intellegens

Solving the 'small data' problem
for formulations, materials, and processes

Webinar will begin shortly

intellegens

Solving the 'small data' problem
for formulations, materials, and processes

Webinar will begin in one minute

intellegens

Solving the 'small data' problem
for formulations, materials, and processes

Webinar - 13 July 2021

Today's live, interactive session

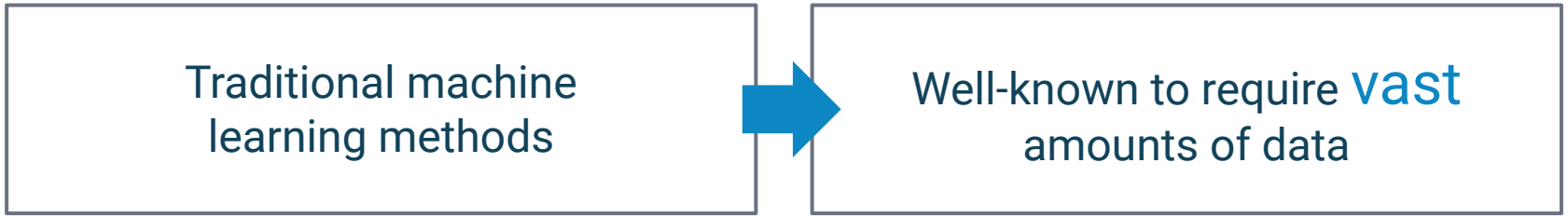
Host Stephen Warde, Intellegens Marketing

Speaker Dr Gareth Conduit, CTO and co-founder

Please ask questions at any time in the control panel box, we will answer these at the end of the webinar

Look out for a follow-up email with links to the presentation slides and a recording of the webinar

Introduction: traditional machine learning



Introduction: real-life discovery projects

Traditional machine learning methods

Well-known to require vast amounts of data

- Material & chemical discovery
- Design of formulations
- Novel processes e.g. AM

Data is expensive and time-consuming to collect so is inevitably sparse

Introduction: Alchemite™ machine learning

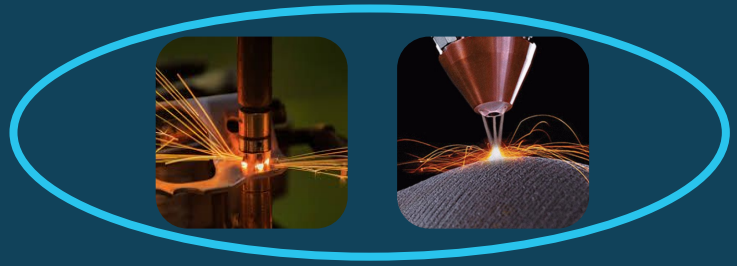
Traditional machine learning methods → Well-known to require vast amounts of data

- Material & chemical discovery
- Design of formulations
- Novel processes e.g. AM

→ Data is expensive and time-consuming to collect so is inevitably sparse

Alchemite™ machine learning from Intellegens exploits four methods to deliver deep insights in the face of sparse data

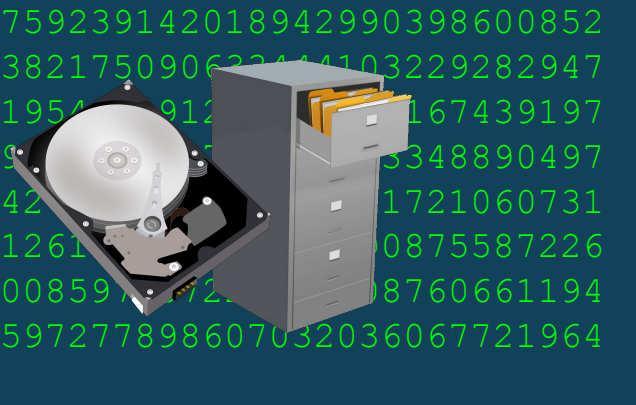
Property-property correlations



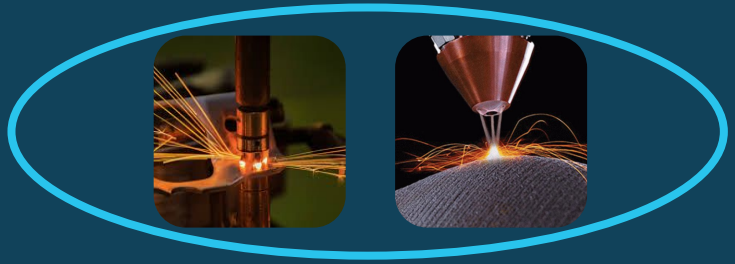
Design of experiments

Uncertainty

Access to data



Property-property correlations

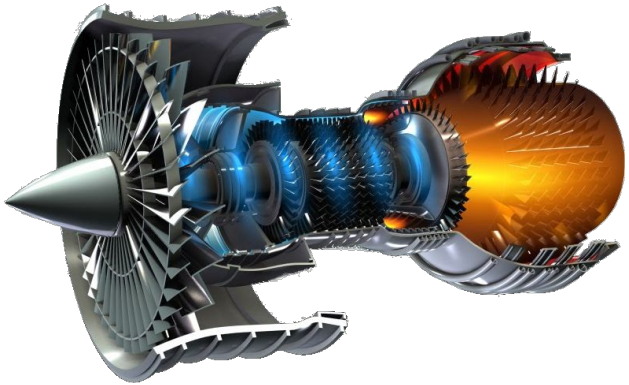


Design of experiments

Uncertainty

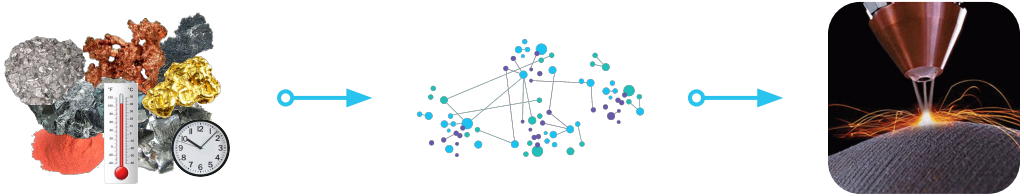
Access to data

Additive manufacturing components for engines



Direct prediction of 3D printing

10 entries



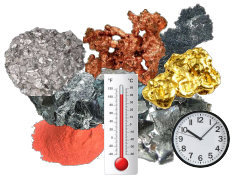
Composition and heat treatment space 30 dimensional

Requires 31 points to fit a hyperplane

Just 10 data entries available to model defect density

Predicting a proxy property: welding

1000 entries

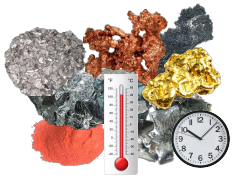
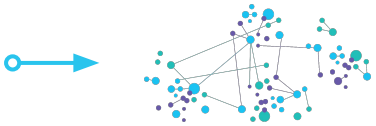


1000 weldability entries to understand complex composition → weldability model

Property-property correlations

1000 entries

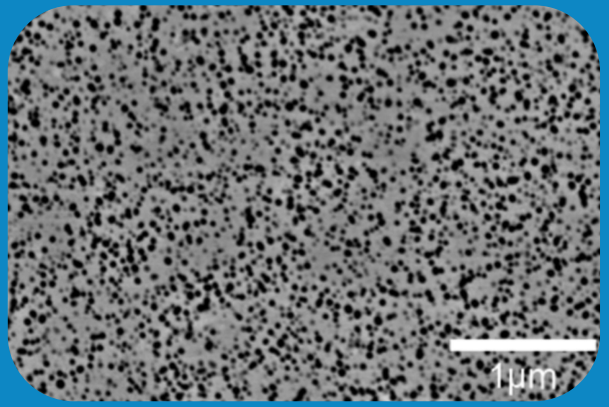
10 entries

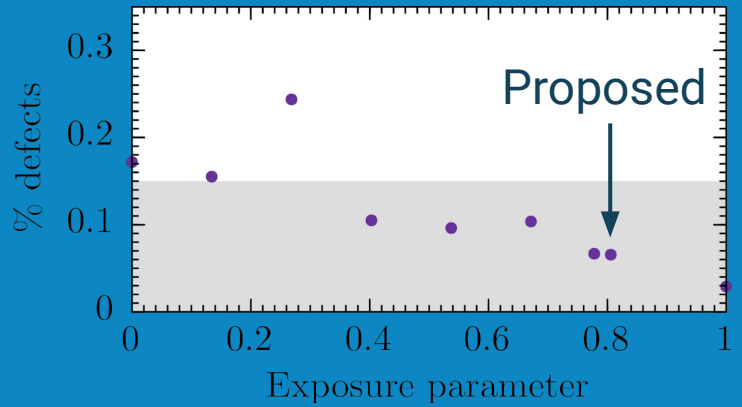




1000 weldability entries to understand complex composition → weldability model

10 defects entries capture the simple weldability → defect relationship

Two interpolations give composition → defects extrapolation





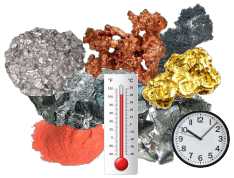
Alloy for additive manufacture

Exploited property-property correlations to design alloy

Eight properties experimentally verified by Rolls Royce

Published in Materials & Design 168, 107644 (2019)

