



intellegens

Applied machine learning

Information alchemy: extracting value from real-world experimental data in materials R&D

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Introducing Intellegens



Unique **deep learning** software and expertise

- Value from sparse, noisy experimental / process data, where other methods fail
- Spin-out from University of Cambridge

Key focus areas: **materials, chemicals, formulations, manufacturing**

- Optimise products & processes; save time & cost (up to 90% less experimentation)
- Easy-to-deploy platform to enable real-world application

Typical headaches in materials R&D



“My competitor could design a better material tomorrow”

“Can we get more value from the millions spent on testing and characterisation?”

“How to respond to environmental regulations *and* improve performance?”

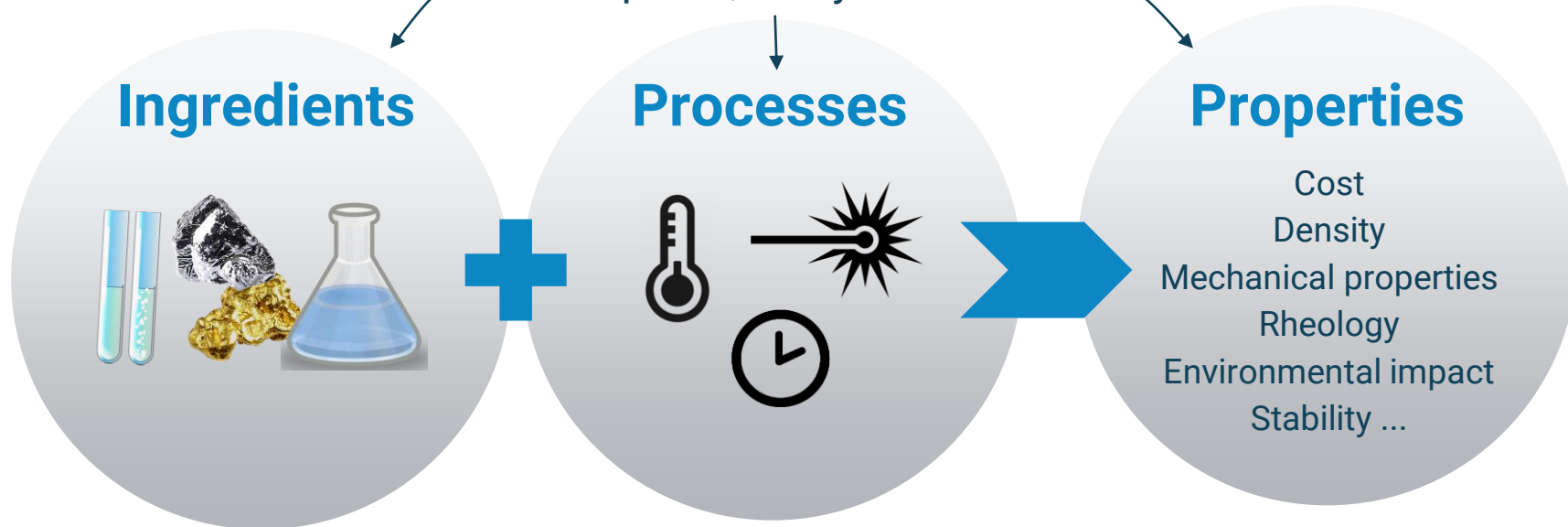
“Our most exciting innovative processes need to be more reliable / repeatable”

“We’re losing vital knowledge when our specialists retire or leave”

The formulation / materials design problem



High-dimensional,
sparse, noisy data



*Chemicals, plastics, pharmaceuticals,
alloys, foods, paints, cosmetics...*

High reliance on costly, time-
consuming experiment

How to design a new formulation / material?



**Try every
possible
formulation**

Guaranteed to
find the best
formulation

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

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Ask an expert

Uses knowledge from past projects

- Expensive resource
- May eventually retire or leave
- Human after all!

