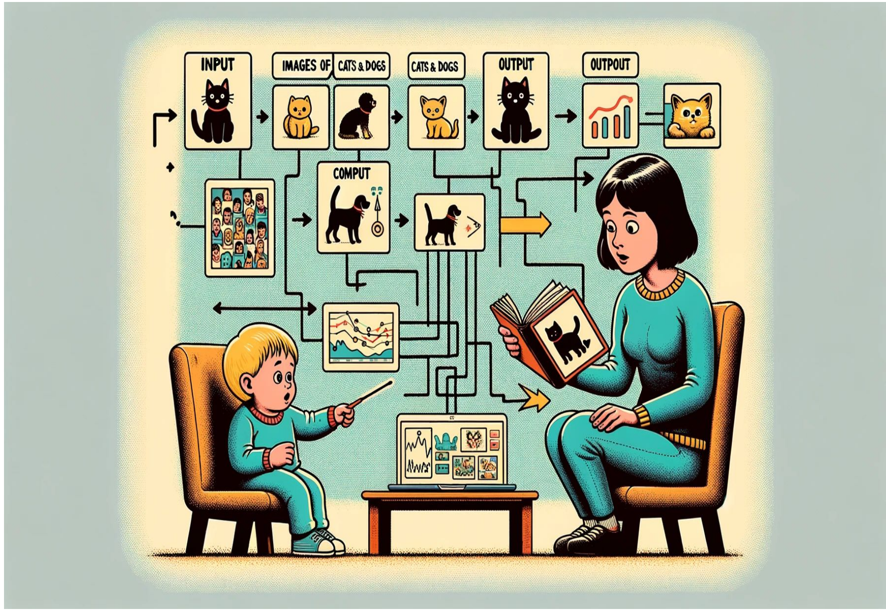
How can Machine Learning Help?

Introduction to Machine Learning

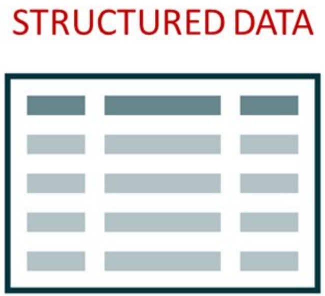
Definition: Machine Learning (ML) is a branch of AI where computers learn from data to make predictions or decisions.

Core Idea: ML algorithms identify patterns in data and make decisions with minimal human input.

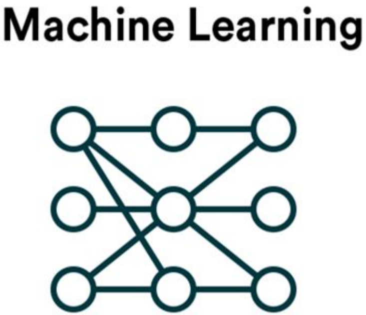
Applications: Used in image and speech recognition, recommendations, autonomous vehicles, etc.



Machine Learning - A Primer



Inputs + Outputs

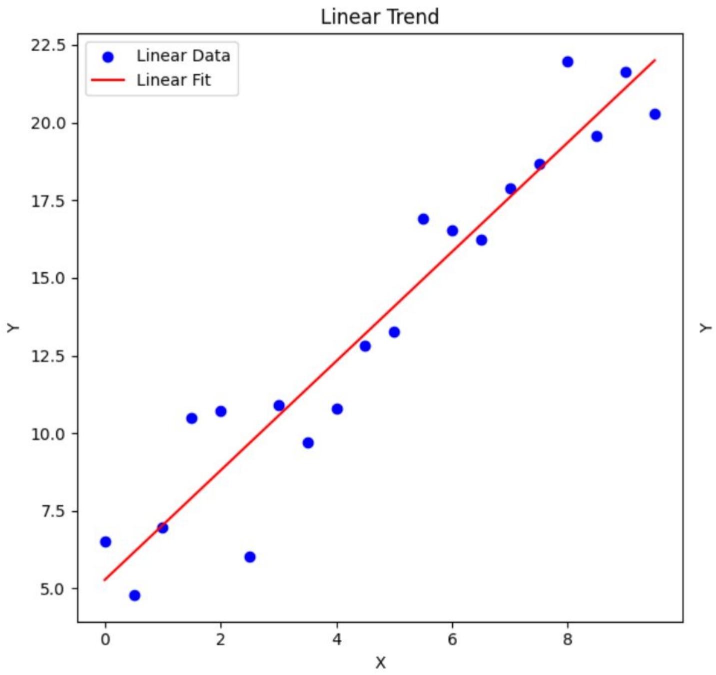


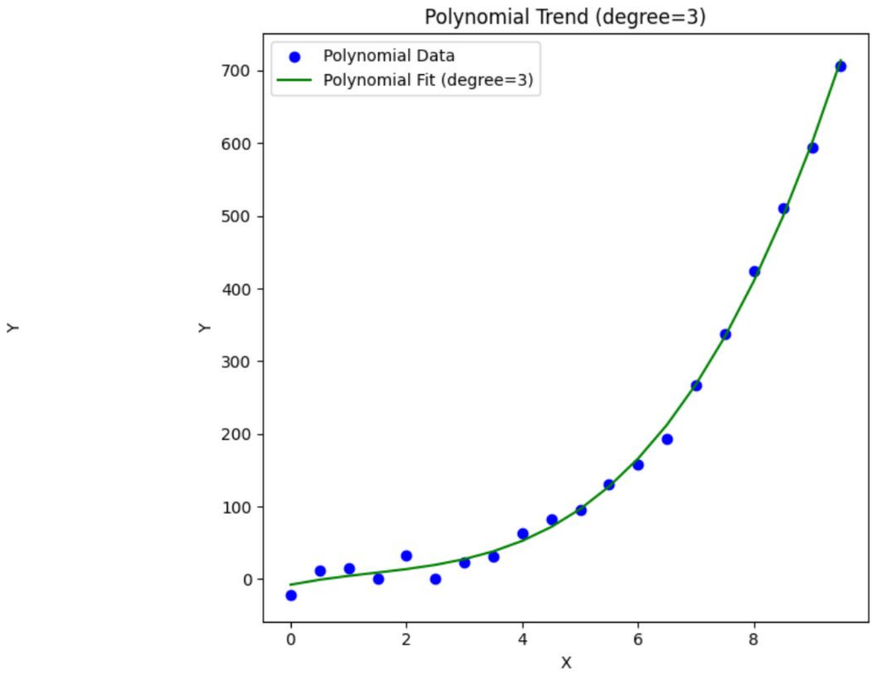
Machine learning allows us to automatically create a ‘model’ to learn relationships between your inputs and outputs.

Extract **insights**
Make **predictions**

Simple Machine Learning Examples

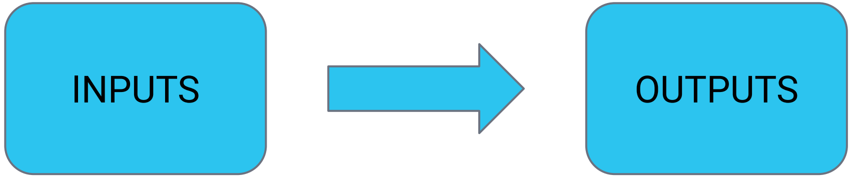
We all use machine learning everyday without necessarily knowing. For instance:





Quadratic Equation

We can apply machine learning to determine the best values for a, b, and c to predict y most accurately across all training examples.



$$ax^2 + bx + c = y$$

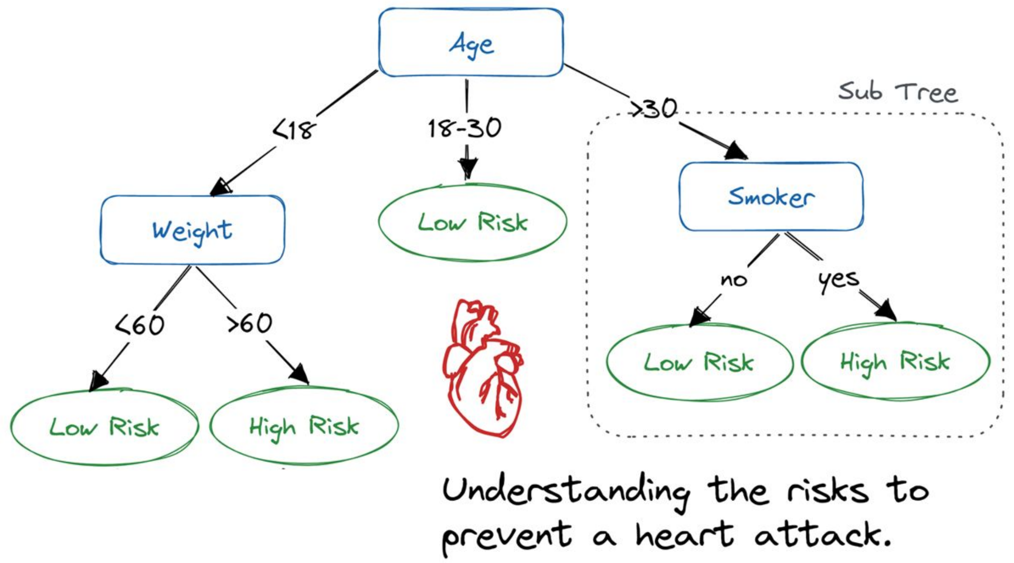
However, such a simple equation may struggle to capture complex relationships.

