intellegens

Applied machine learning

Turning uncertainty into good decisions for chemical, materials, and formulations R&D

14 June 2022

Today's live, interactive webinar

Host
Stephen Warde
Intellegens Marketing

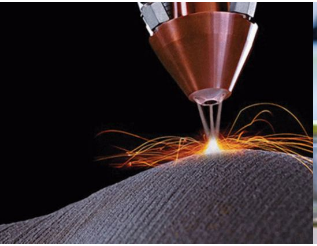
Presentation
Dr Gareth Conduit
CSO

Please ask **questions** at any time

- Use the "Questions" box on the control panel
- Questions will be answered 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

Alchemite™ machine learning



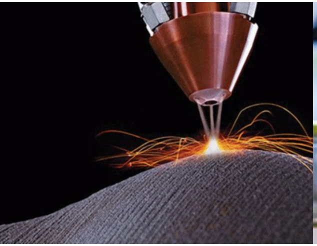



Alchemite™ designs formulations for multiple target properties

Merge simulations, analytics, and experimental data to exploit all knowledge

Exploit uncertainties to deliver most robust predictions to customers

Alchemite™ machine learning






Alchemite™ designs formulations for multiple target properties

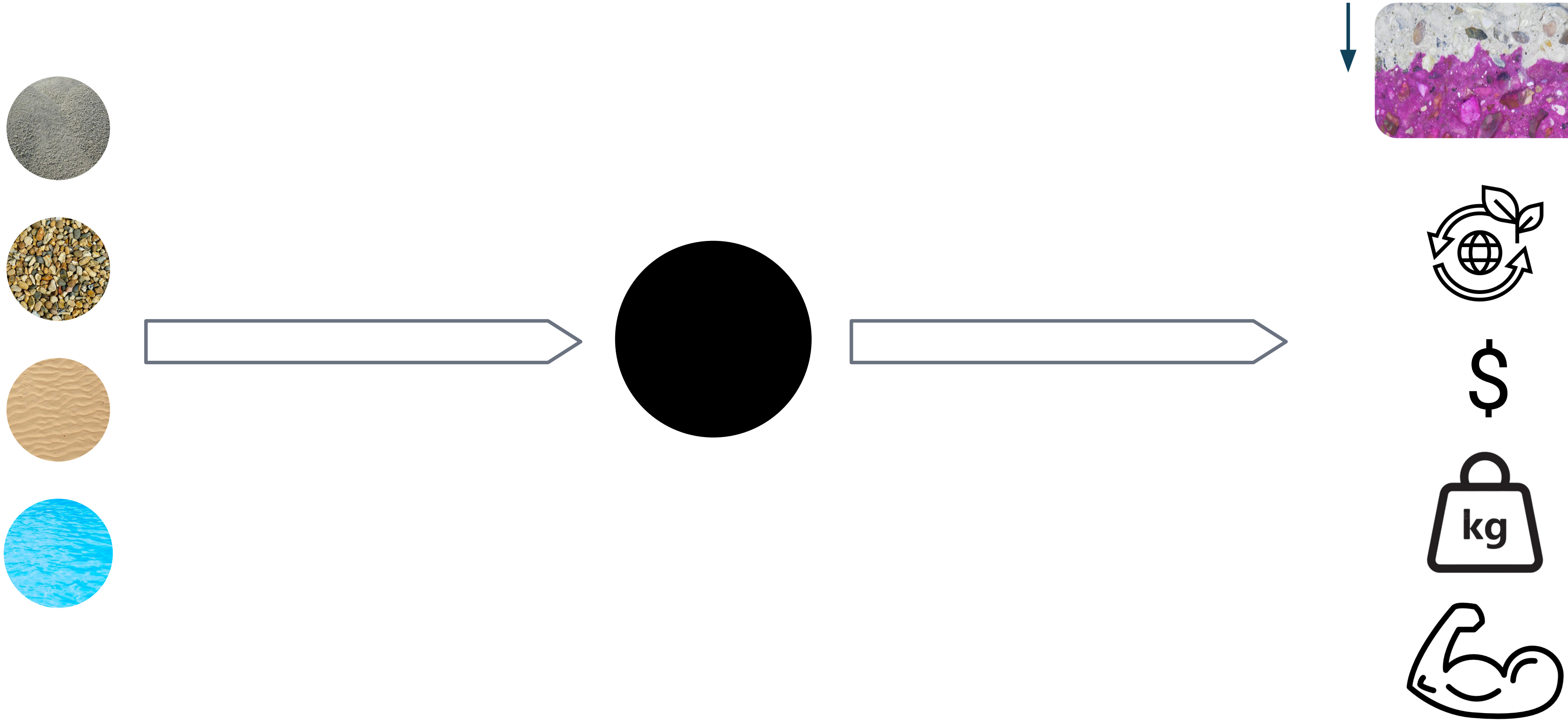
Merge simulations, analytics, and experimental data to exploit all knowledge