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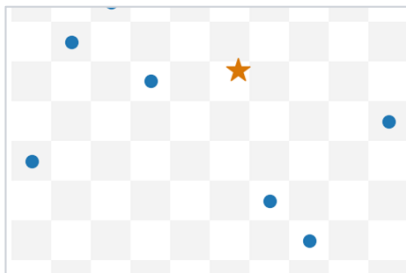
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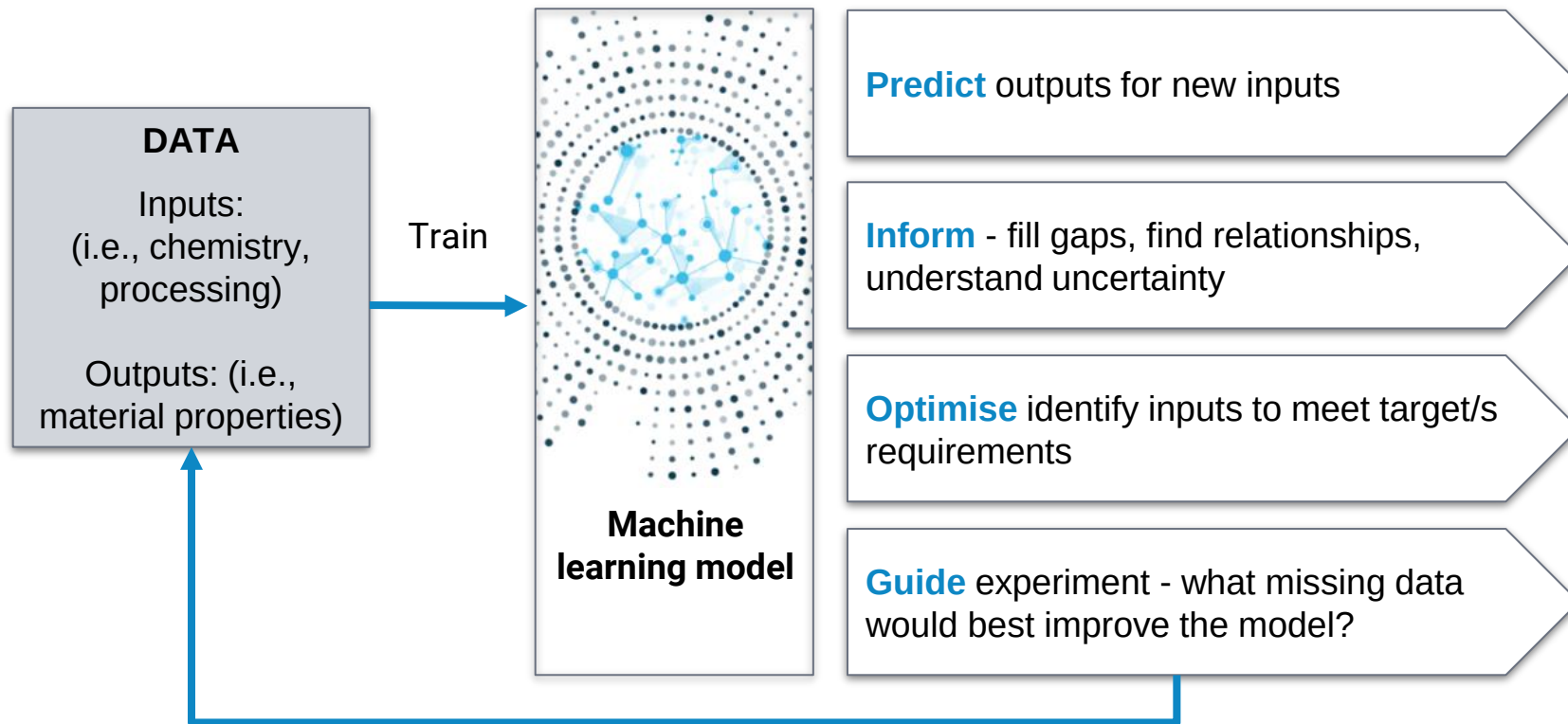