More Complicated Machine Learning Example

Decisions trees allow us to model nonlinear relationships with many variables.

Relating age, weight, and smoker etc. (**inputs**) -> *to the risk of heart attack* (**output**).

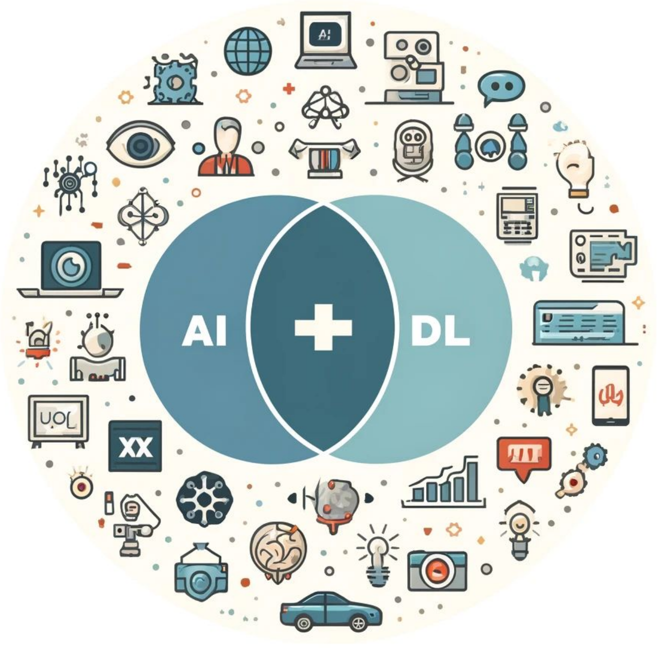
These models can capture more complicated relationships.



The Steps to Train and Deploy a Machine Learning Model

Steps:

- **Data Collection:** Gathering data.
- **Preprocessing:** Cleaning and preparing data.
- **Model Selection:** Choosing the right algorithm
- **Training:** Teaching the model with data.
- **Evaluation:** Testing the model's accuracy.
- **Deployment:** Using the model for predictions.



How can machine learning enhance adaptive experimental design?

How machine learning can help in R&D

How machine learning can help in R&D

Collect an initial dataset to train a preliminary machine learning model.

How machine learning can help in R&D

Collect an initial dataset to train a preliminary machine learning model.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149
Experiment 2	98.6		0.9			80	170
Experiment 3		0.42		1100			179
Experiment 4	98.4	0.55	0.8		118	70	

How machine learning can help in R&D

With the initial model we can make predictions and fill in missing values.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76	**64±2**	149
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Experiment 3	**98.8±0.8**	0.42	**0.7±0.1**	1100	**91±9**	**77±3**	179
Experiment 4	98.4	0.55	0.8	**980±38**	118	70	**241±6**

How machine learning can help in R&D

We can apply constraints to our inputs to refine our design space and set requirements for outputs.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76	**64±2**	149
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Experiment 4	98.4	0.55	0.8	**980±38**	118	70	**241±6**
Requirement		0.2-0.5			>115		>230

How machine learning can help in R&D

Using the constraints and targets, the model makes a suggestion for a new experiment.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76	**64±2**	149
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Experiment 4	98.4	0.55	0.8	**980±38**	118	70	**241±6**
Suggestion	98.7	0.45	0.8	1010			

How machine learning can help in R&D

The model predicts the performance of this virtual formulation.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
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Suggestion	98.7	0.45	0.8	1010	105±4	81±3	230±10

How machine learning can help in R&D

We measure the real composition, processing, and properties.

Tens of properties

Thousands of materials

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Experiment 5	98.7	0.45	0.8	1010	110	**81±3**	238

How machine learning can help in R&D

We check our requirements.

Tens of properties

Thousands of materials

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How machine learning can help in R&D

Is HBW > 230?

Tens of properties

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	COMPOSITION			PROCESS	PROPERTIES		
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Experiment 1	99.1	0.27	0.6	842	76	**64±2**	149
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Experiment 3	**98.8±0.8**	0.42	**0.7±0.1**	1100	**91±9**	**77±3**	179
Experiment 4	98.4	0.55	0.8	**980±38**	118	70	**241±6**
Experiment 5	98.7	0.45	0.8	1010	110	81±3	238

How machine learning can help in R&D

Is TS > 115?

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76	**64±2**	149
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How machine learning can help in R&D

If goals aren't achieved, we can use this new data to update the model, and then repeat the process.