Exploit uncertainties to deliver most robust predictions to customers

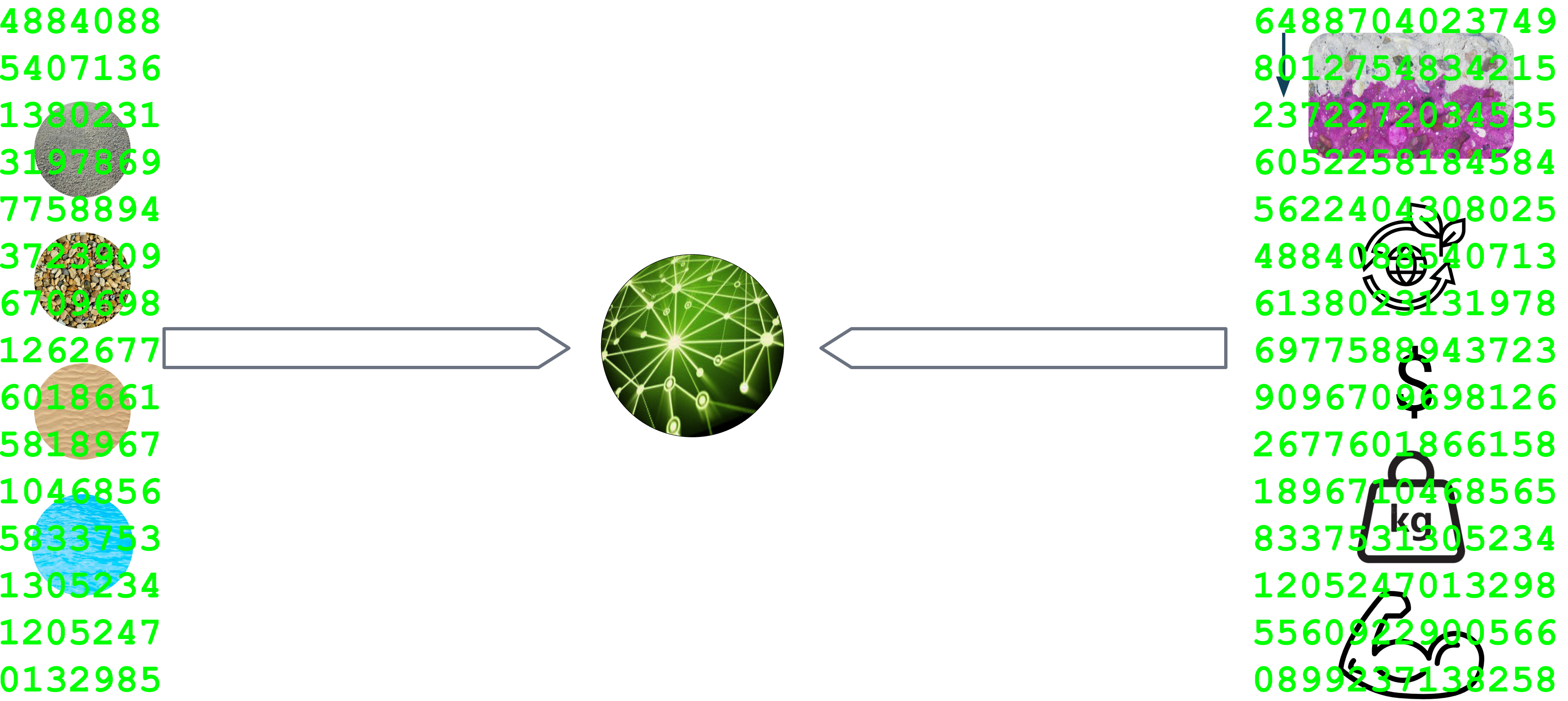
Extract information from noise itself

Training a machine learning model