Computer simulation-property correlations



100,000 entries

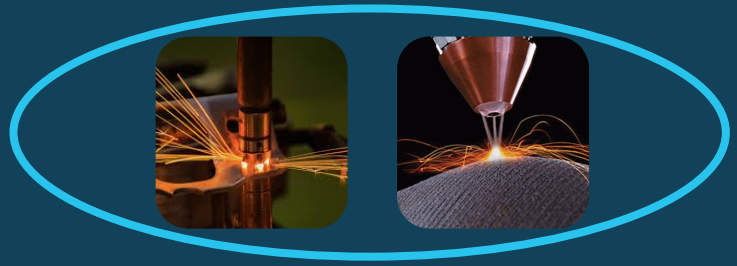
100 entries

100,000 computer simulations results to understand phase behavior

100 entries capture the fatigue life

Merge inexpensive computer simulations with expensive experiments

Property-property correlations

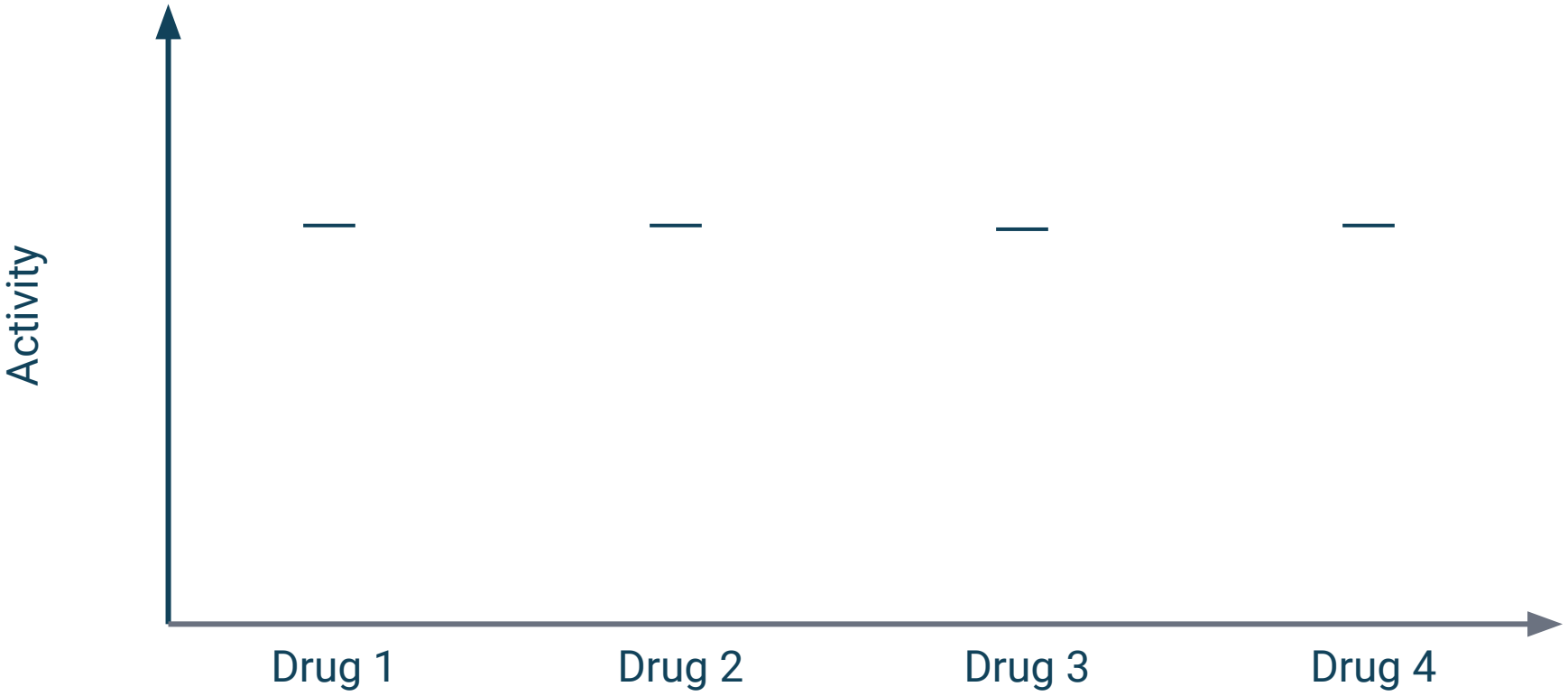


Design of experiments

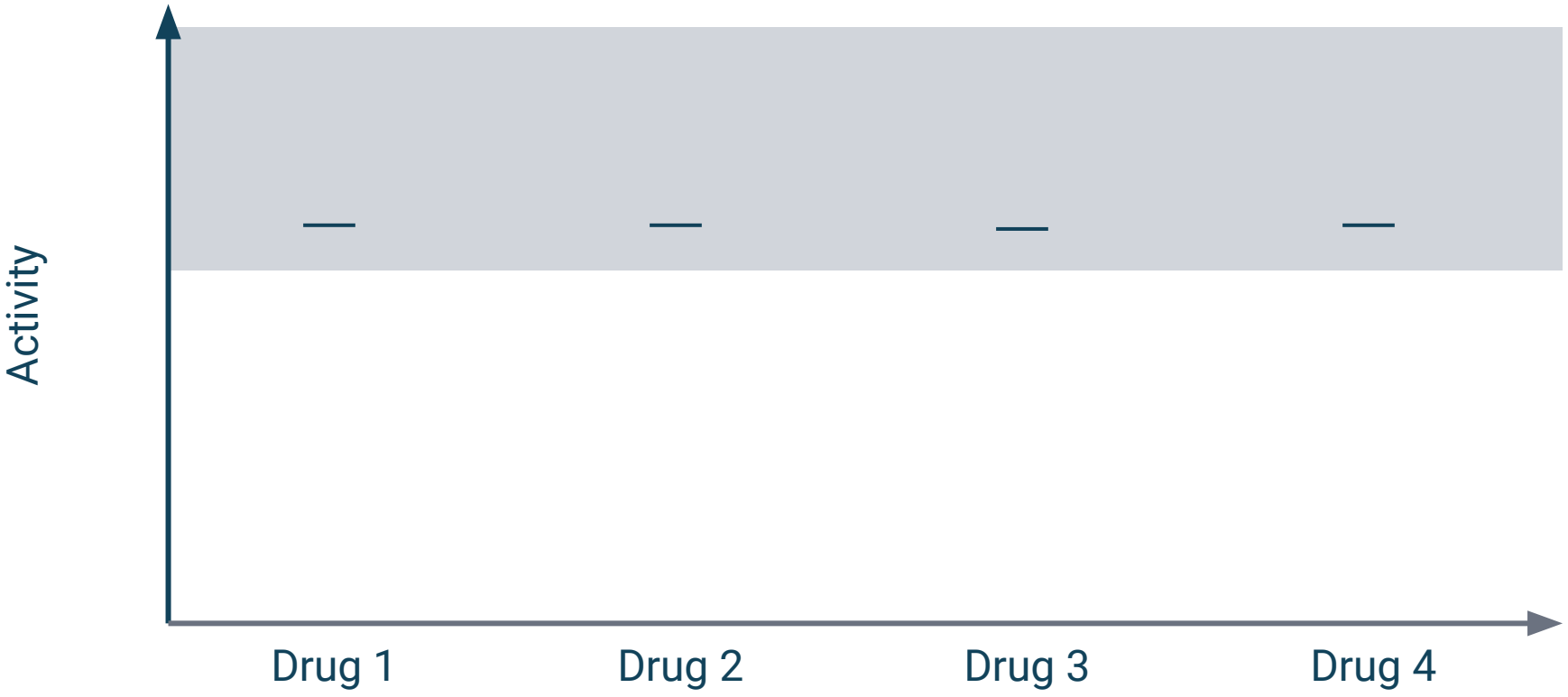
Uncertainty

Access to data

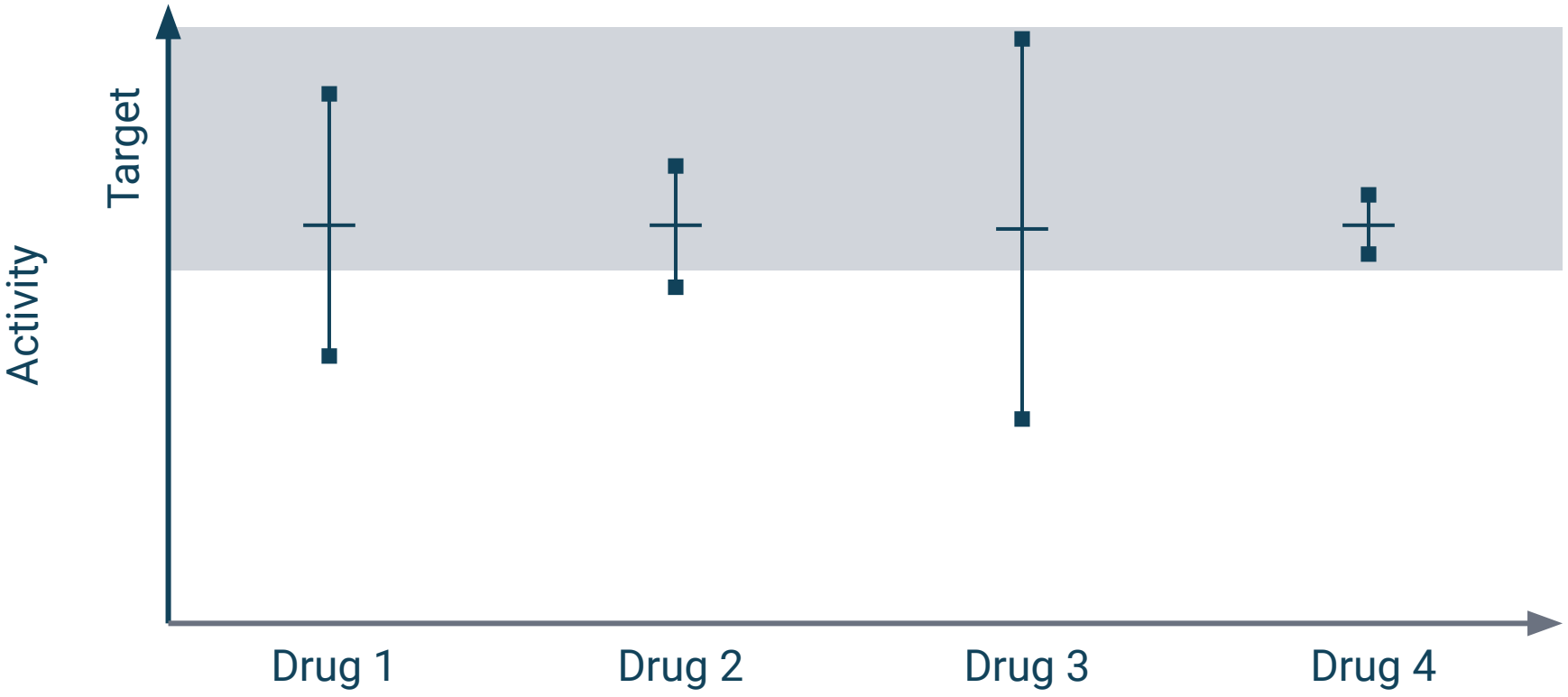
Predictions



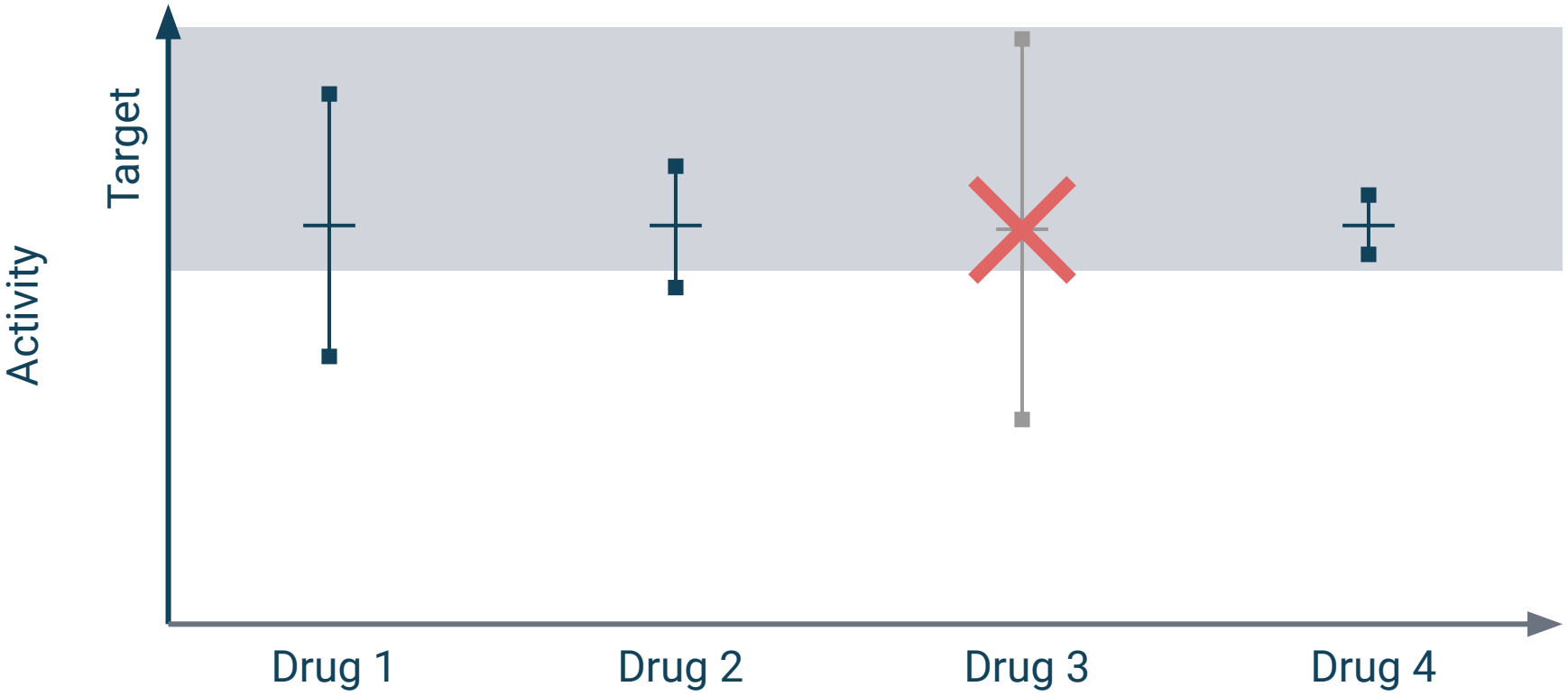
Target activity