Tens of properties

Thousands of materials

	COMPOSITION			PROCESS	PROPERTIES		
	Iron	Carbon	Mn	Temp (C)	TS	YS	HBW
Experiment 1	99.1	0.27	0.6	842	76		149
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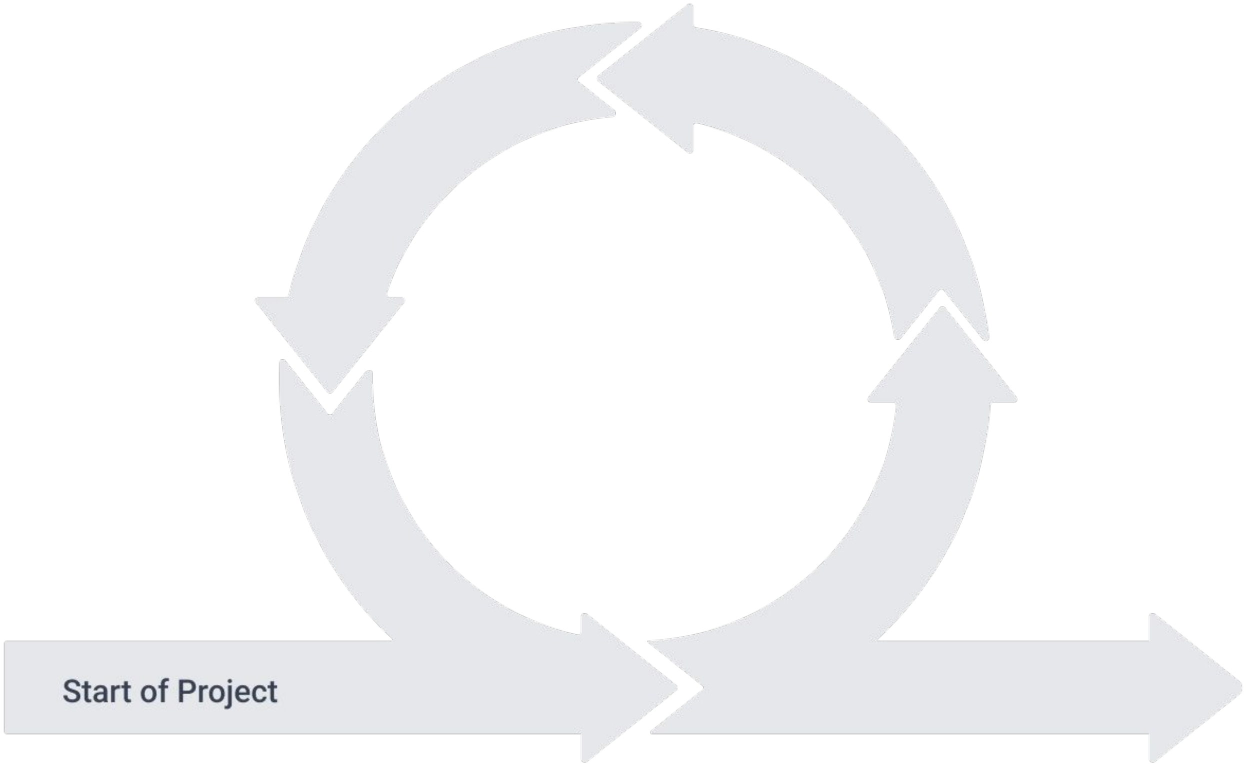
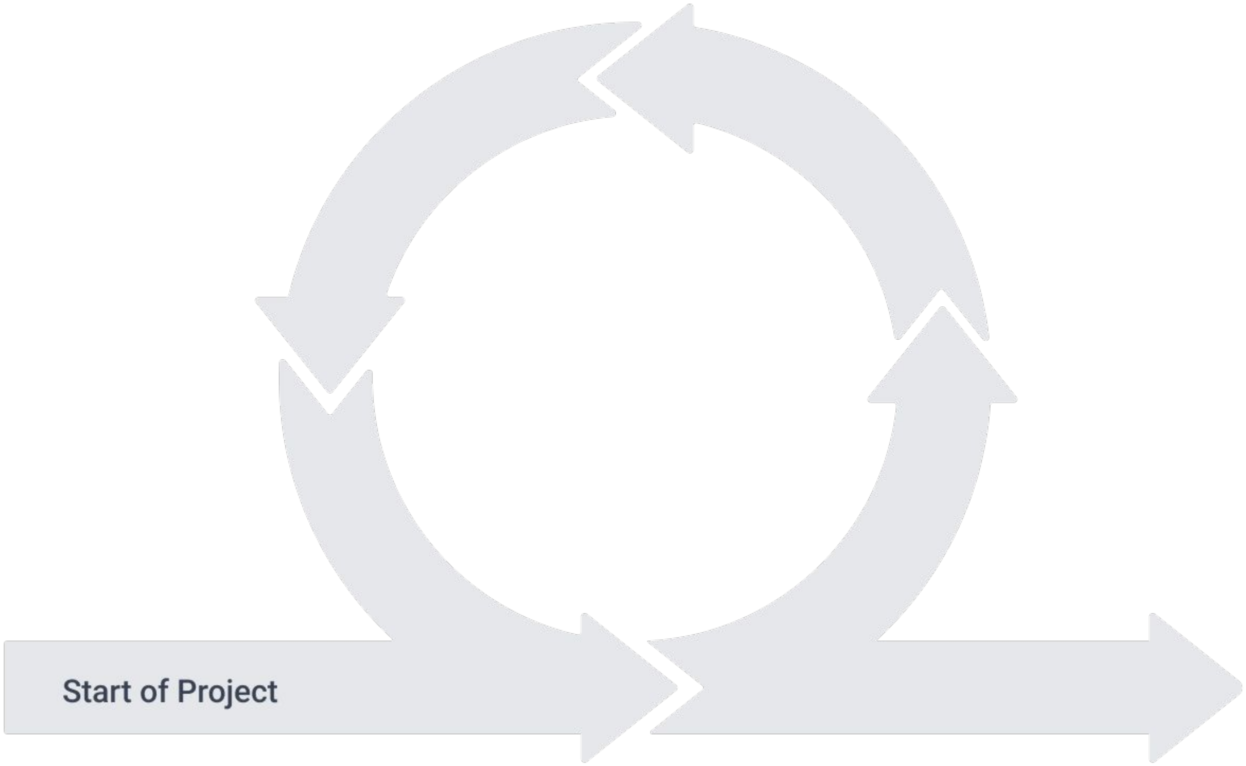
Experiment 5	98.7	0.45	0.8	1010	110		238