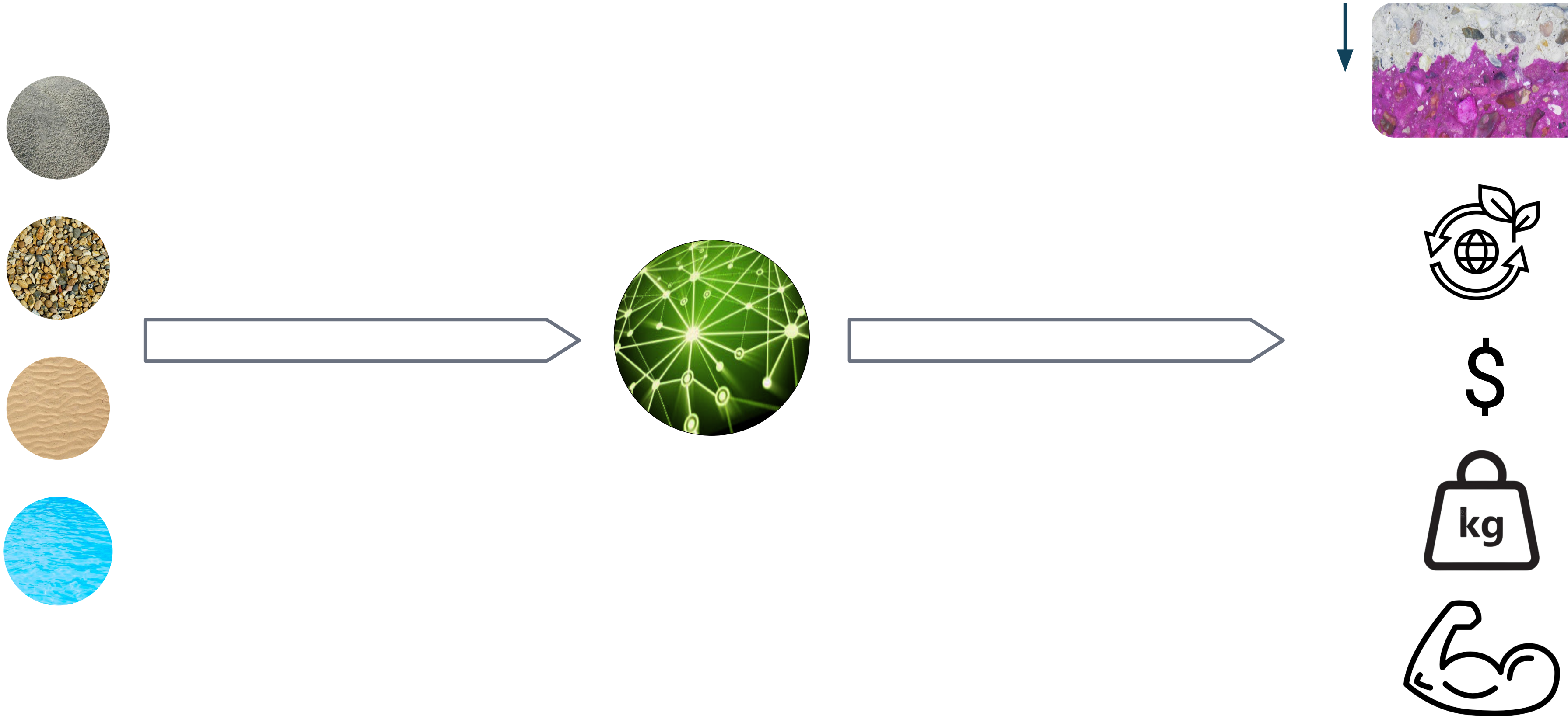
Machine learning



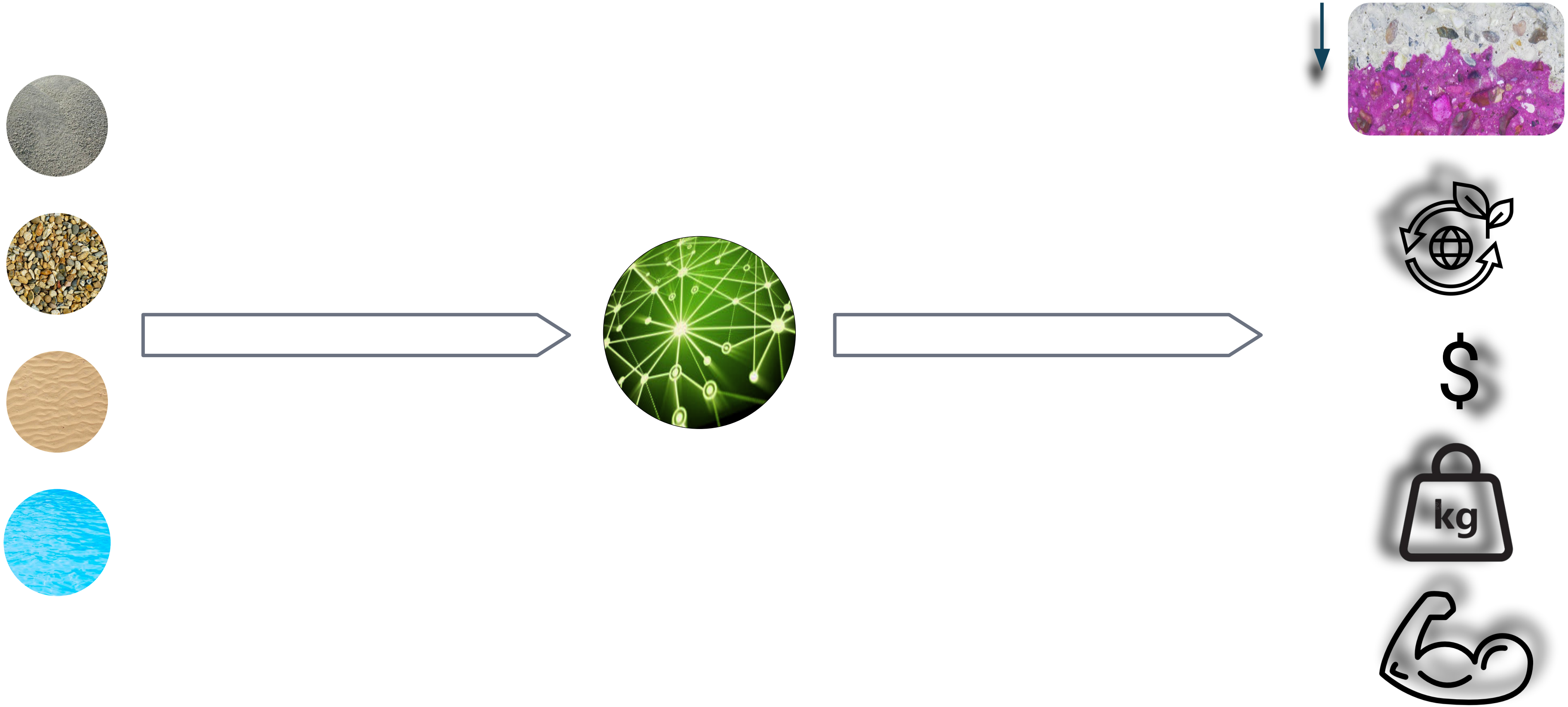
Train the machine learning



Use the machine learning



Machine learning estimates uncertainty