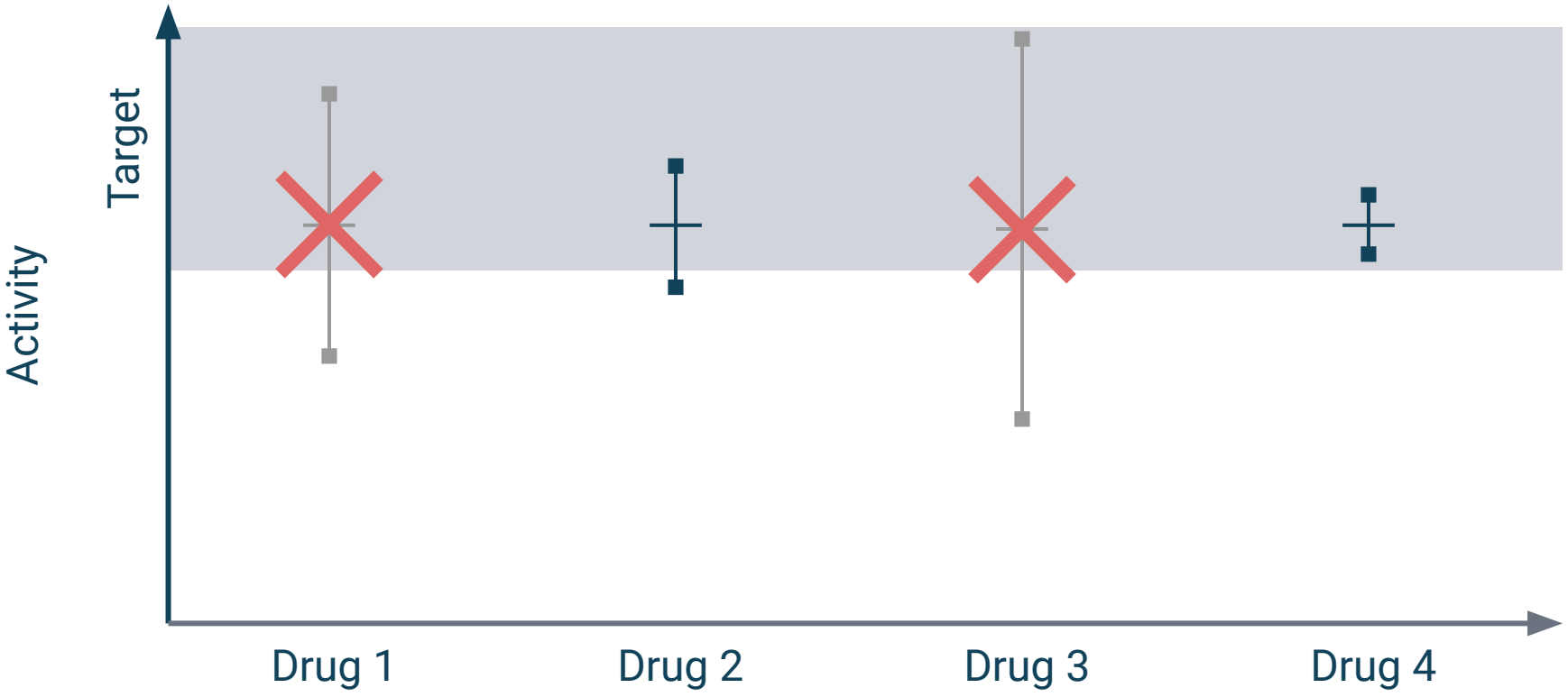
Uncertainty in the predictions



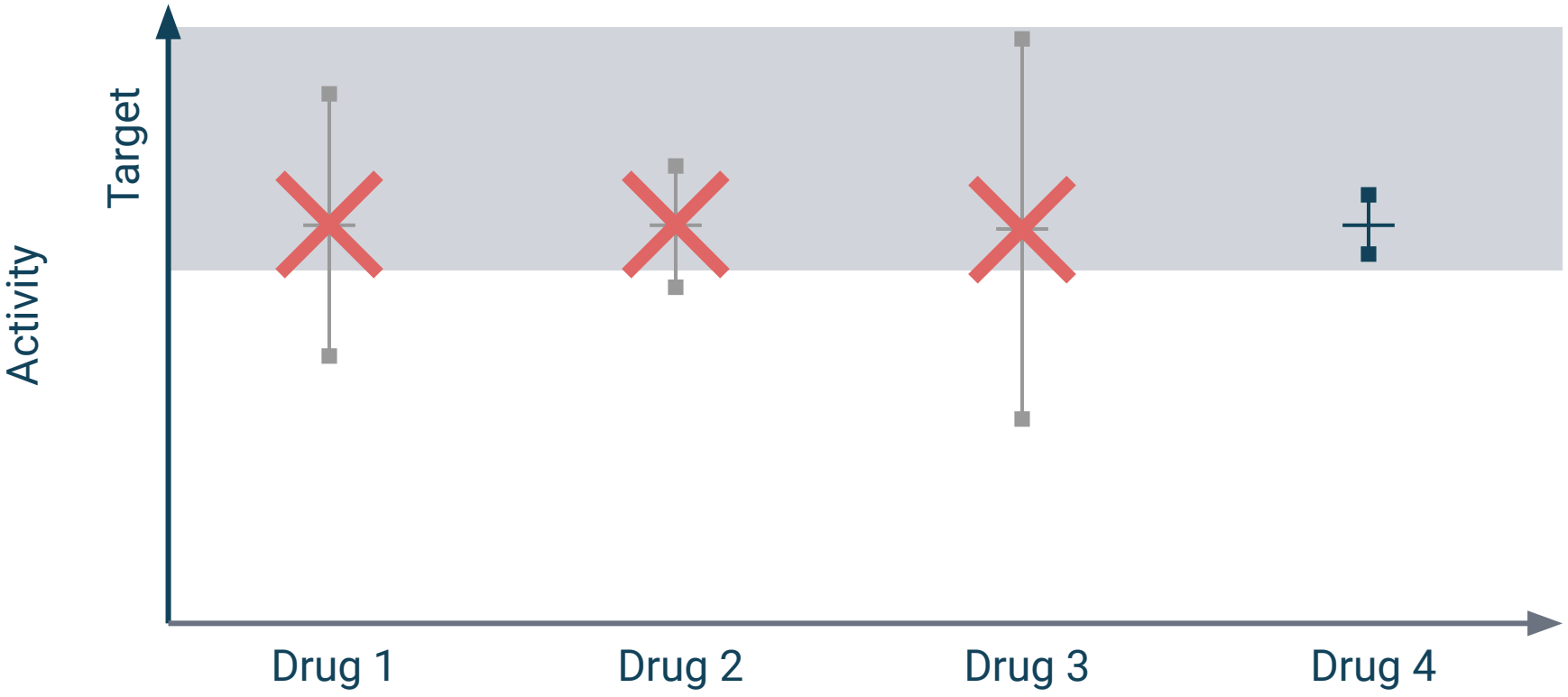
Reject worse quartile of predictions



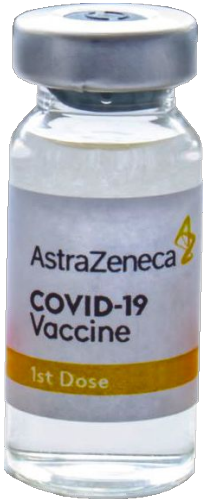
Retain the 50% most accurate predictions

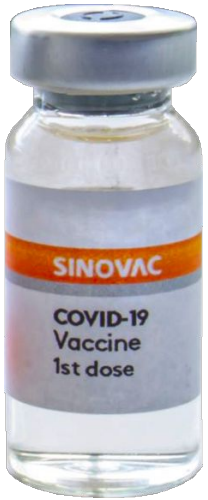


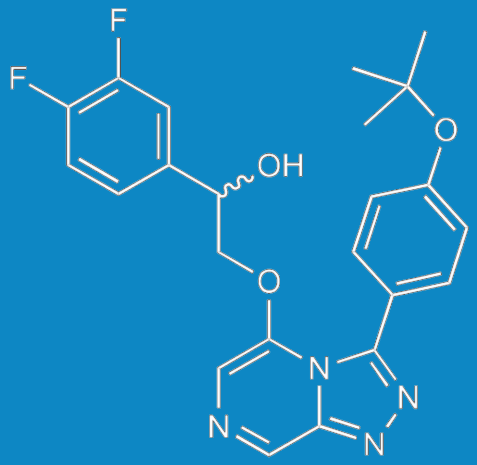
Retain the best quartile of results



Many vaccines have been developed for COVID-19







“It’s great to see that the Optibrium/Intellegens’ strong modelling results from phase 1 could be complemented with generative methods and held up in in vitro testing.”