Now visualised

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

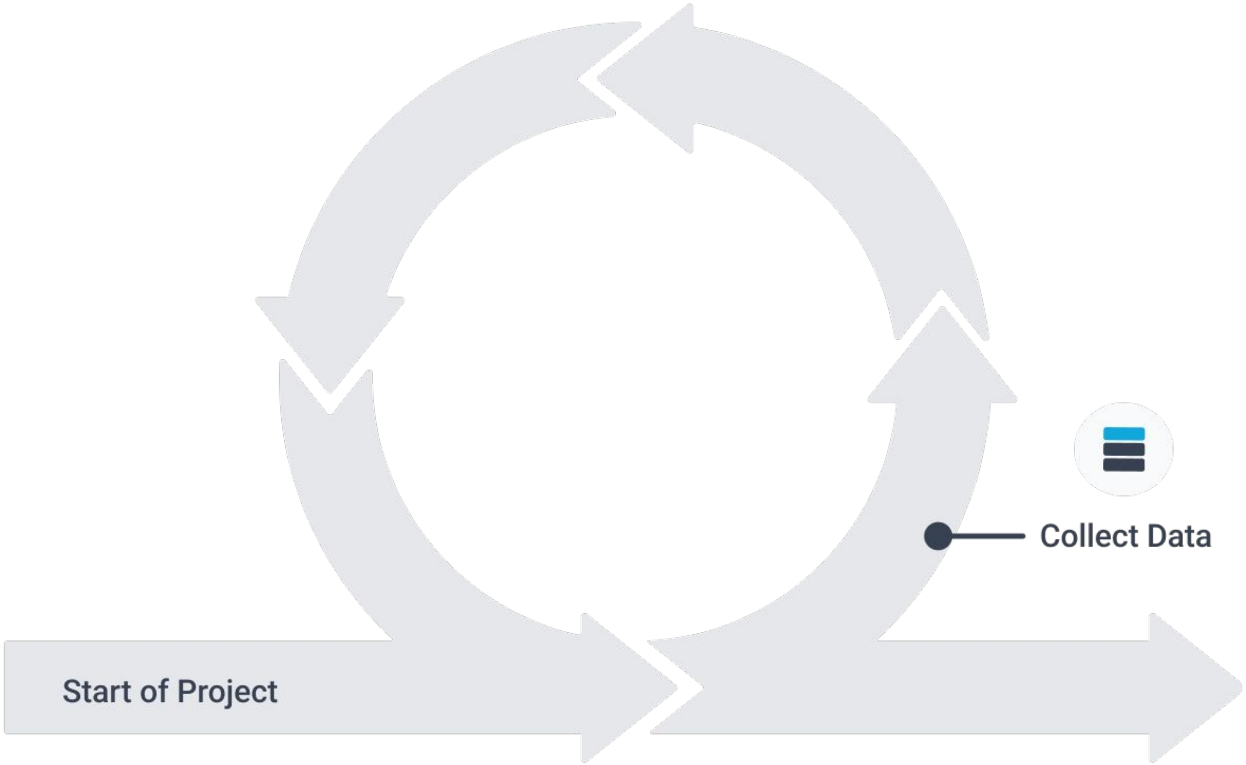


Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

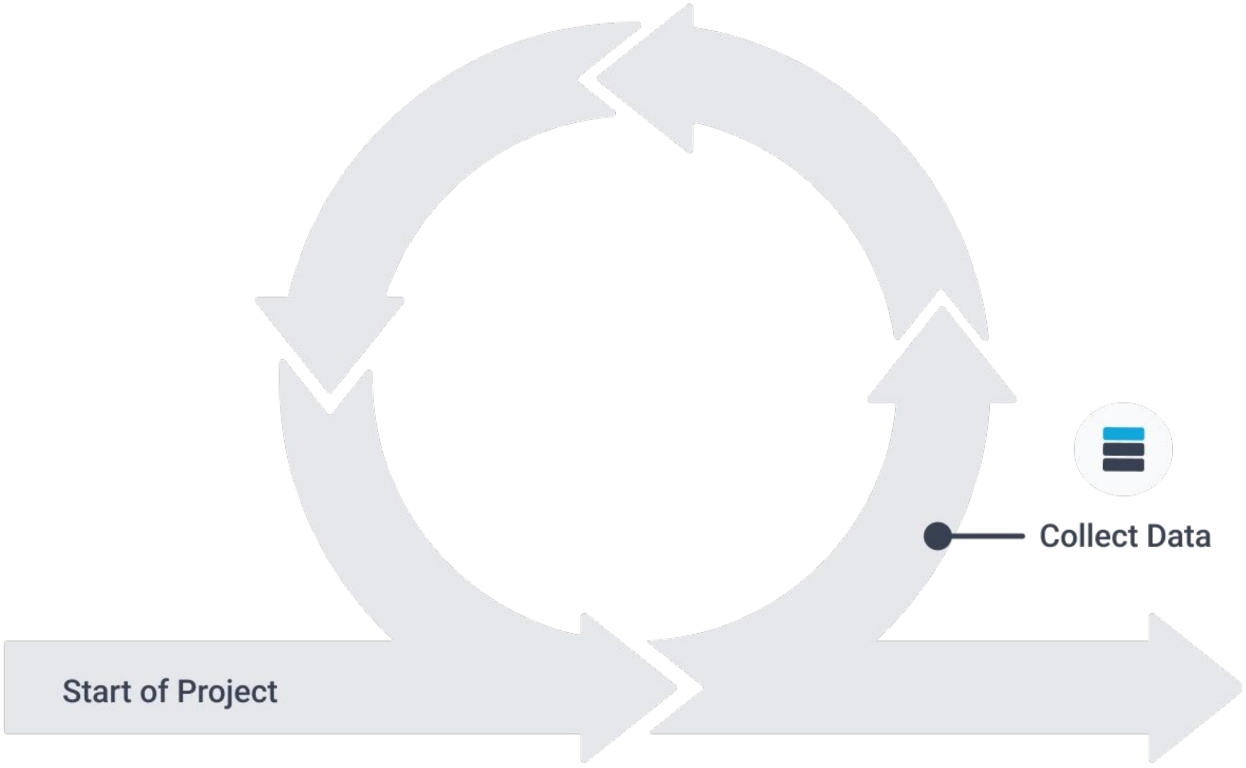


Set Requirements

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

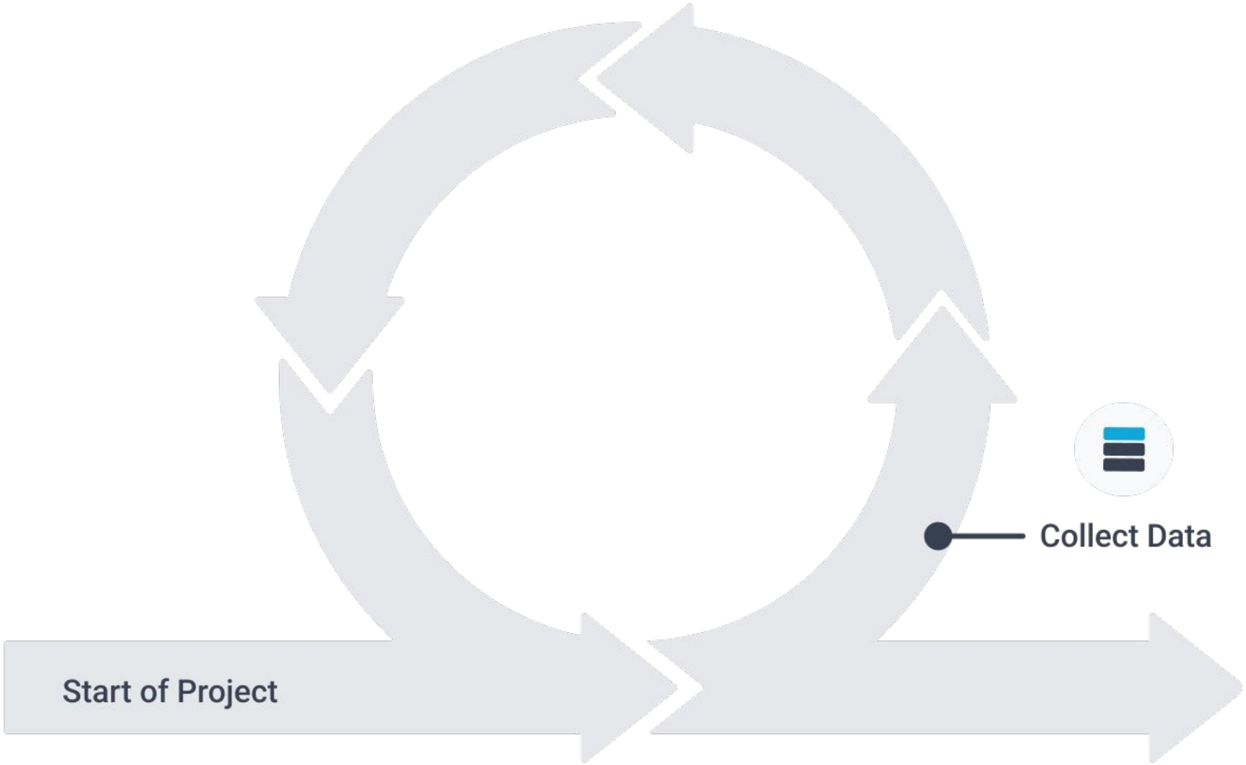


Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

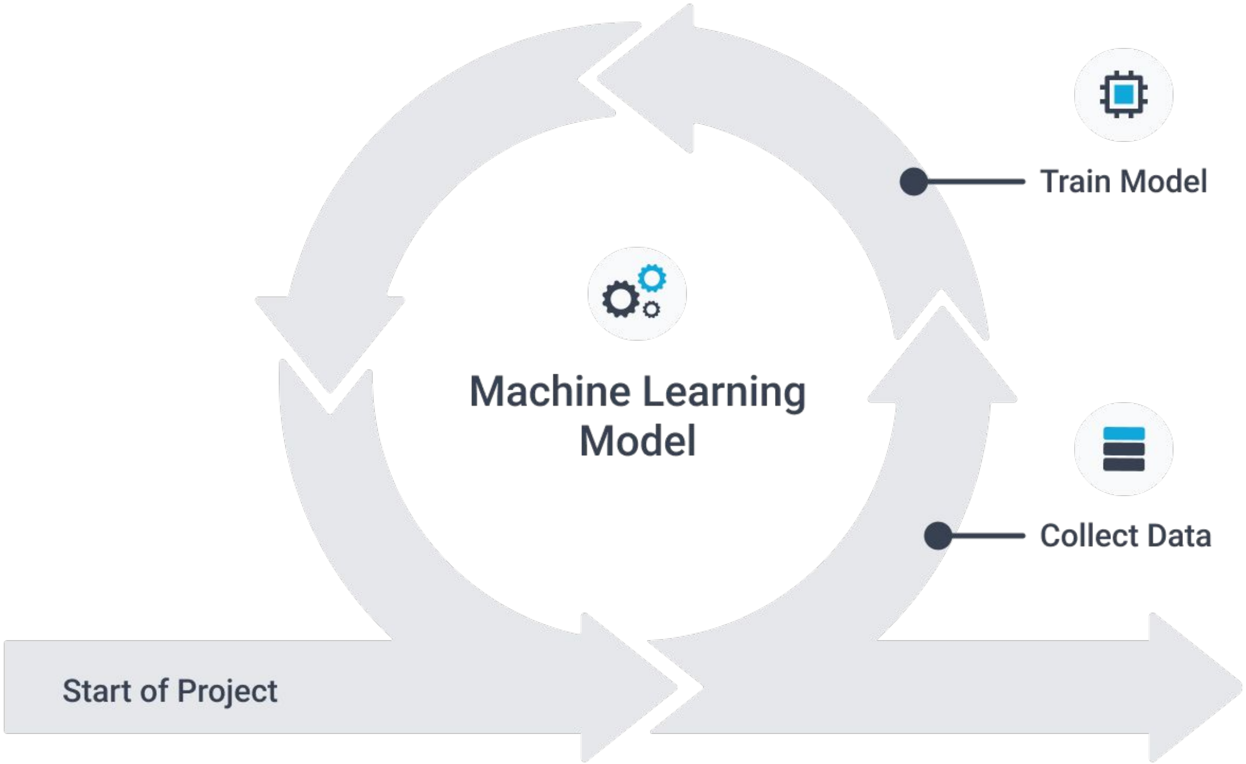