Handling uncertainty

Design formulations

Design of experiments

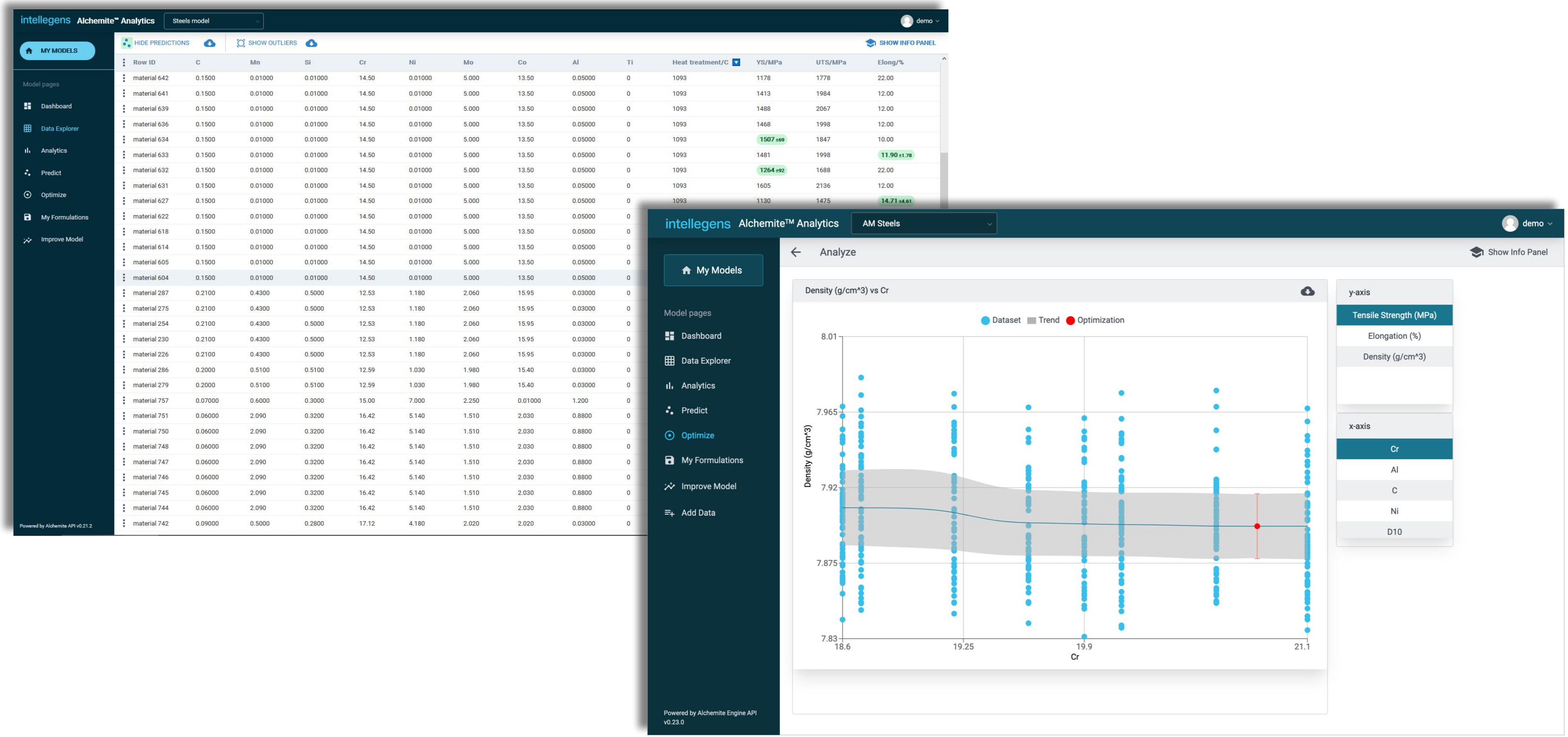
Outlier detection

Unveil the unseen

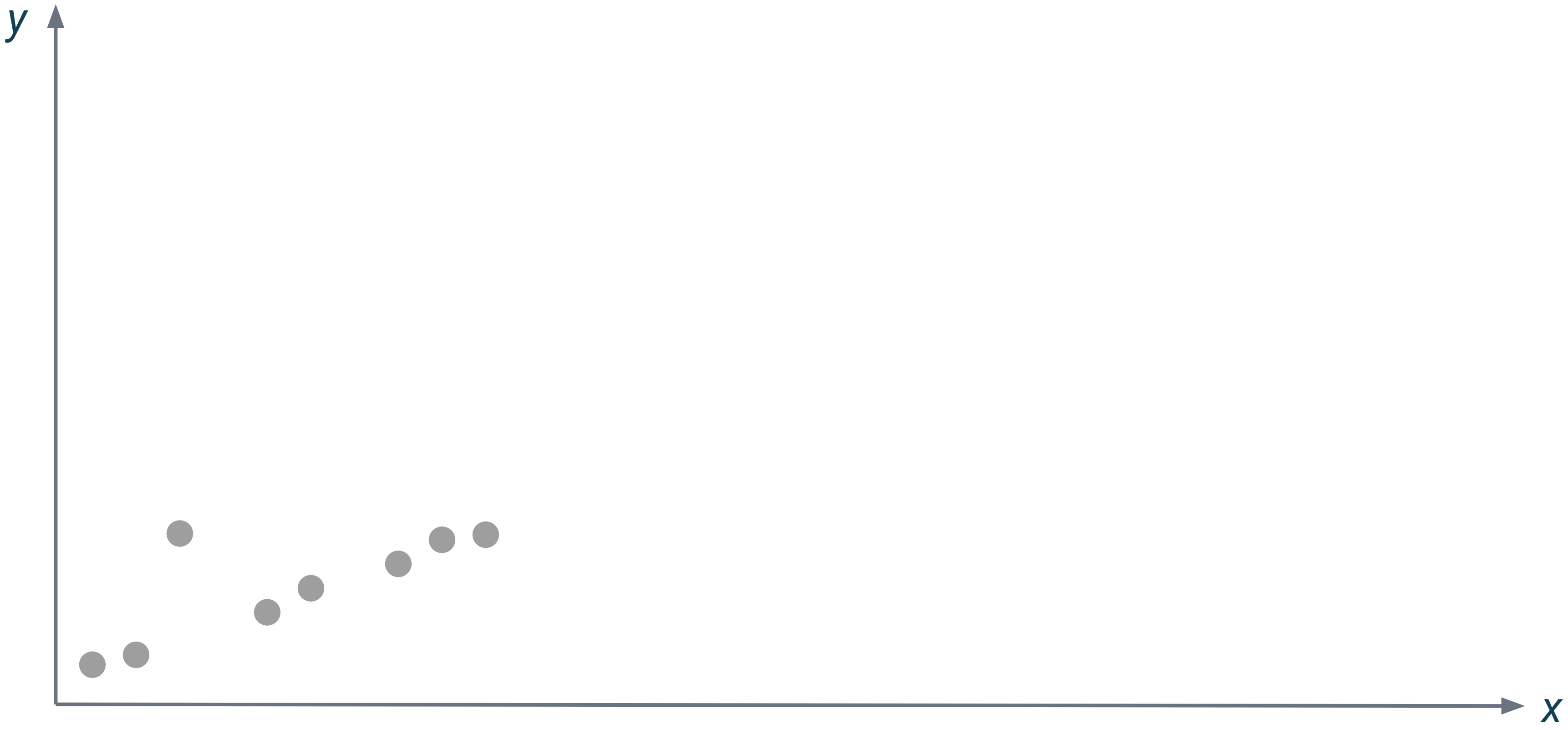