Professor Matthew Todd
University College London

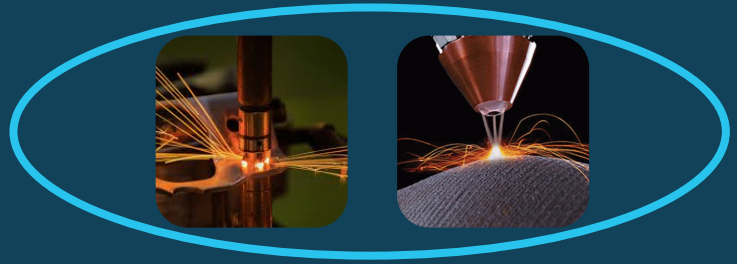
Open Source Malaria competition

Data-driven approach identified new candidate molecules

Focus on drug most likely to work

OPEN SOURCE MALARIA
Looking for New Medicines

Property-property correlations

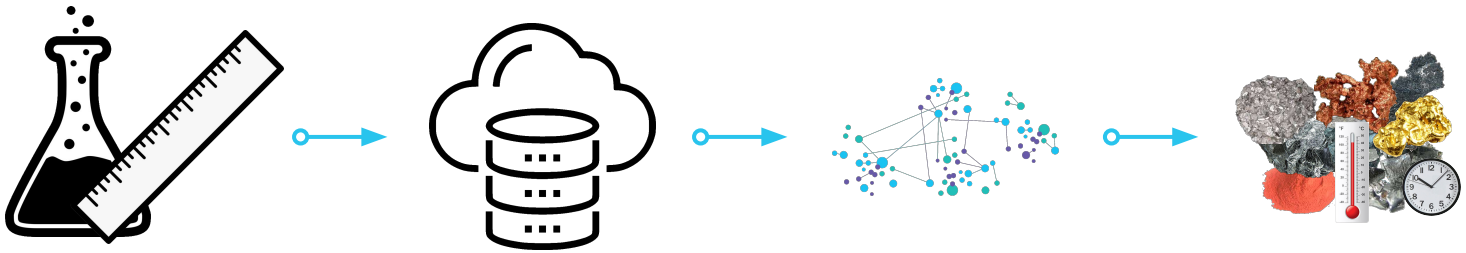


Design of experiments

Uncertainty

Access to data

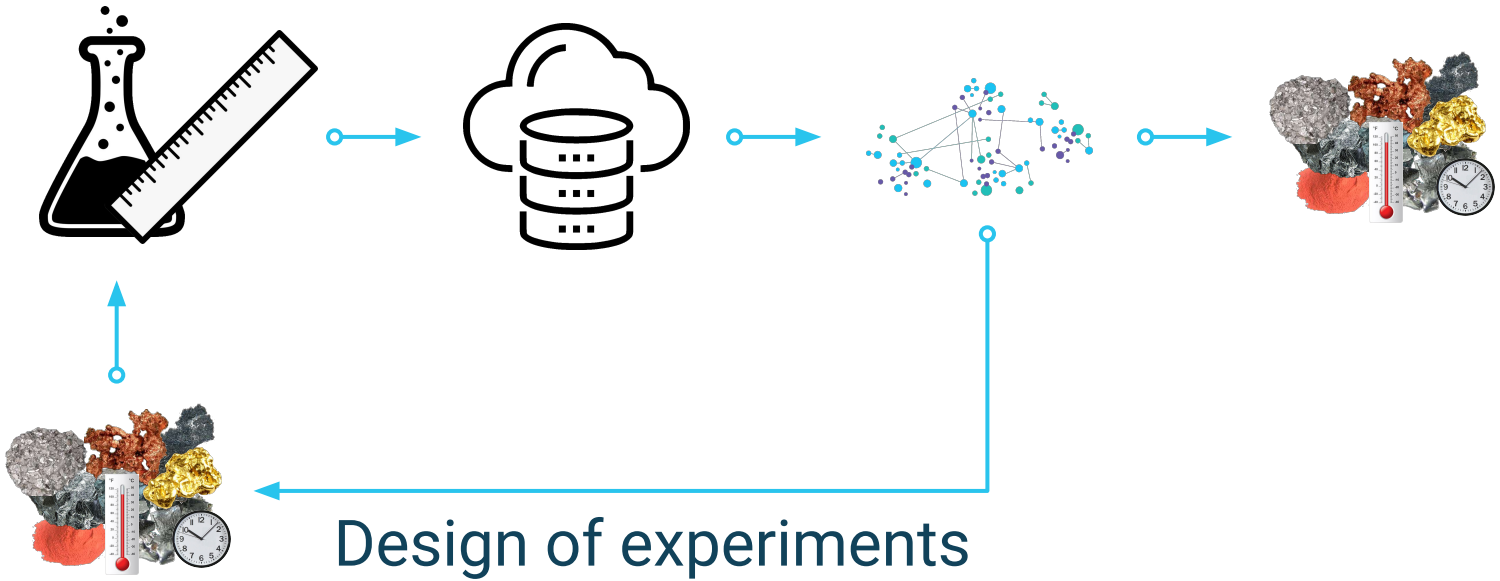
Standard approach to machine learning



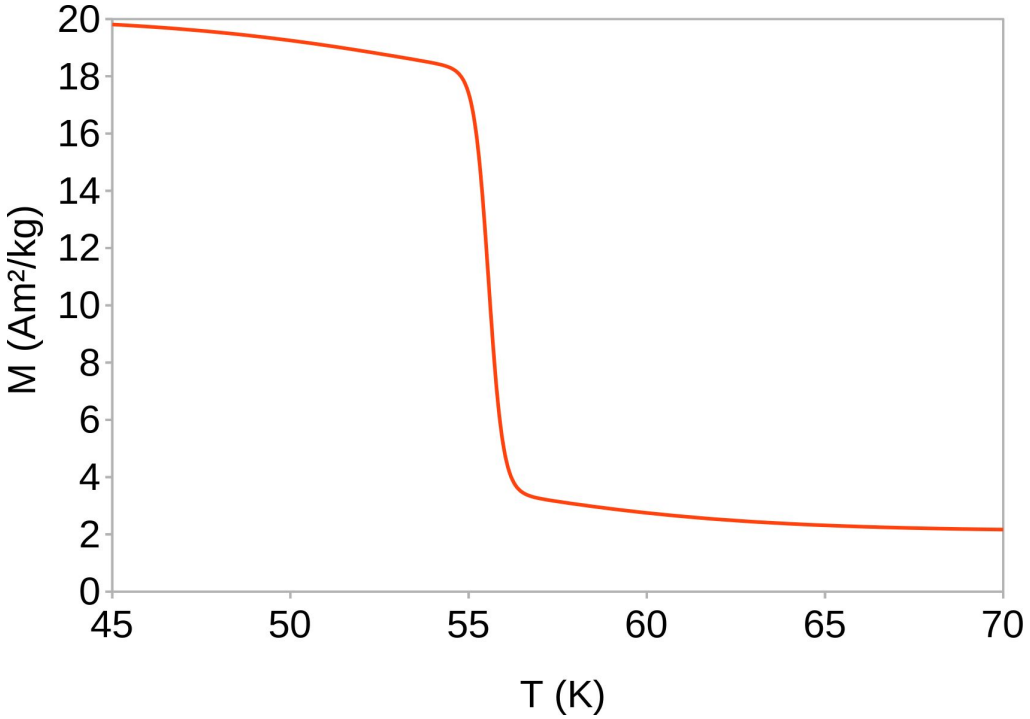
Data is difficult and expensive to collect so is sparse