Start from zero
or use
historical data

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

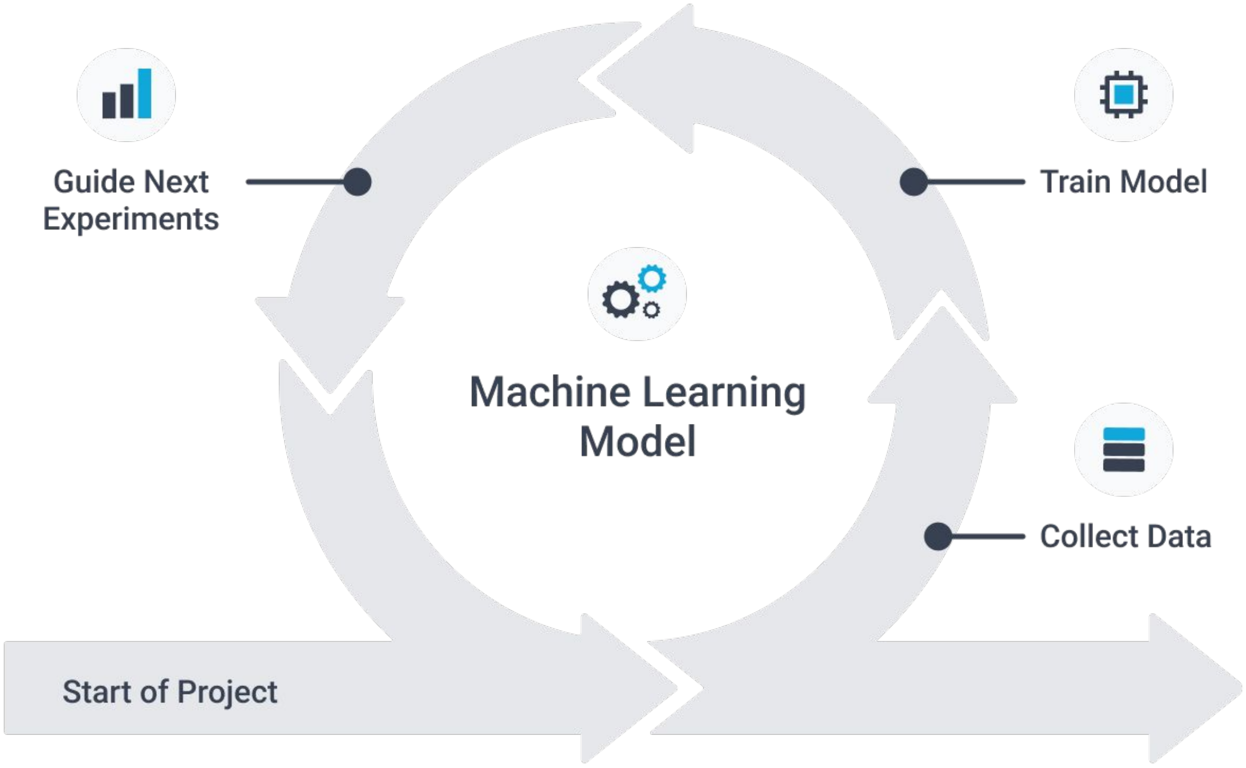


Machine Learning Enhanced Adaptive Experimental Design (ML-AED)



Given your data, learn how to predict outputs using inputs (train a model)

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)



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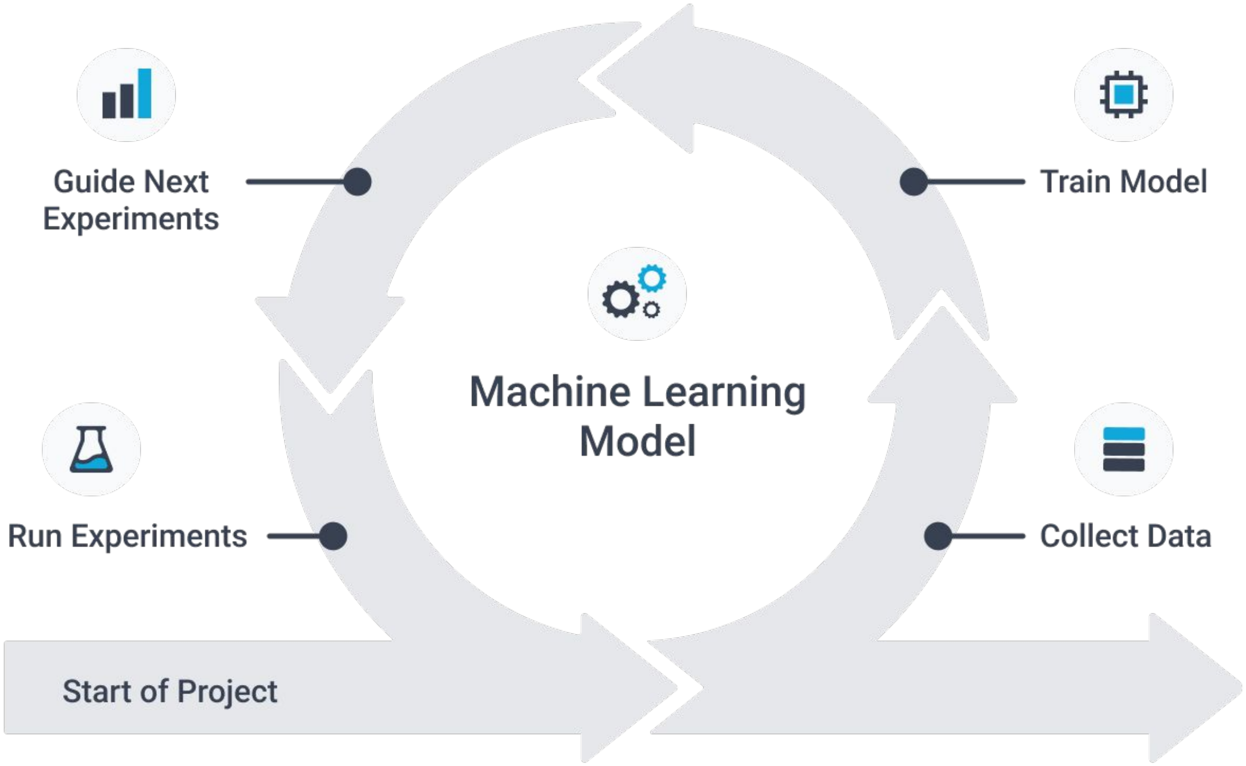