Exploit information hidden in noise

Handling uncertainty

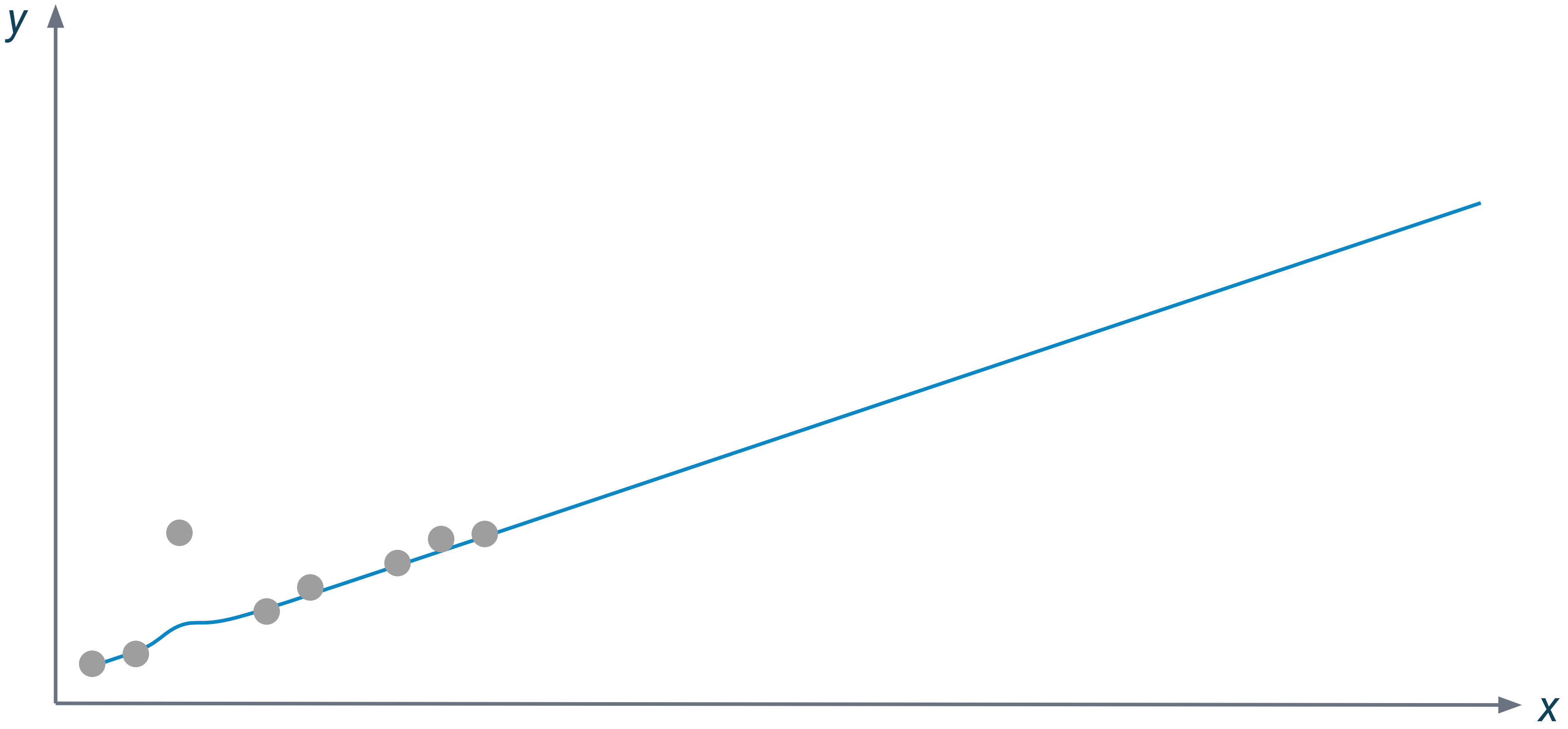
Model within Alchemite™



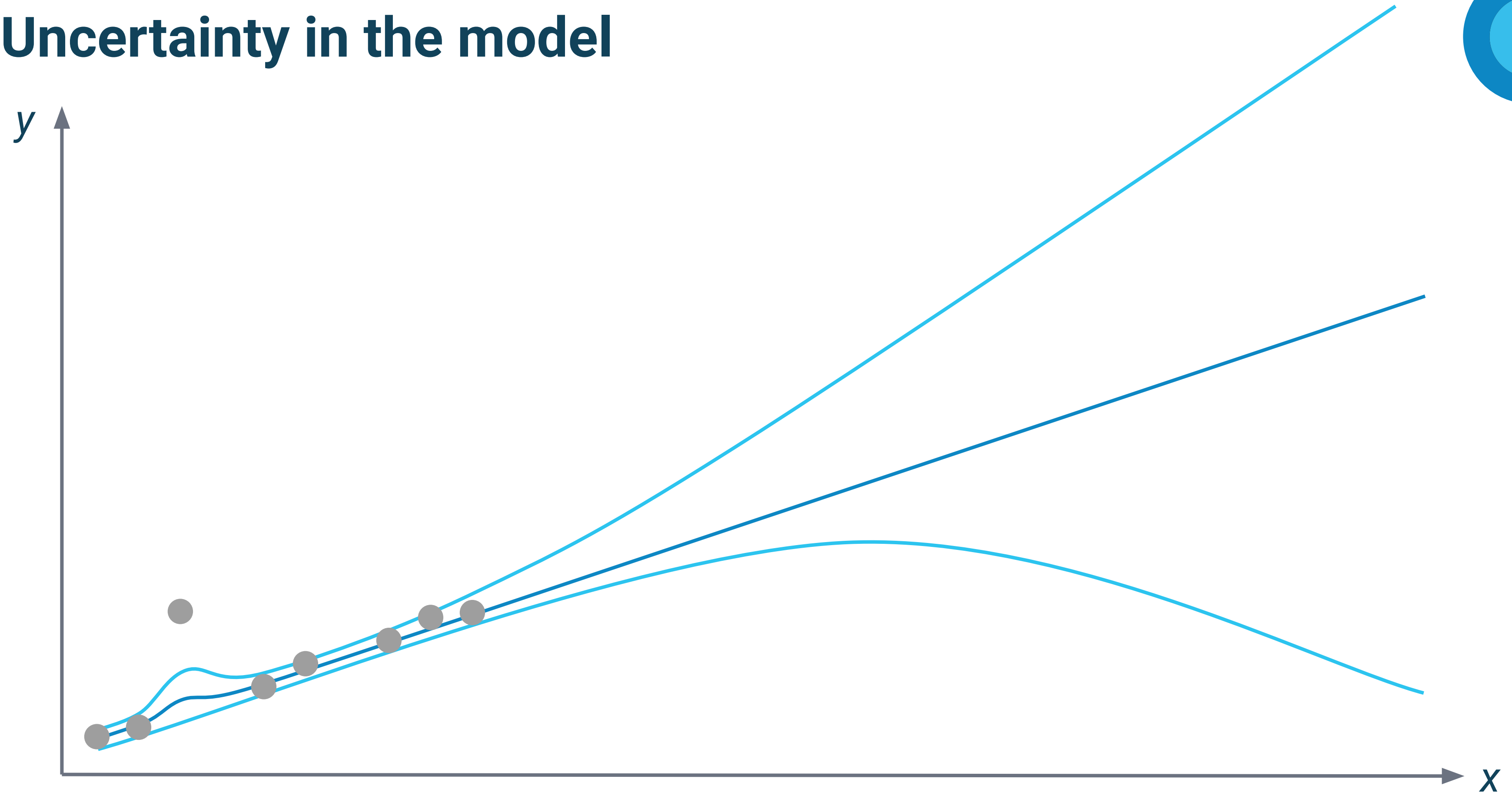
Training data