Structured design / DoE

Efficiently covers design space

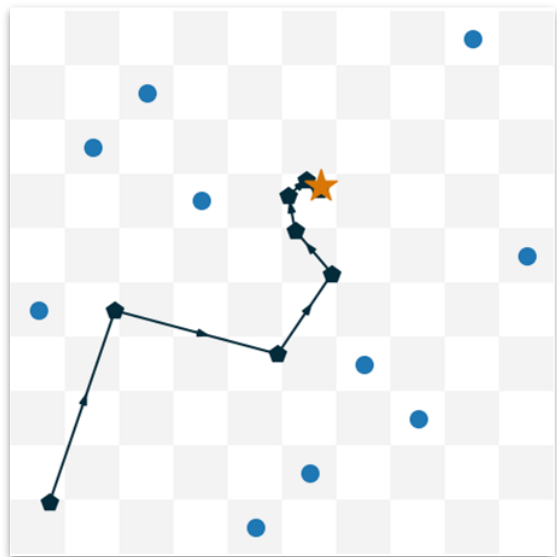
- May require a large number of experiments
- Requires statistical knowledge

How should machine learning help... in theory?



Model can continue to learn

Adaptive Experimental Design



Machine learning-driven
Adaptive Experimental Design



Target-driven: actively search for successful materials



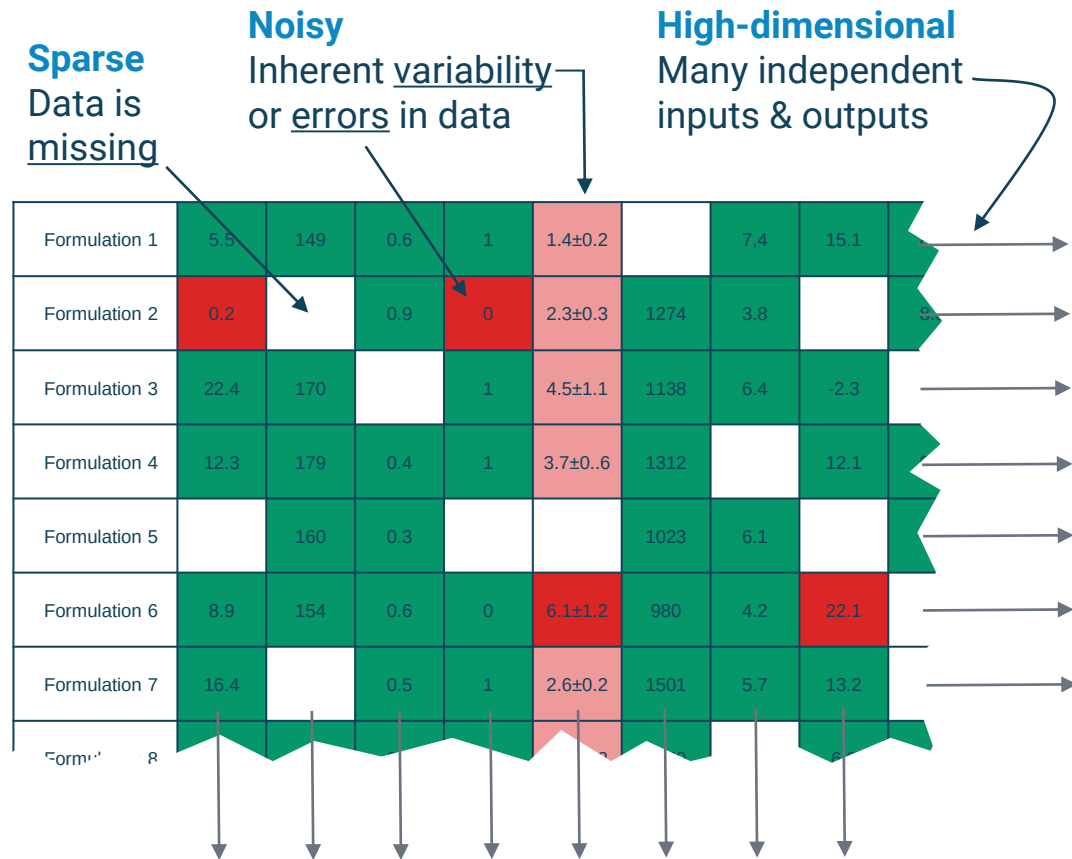
Natively handle 100s or 1000s of variables