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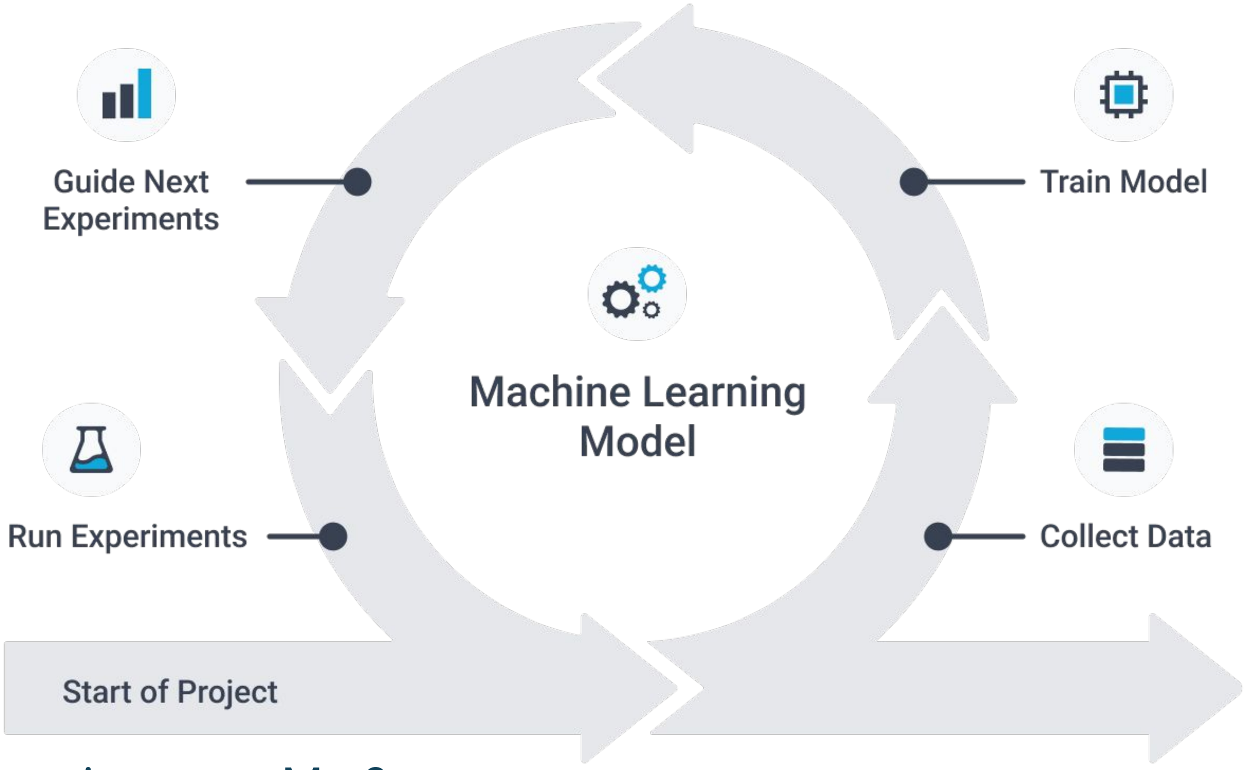
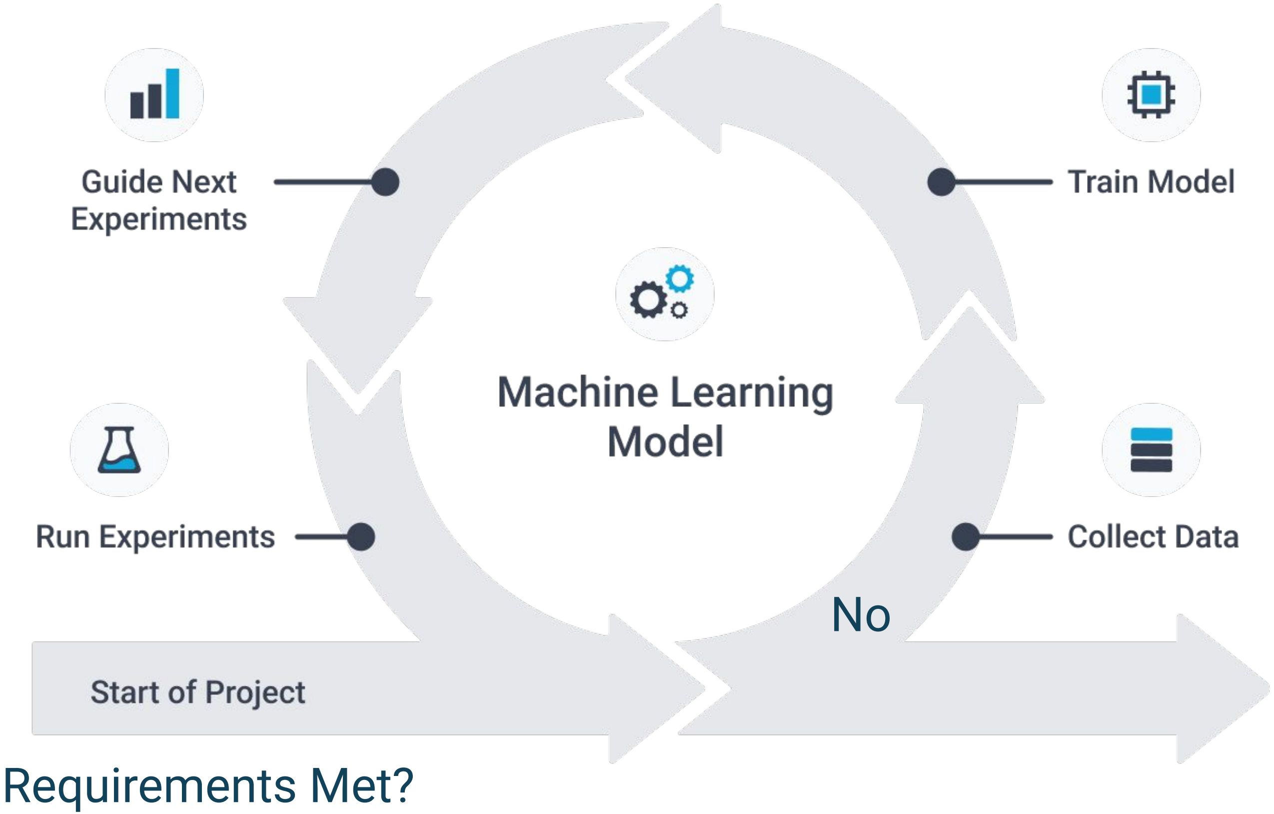


Requirements Met?

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)