Use Alchemite™ to guide what data to collect

Design of experiments cycle

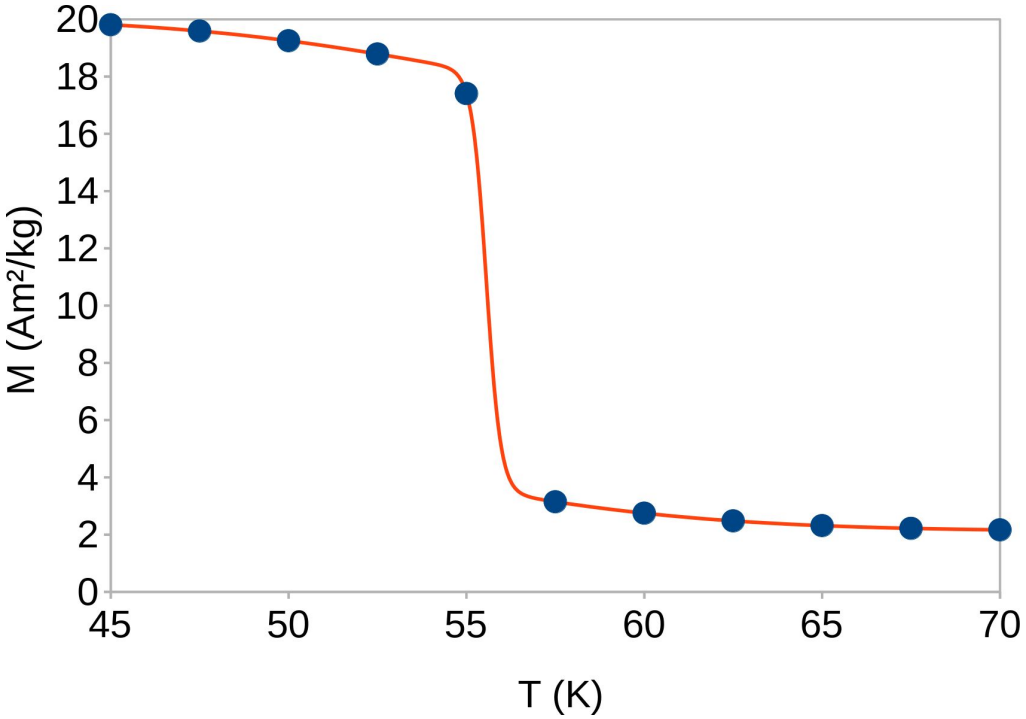


Underlying experimental curve

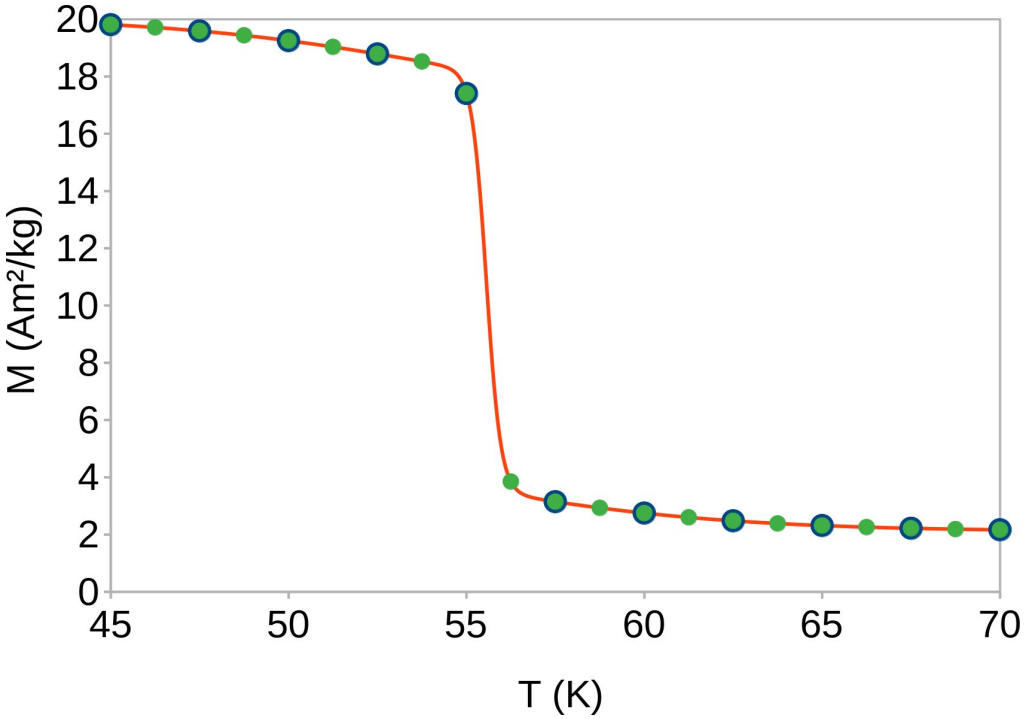


Non-hysteretic first-order phase transition with large latent heat and giant low-field magnetocaloric effect, Nature Communications **9**, 2925 (2018)