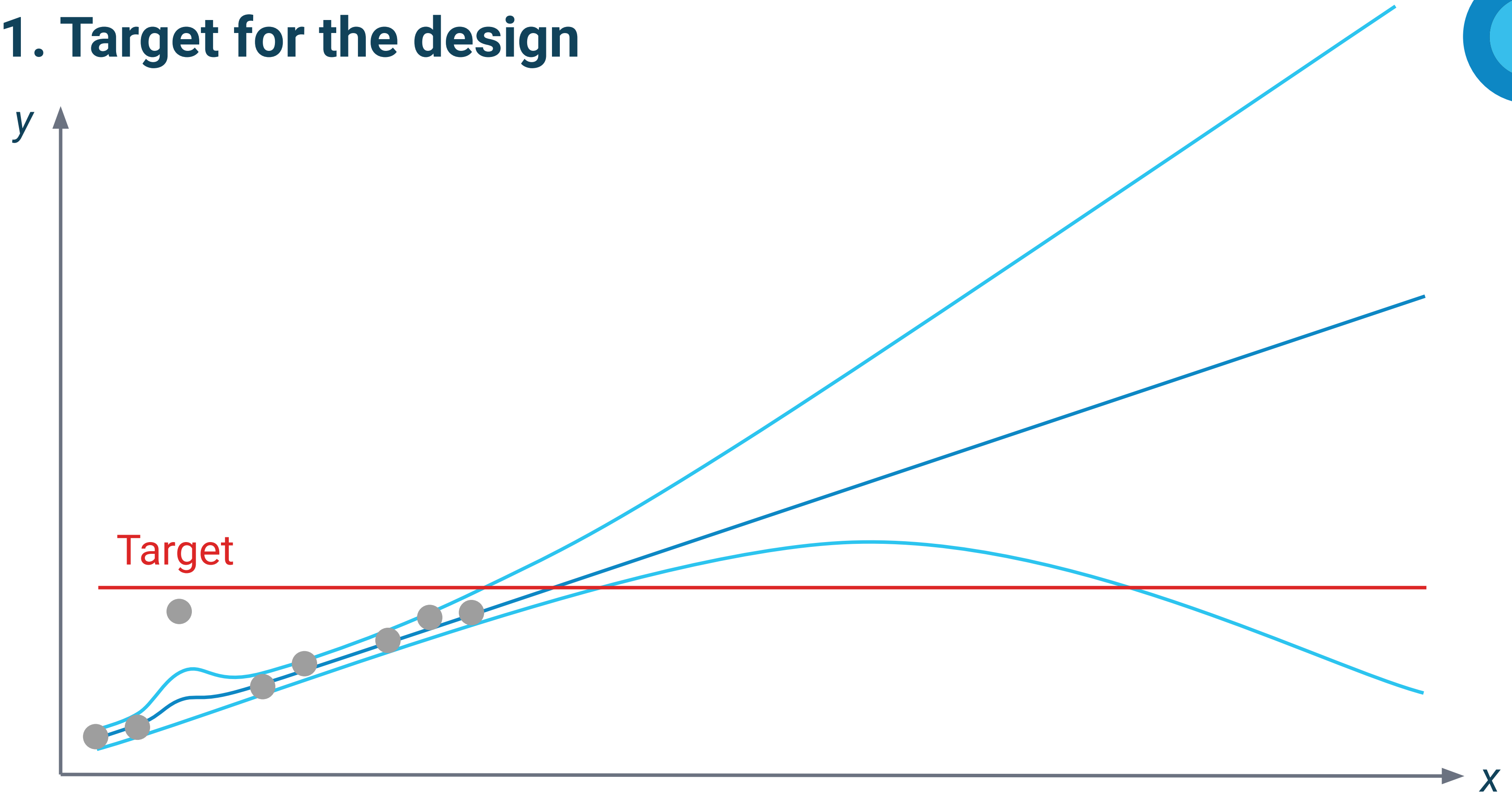
Machine learning model



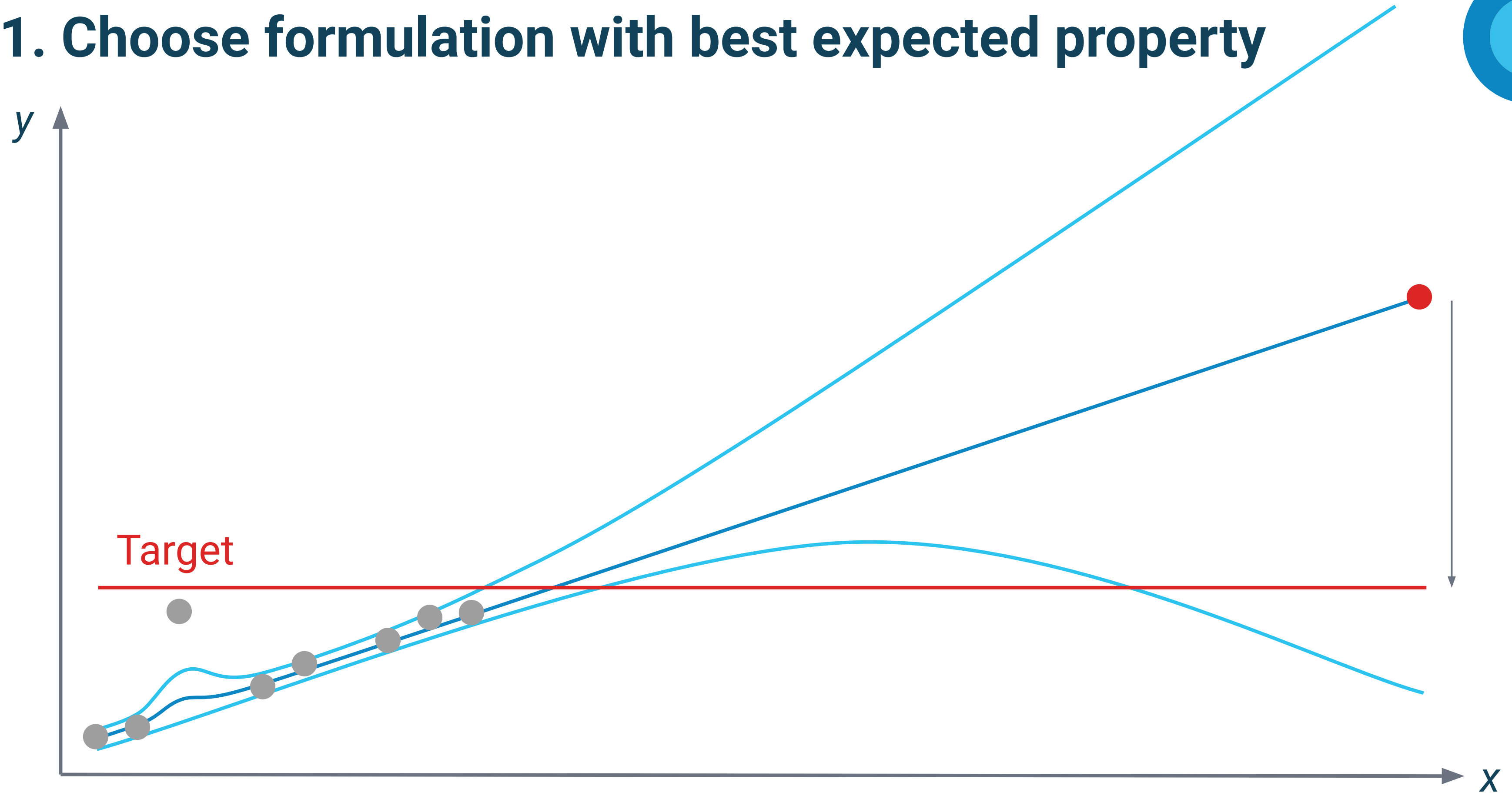
Uncertainty in the model



1. Target for the design



1. Choose formulation with best expected property