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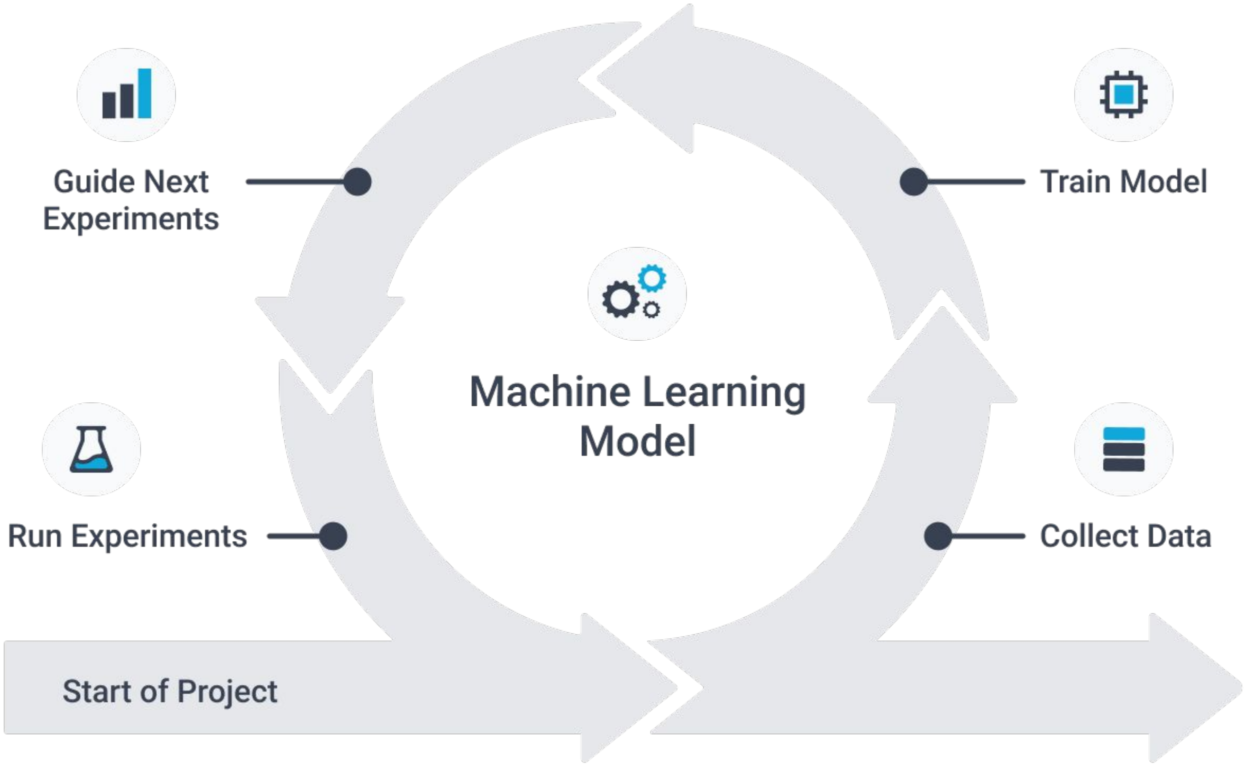
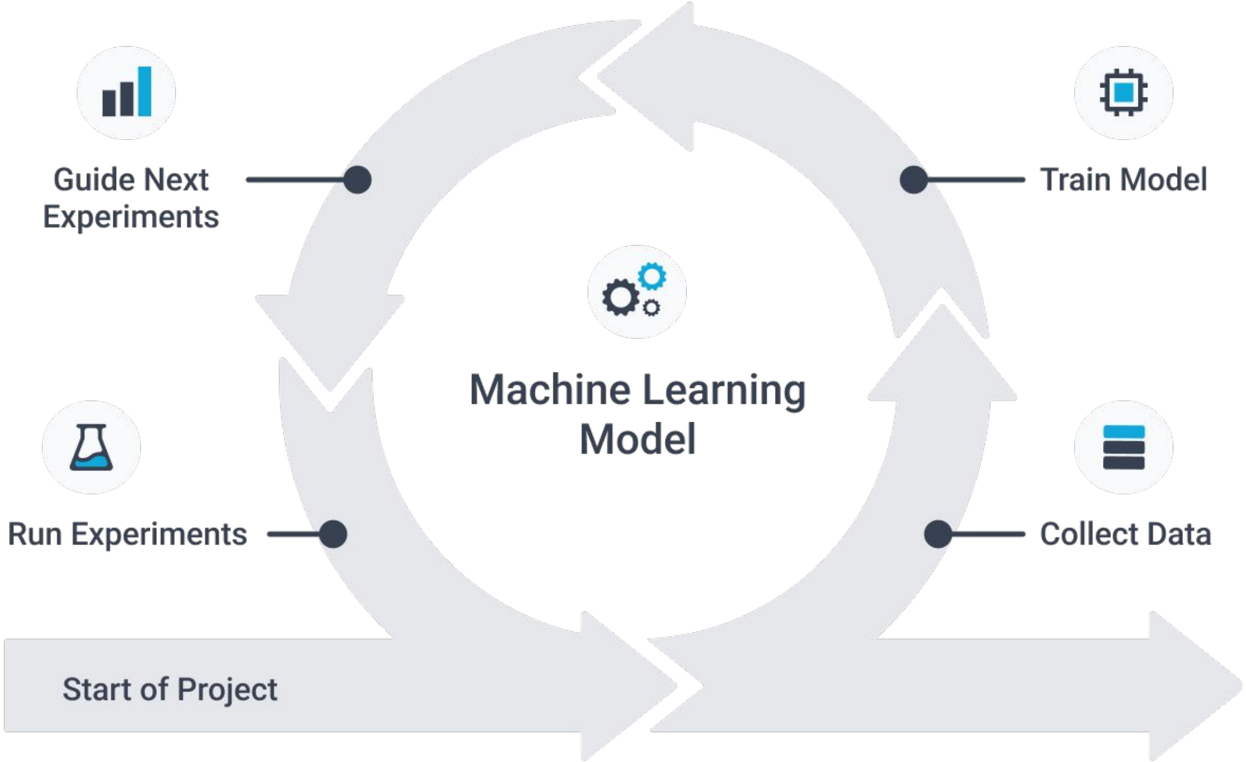
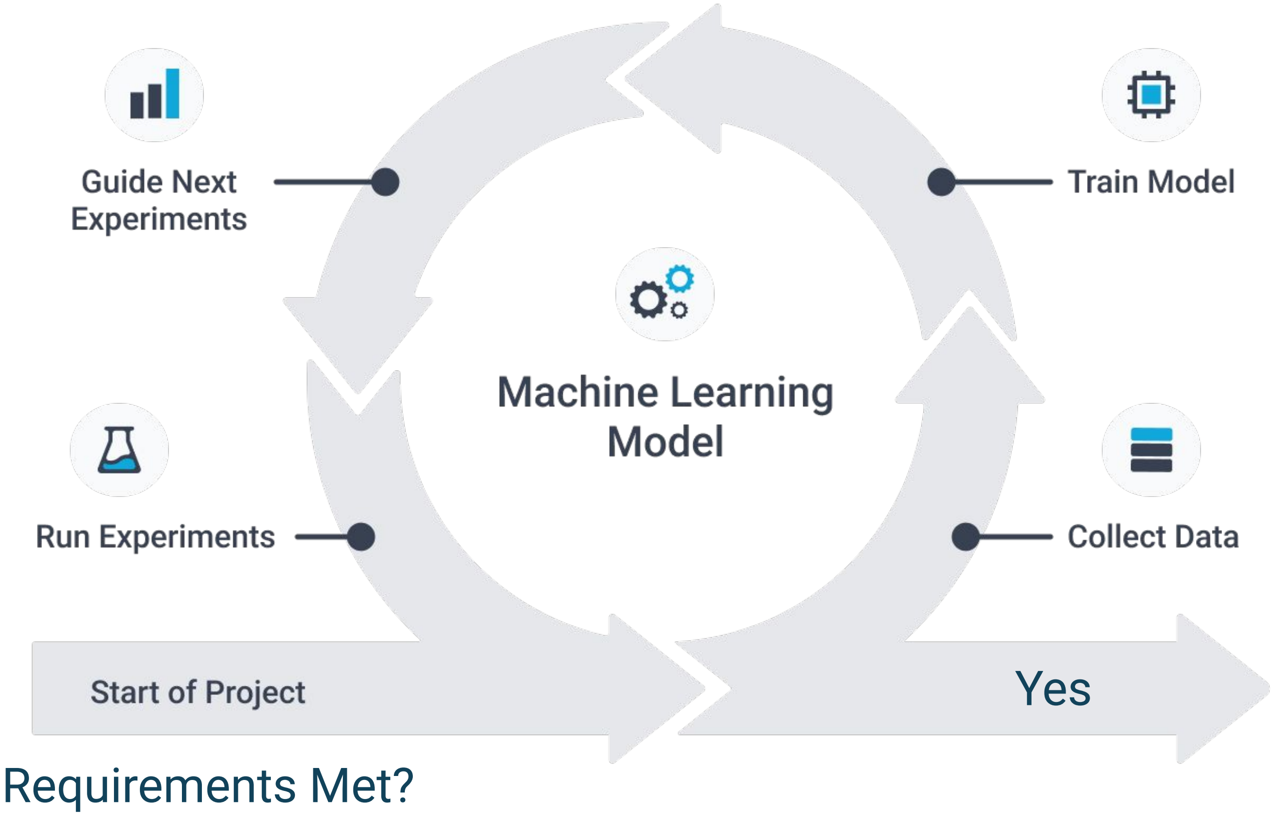


Machine Learning Enhanced Adaptive Experimental Design (ML-AED)

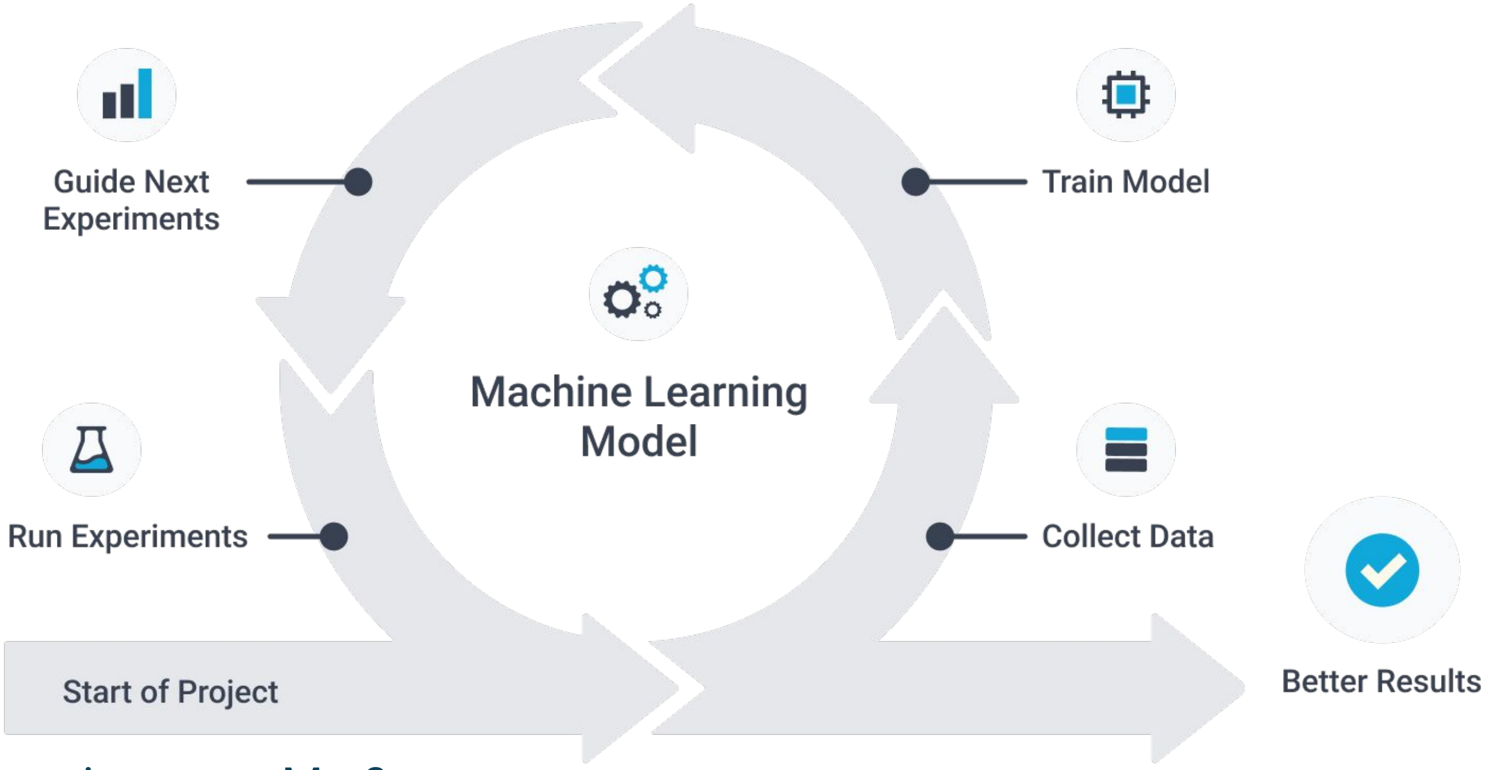


Requirements Met?