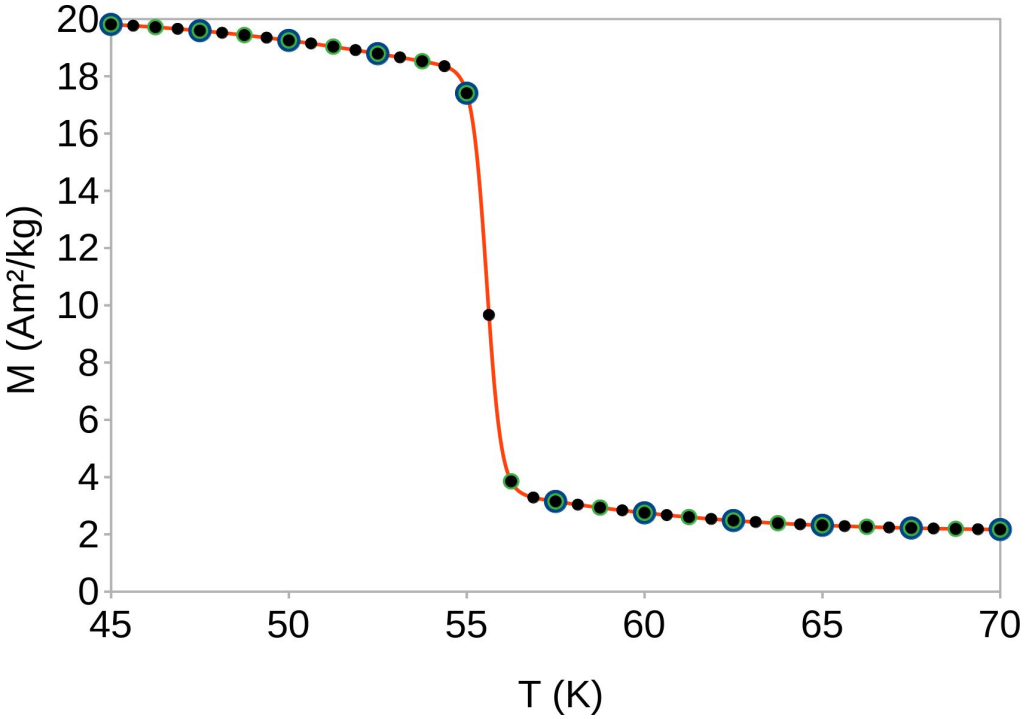
Full factorial



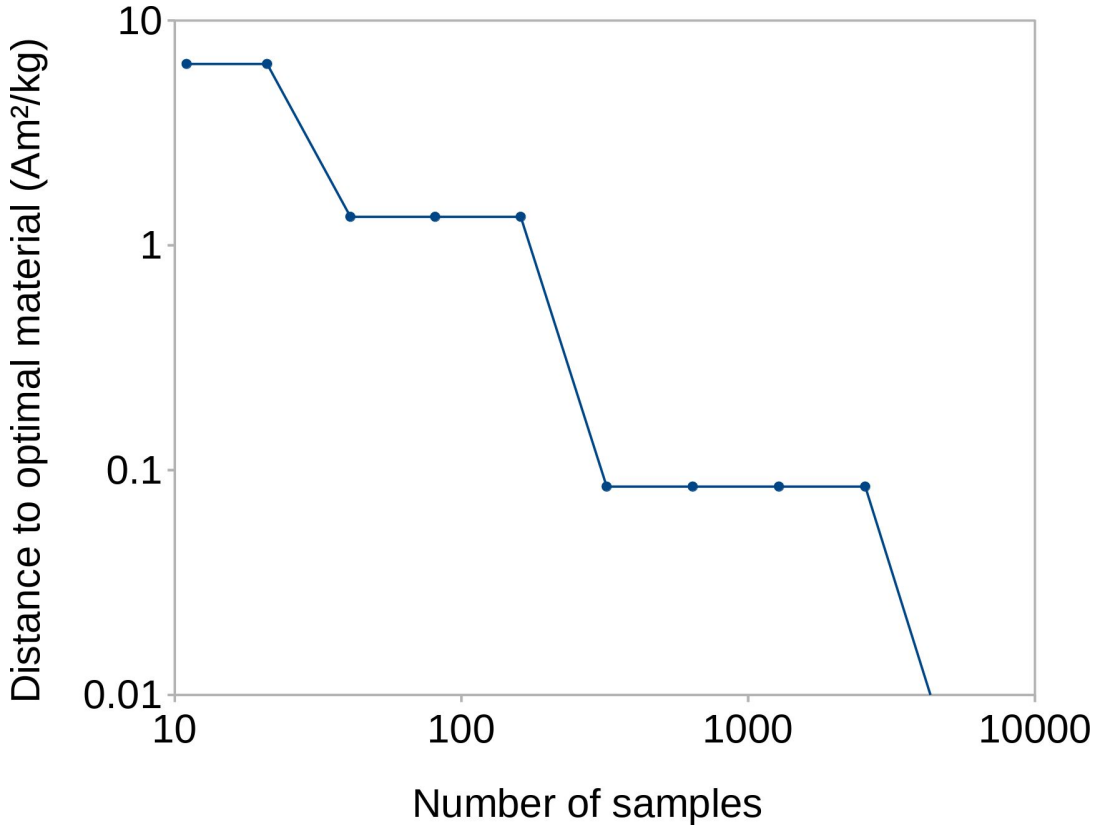
Second round of full factorial



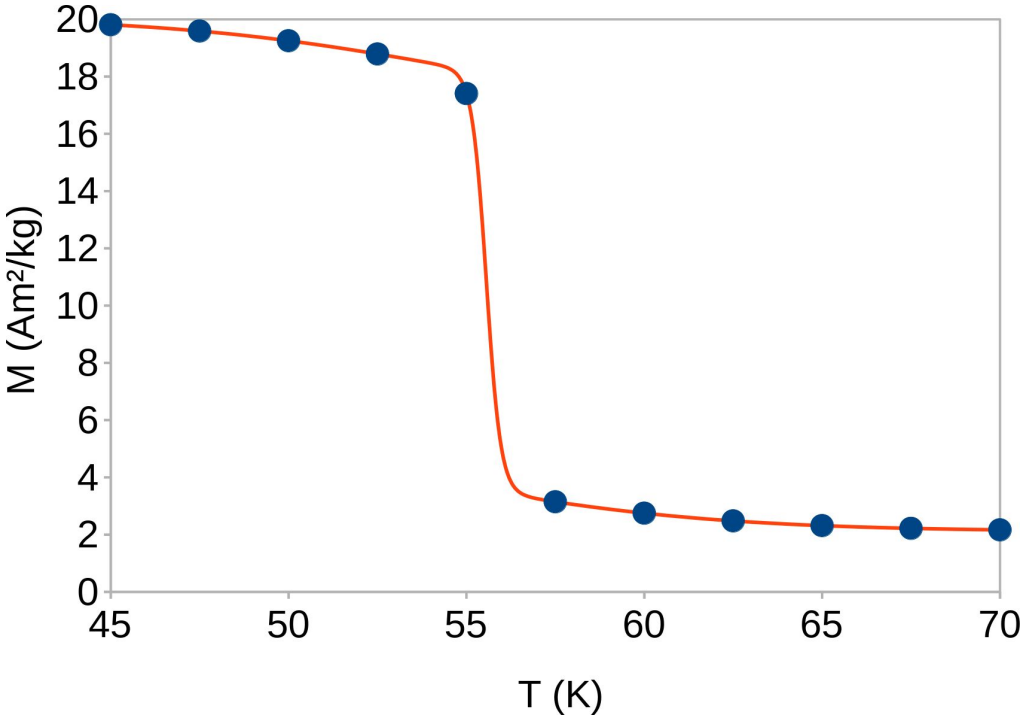
Third round of full factorial



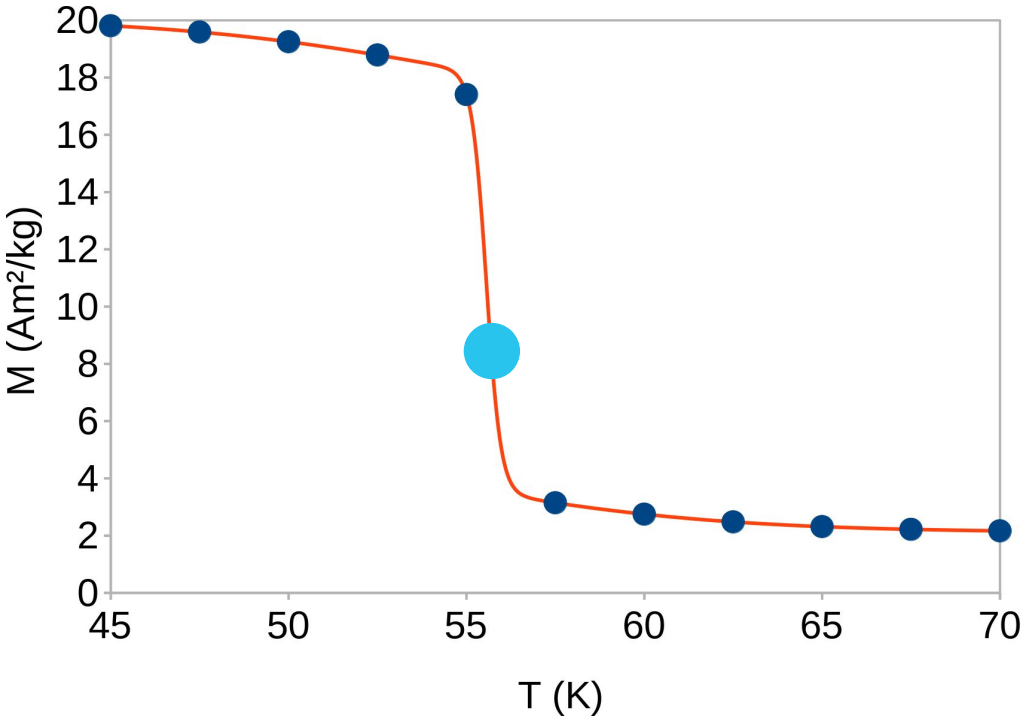
Design of experiments



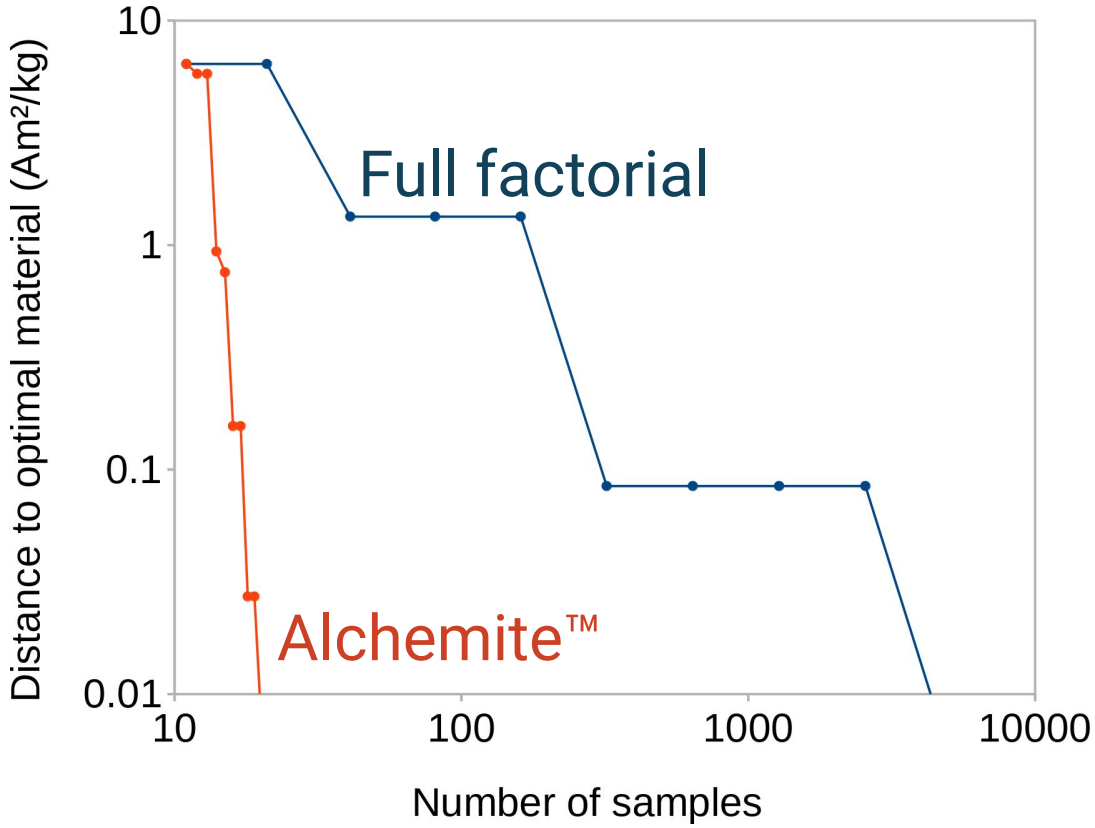
Judiciously put point in the center



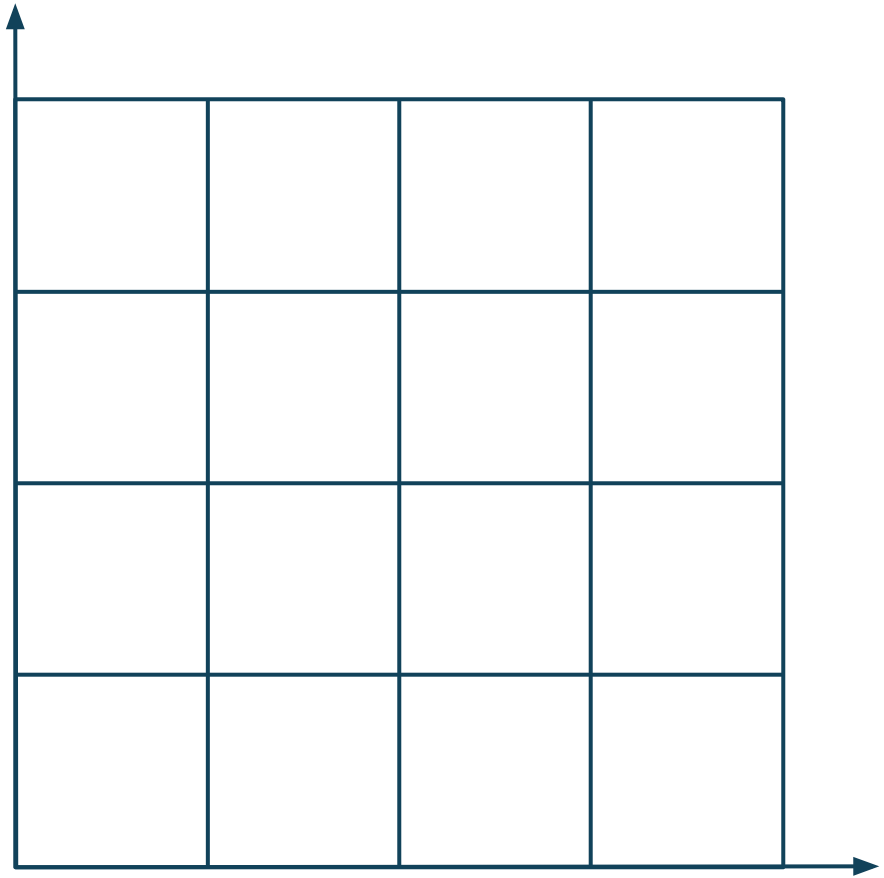
Judiciously put point in the center



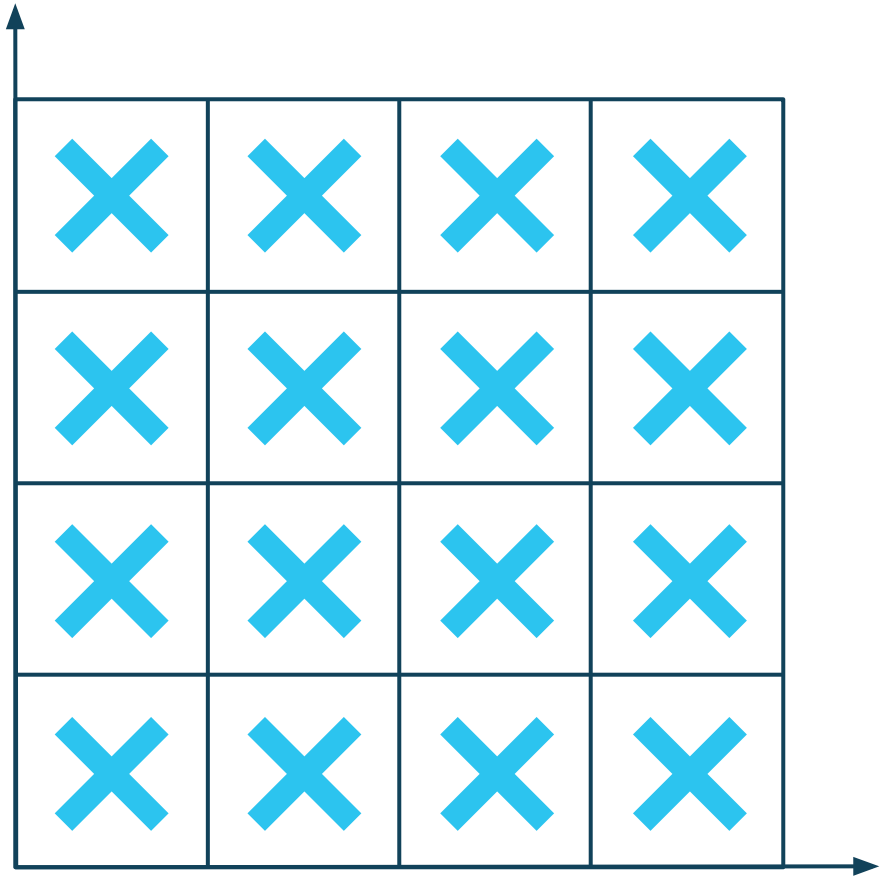
Design of experiments



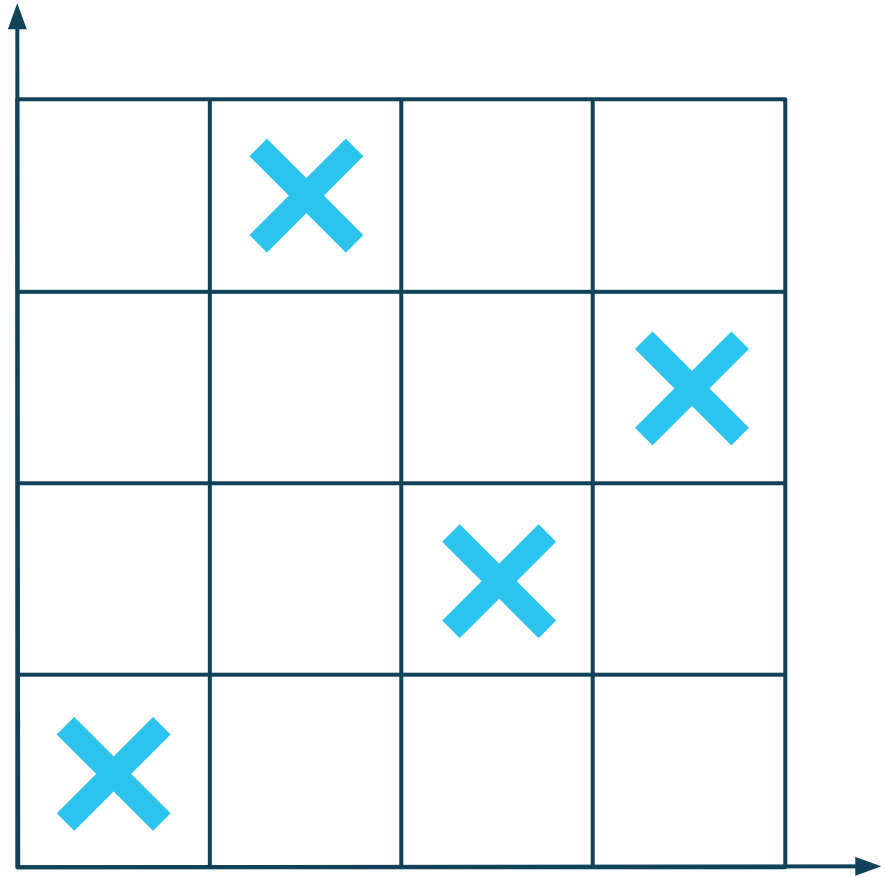
What if there is no data to motivate measurements?

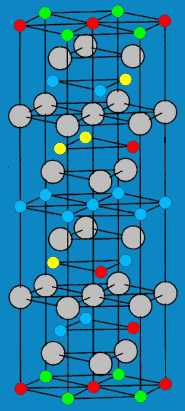


Full factorial distribution



Latin hypercube distribution





Alchemite™ design of experiments used

x10 fewer calculations

Battery design

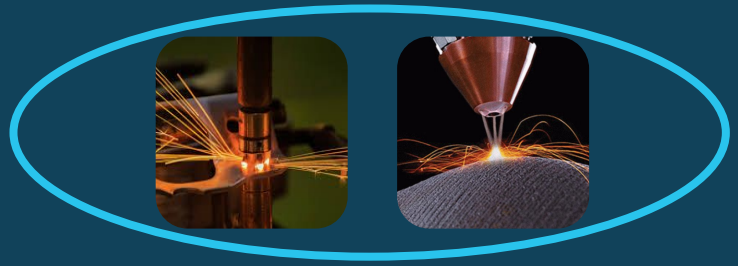
Blend experimental and computational data to predict many important properties of batteries

Further opportunities in battery management software

Predicting the State of Charge and Health of Batteries using Data-Driven Machine Learning

Nature Machine Intelligence **2**, 161 (2020)

Property-property correlations



Design of experiments

Uncertainty

Access to data

Validate new data

You will always want to get more data from any available source, Alchemite™ can help to validate the data

Part of a broader collaboration with Ansys led to the paper

Materials data validation and imputation with an artificial neural network
Computational Materials Science 147, 176 (2018)

See also our data quality case study with Matmatch

Access more data

You will always want to get more data from any available source, Alchemite™ can help to validate the data