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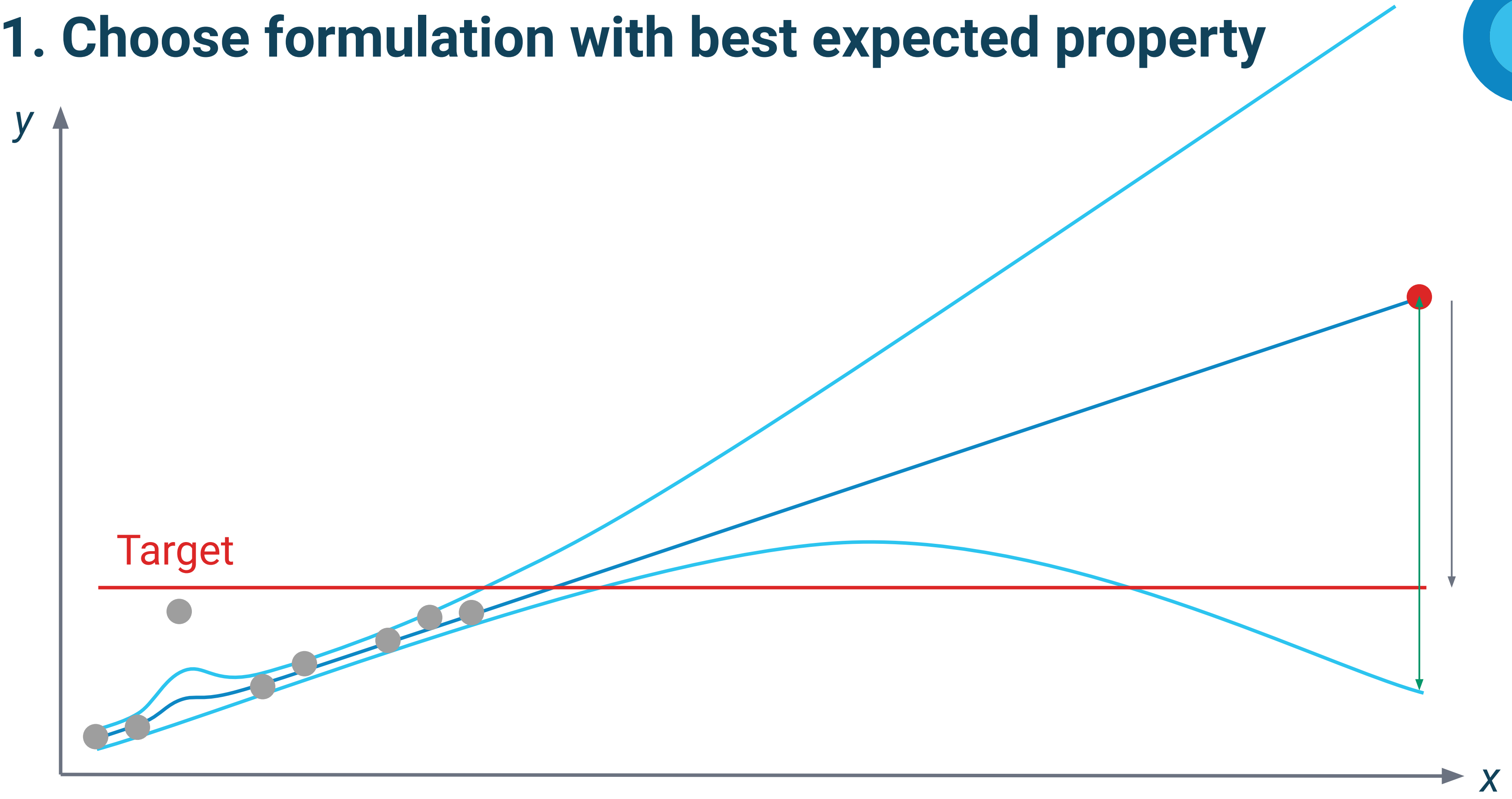
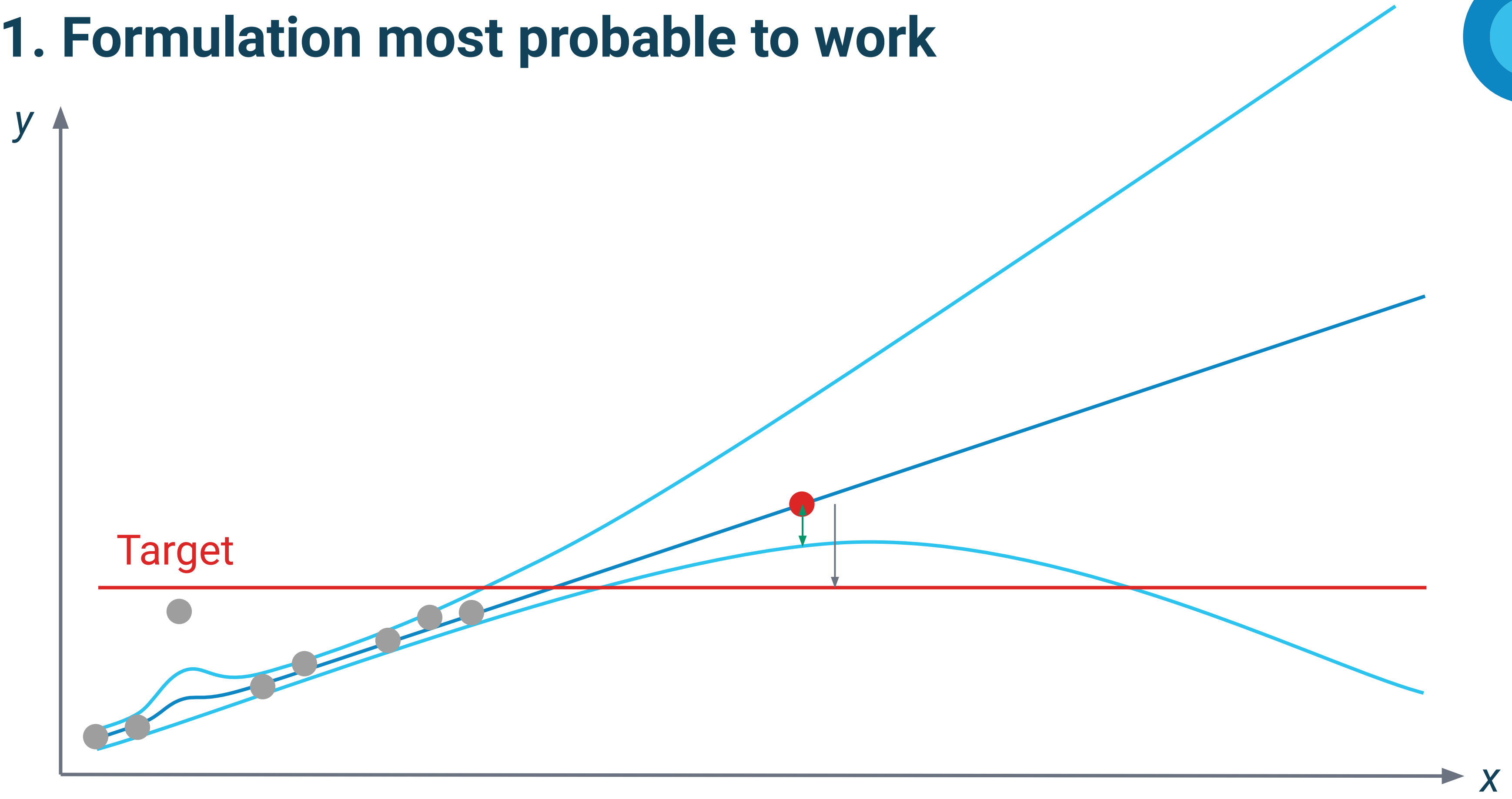
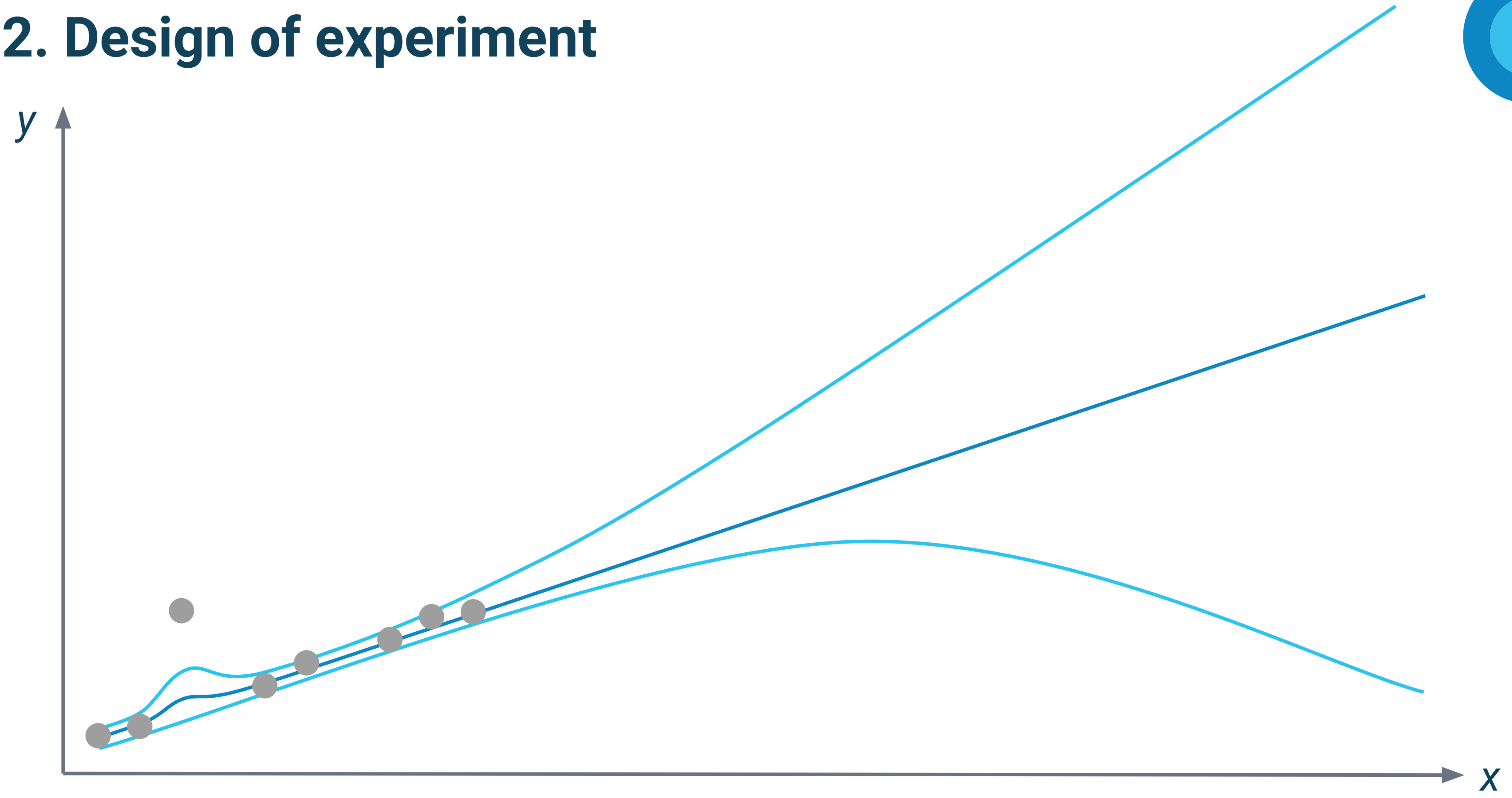