Machine Learning Enhanced Adaptive Experimental Design (ML-AED)



Machine Learning Enhanced Adaptive Experimental Design (ML-AED)



Requirements Met?

Why Machine Learning is Ideal for R&D

Learns Nonlinear Relationships: Understands complex patterns in data.

Handles High-Dimensional Data: Efficiently processes large and complex datasets.

Robust to Noise and Missing Data: Maintains performance despite data imperfections.

Suggests New Experiments: Recommends new experimental points to optimize outcomes.

Continuously Improves: Adapts and enhances models with new data.

Section 3 Questions

Why Alchemite™?

Why is there not greater adoption of ML?

It doesn't work with (sparse, noisy) **real data** from experiments or processes

It doesn't fit well into the **workflows** of our scientists

It's a 'black box'... can we **trust** it?

Why Alchemite™?

1. Setting up a machine learning framework for adaptive experimental design is hard.
2. Deploying models to teams is even harder.
3. The speed benefits of ML-AED are only realized with a platform.
4. If each chemist needed to know machine learning to set up the framework for ML-AED, they wouldn't be doing any R&D…
5. That's why we have Alchemite™ – a tool to handle the machine learning for you.

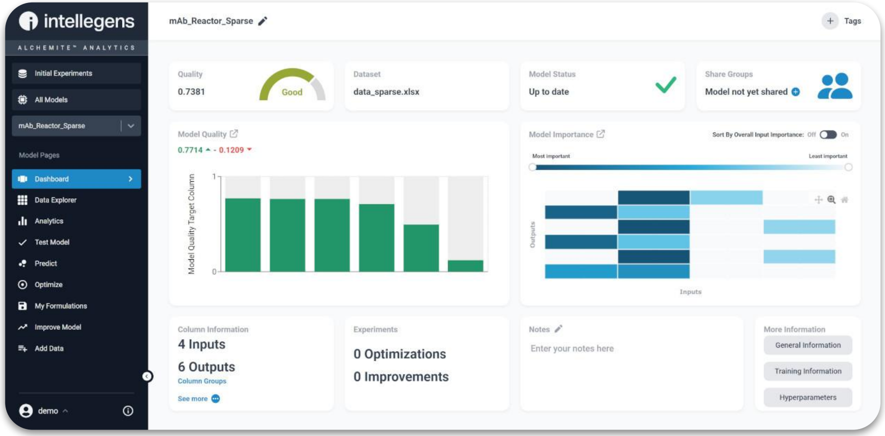
What is Alchemite™

Alchemite provides the following:

1. Alchemite is a no code tool that allows adaptive experimental design to be applied to R&D data
2. It is built on top of the ML-AED framework
3. It is a platform that allows machine learning models to be built on noisy, sparse, and high dimensional structured data
4. It provides accurate uncertainty quantification to guide experimental design
5. It leverages the ML-AED framework to accelerate R&D

Products and Successful Applications of the Technology

Alchemite™ – *ML design platform*



Real data

- Unique method for sparse, noisy data
- Accurate uncertainty quantification
- Complex, multi-dimensional problems

Fit to workflow

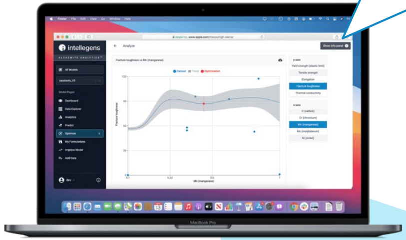
- Simple-to-use web user interface
- Designed for key analysis tasks
- Coding not required (optional API)

Trust

- Alchemite™ Success Team
- Explainable AI tools
- Proven - case studies, pilot projects

The Alchemite™ Products

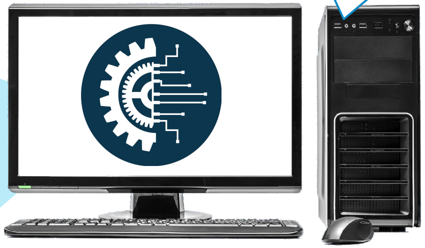
Scientists & engineers



Alchemite™ Analytics

- Web UI – insights on your desktop
- Optimise products, extract value from data, guide experiment

Data scientists



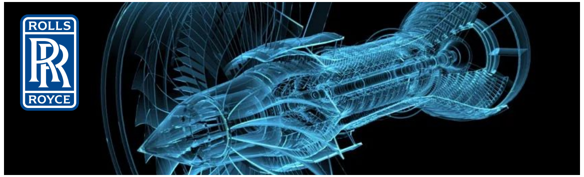
Alchemite™ Engine

- Integrate into your workflows (API, Python)
- Advanced configuration, deploy models

Alchemite™ Success

- Use our expertise in applying ML
- Ranging from ‘getting started’ advice to full project management

Successful applications



Design of an aero alloy

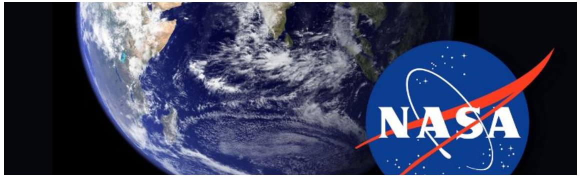
Multi-million $ savings in discovery of new alloy

Ink reformulation

Cut experimental timescales from months to minutes

Drug discovery

Predict pharmacokinetics to improve compound selection



Component design

Validating Alchemite™ for advanced engineering at NASA

Additive manufacturing

Reduce the number of tests by an order of magnitude

Flavours and fragrances

Predict the sensory properties of compounds

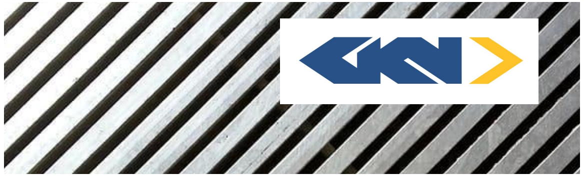
Successful applications

Optimising steels

Arcelor joint venture - insights from microstructure data

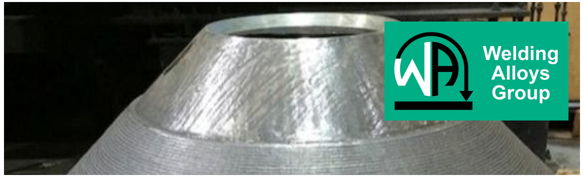
Drug discovery

Optimising kinase profiling programs despite sparse data



Virtual experimentation

Exploring new parts of material property space



Combatting wear

Better surface treatments with fewer alloying elements

Materials and processes

Drive efficiency in the use of simulation and experiment

Automotive catalysts

Reducing the amount of experimental work required

Customers, collaborations, and partnerships

Selected case study examples

Integration partners

Some other customers

- Fast-moving consumer goods corporation
- Biotech
- Plastics, paints & coatings maker
- Global petrochemicals producers
- Construction chemicals provider
- Battery manufacturer
- Major food & beverages corporation
- Plant-based foods innovator
- Leading steelmaker
- Advanced materials organisation
- Mining and cement company
- Additive manufacturing specialist

BREAK

Demo

What's next?

info@intellegens.com

/company/intellegensai

Further information

intellegens.com/doe-made-easy/

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