Part of a broader collaboration with Ansys led to the paper

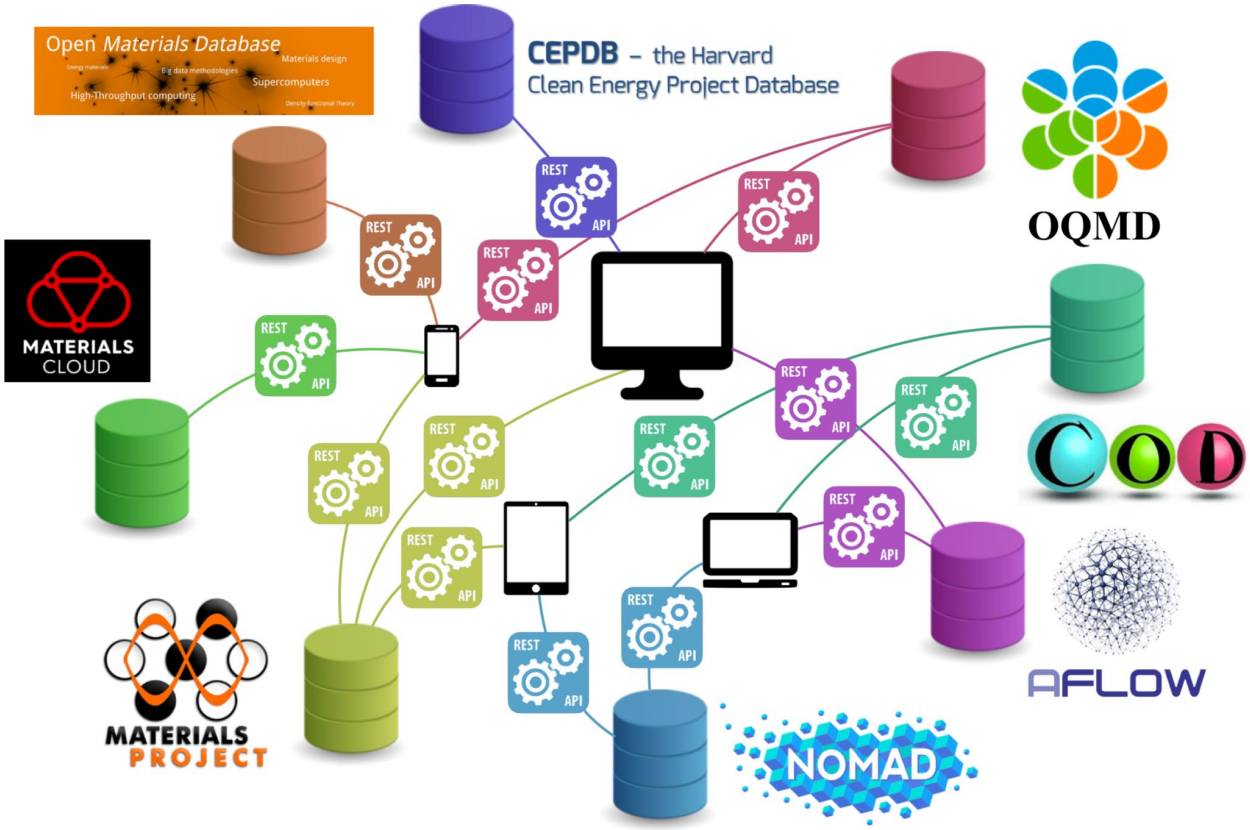
Materials data validation and imputation with an artificial neural network
Computational Materials Science 147, 176 (2018)

See also our data quality case study with Matmatch

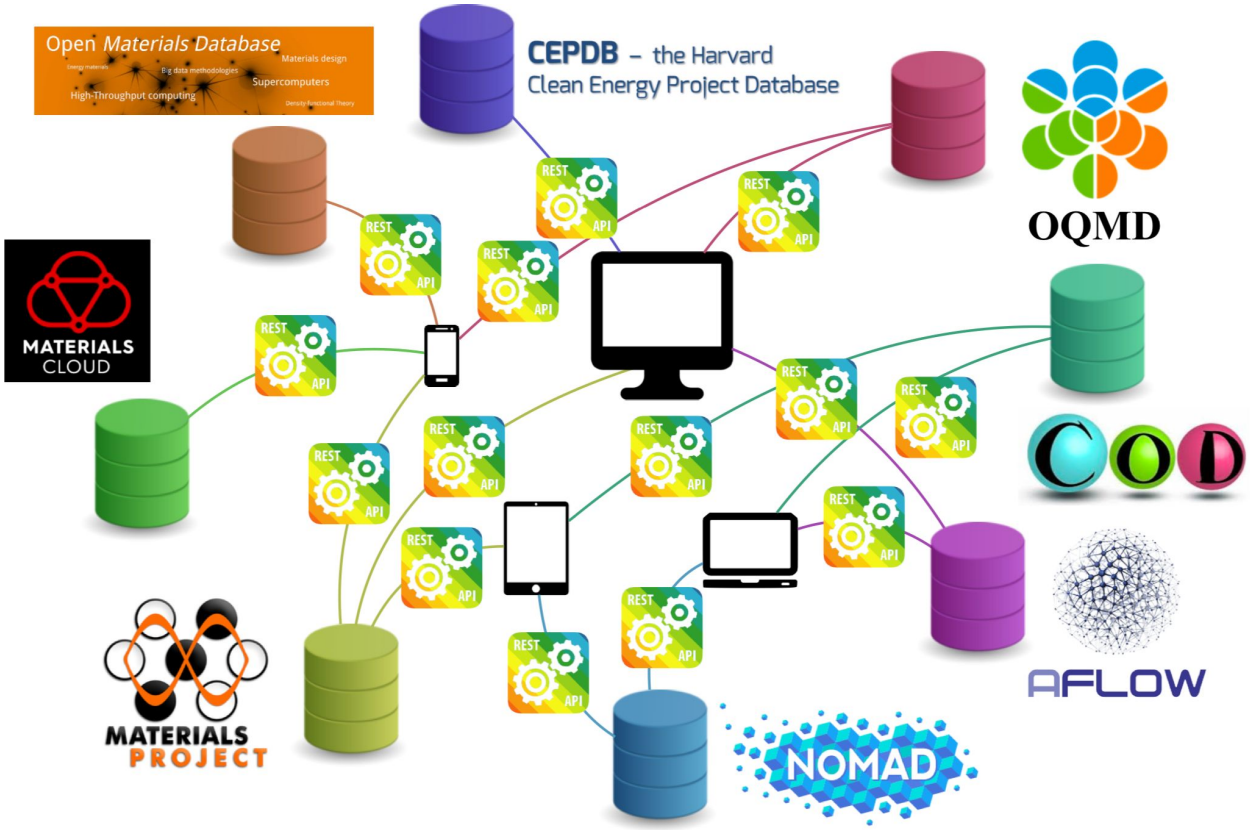
Wide range of research databases are available, the OPTIMADE projects enables access through a common interface

Many sources of data

Each repository has its own API



Common OPTIMADE API enables access to all data



OPTIMADE

Open Databases Integration for Materials Design

The Open Databases Integration for Materials Design (OPTIMADE) consortium aims to make materials databases interoperable by developing a specification for a common REST API

https://www.optimade.org/

Access >10^8 materials

OPTIMADE: an API for exchanging materials data

Accepted for publication in Nature Scientific Data (2021)

Sparse data, uncertainty & design of experiments

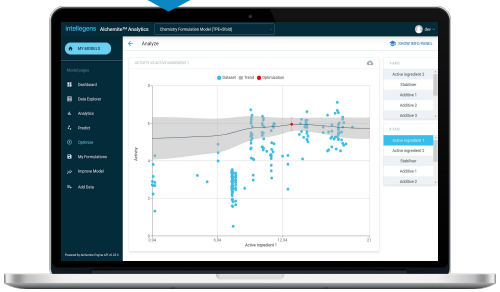
Alchemite™ uses property-property correlations, uncertainty estimates, design of experiments, and broad access to overcome inevitable sparse data

Track record of designing experimentally verified materials with apparently impossibly small amounts of data, including for additive manufacturing

Double winner at the ASME Additive Manufacturing Innovation Awards 2021

Alchemite™ product family

Scientists & engineers
Fast start, easy-to-use, visual



Option to deploy models

Data scientists
Add to your ML toolkit

Optional connectors

- *Lab systems*
- *Software & scripts*
- Sharing & collaboration

Alchemite™ Analytics

Deep data insights on your desktop
Guide experiments, predict, design, optimise

Alchemite™ Engine

Integrate into your workflow (API, Python)
Advanced configuration, enterprise deployment

Alchemite™ Success

Access Intellegens deep learning expertise

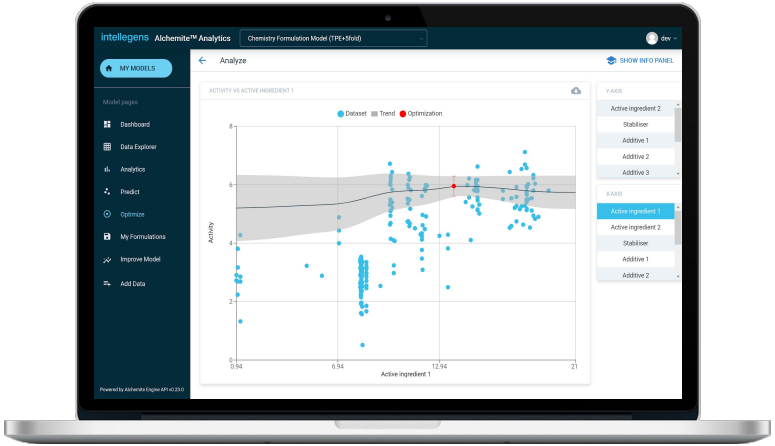
Advice to your data science team or full project management

Next steps

Follow-up email with links to the presentation slides and a recording of the webinar

Request a demonstration

Sign up for our newsletter for notifications of future webinars and events
intellegens.ai/subscribe



info@intellegens.ai

https://intellegens.ai

Question & answer session

Contact gareth@intellegens.ai

Website https://intellegens.ai

Papers https://intellegens.ai/article-type/papers/

Demo https://app.intellegens.ai

@intellegensai

/company/intellegensai