No statistical or ML knowledge needed



The challenge: complex problems, real-world data



**Conventional
machine learning
fails given sparse,
noisy training data**

Solutions to the sparse, noisy data challenge

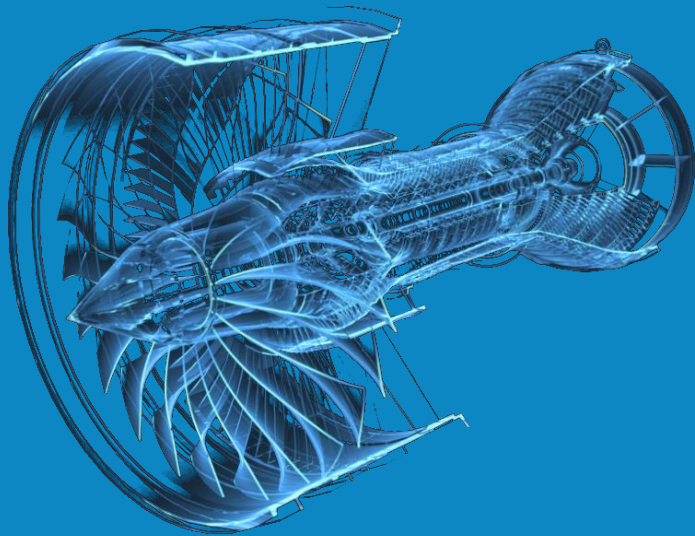


Data manipulation and analysis:

- Specialist data science effort to 'clean' the data to remove missing values and exploit known analytical relationships.
- Focus the analysis on 'complete' parts of the dataset.

A machine learning solution:

- E.g. Alchemite imputation algorithm, developed at University of Cambridge.
- Automatically handles sparse and noisy data, and exploits property/property relationships.



Case study - High temperature alloy



A new alloy design varied 20+ composition / process parameters to satisfy 11 physical criteria and outperform existing alloys

90% fewer costly experiments

Reduced costs by \$10 million

Accelerated typical discovery and validation time from 20 to 2 years

Materials & Design 168, 107644 (2019)



Case study - Composite tooling



The
University
Of
Sheffield.

AMRC
Advanced Manufacturing
Research Centre

Machine learning enabled an
80% reduction in the direct
costs associated with testing

For a new tool / composite pairing:

- Accurately predict failure mechanism and tool life based on 200 tests rather than usual 1,000
- Understand impacts of tool geometry, material selection, and more
- Design experimental campaigns to avoid unnecessary tests
- Cut direct costs, reduce wastage

Case study - Steels



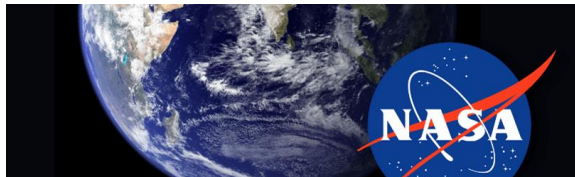
OCAS is a joint venture of global steel leader ArcelorMittal

- Extract hidden information from microstructure images
- Predict properties from structure and property data
- Design a set of processing parameters to achieve target steel properties

“The project has validated the use of the deep learning method for real-world steels applications and provided insights that can help us to improve steel properties and focus valuable experimental resources more efficiently.”

Lode Duprez, *Chief scientific officer, OCAS*

More examples of successful ML application



Component design

Advanced engineering at NASA



Additive manufacturing

Reduce the number of tests by an order of magnitude



Advanced materials

Working on ceramics, plastics, and controlled release systems



Combatting wear

Better surface treatments with fewer alloying elements



Automotive catalysts

Reducing the amount of experimental work required



Recycling plastics

Optimising blend performance for variable recycled content



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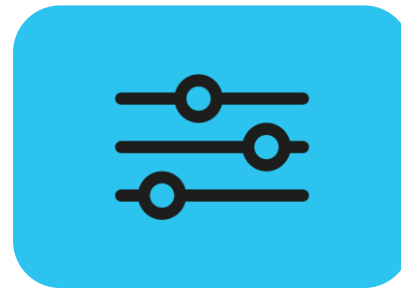
Accelerating innovation for materials, chemicals, manufacturing, and beyond...



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from real-world,
sparse, noisy data



Save time and cost
with up to 90%
fewer experiments



Win with optimised
formulations, products,
and processes