1. Formulation most probable to work

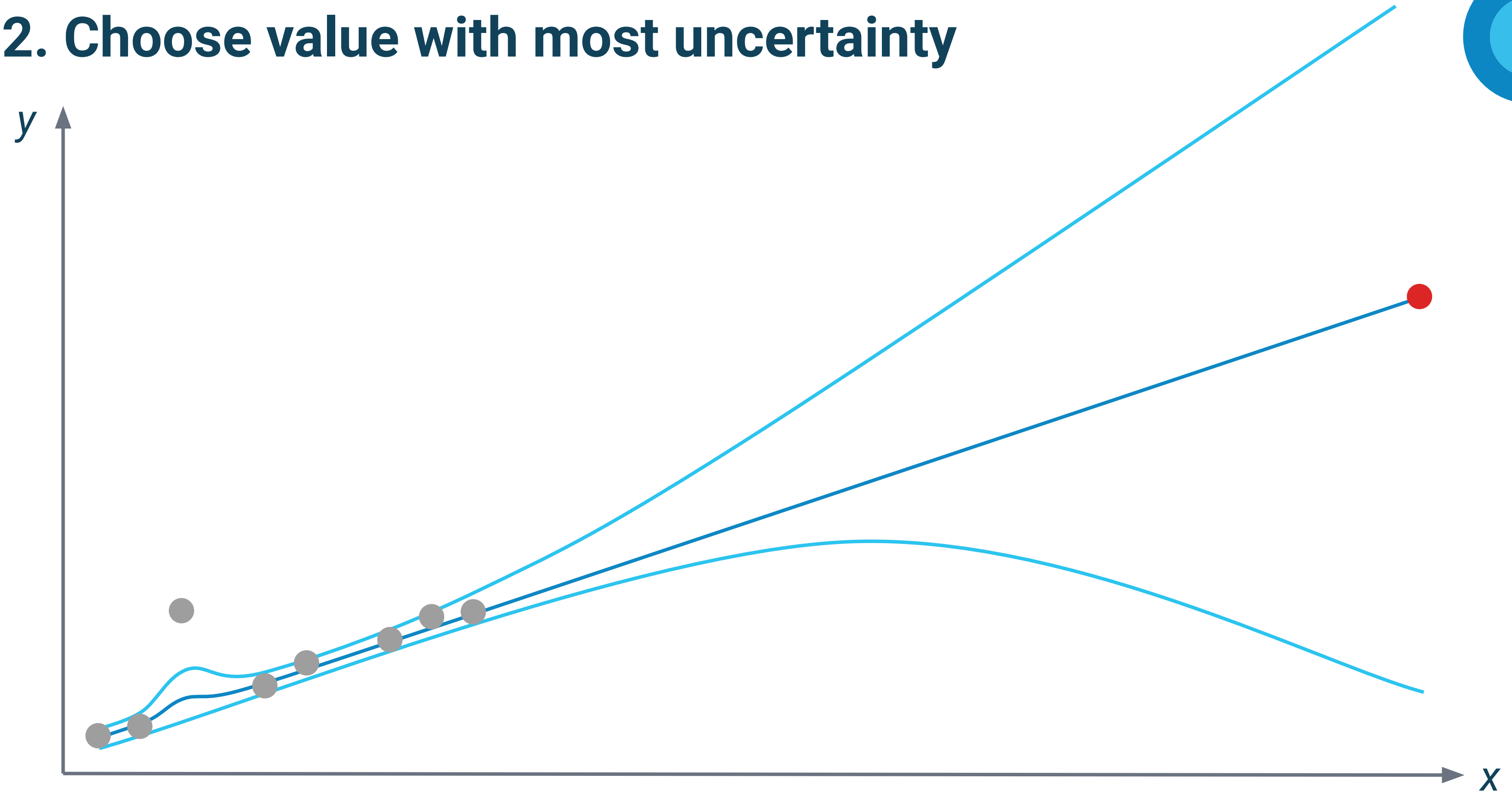


Conduit, Jones, Stone & GJC, Materials & Design **131**, 358 (2017)

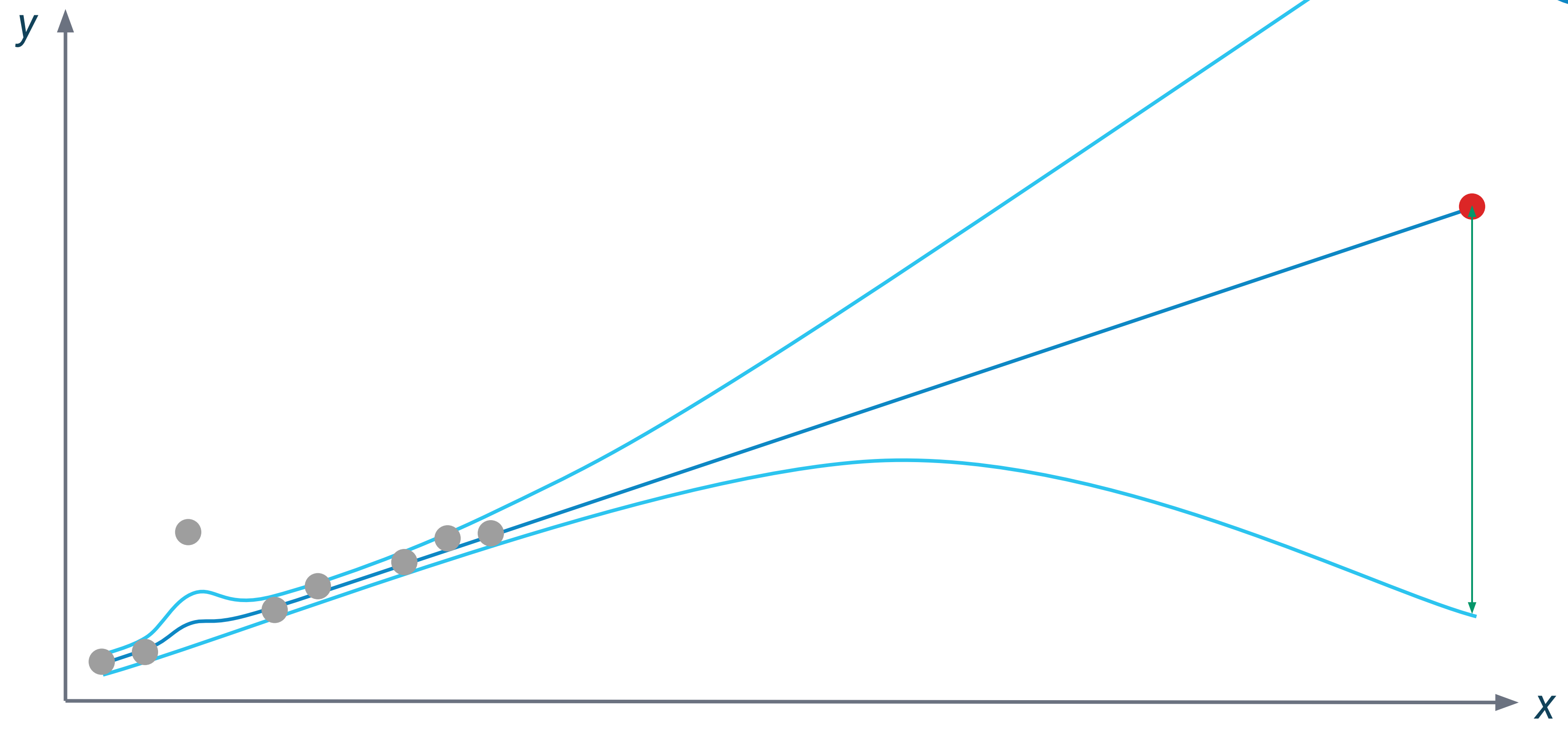
2. Design of experiment



2. Choose value with most uncertainty

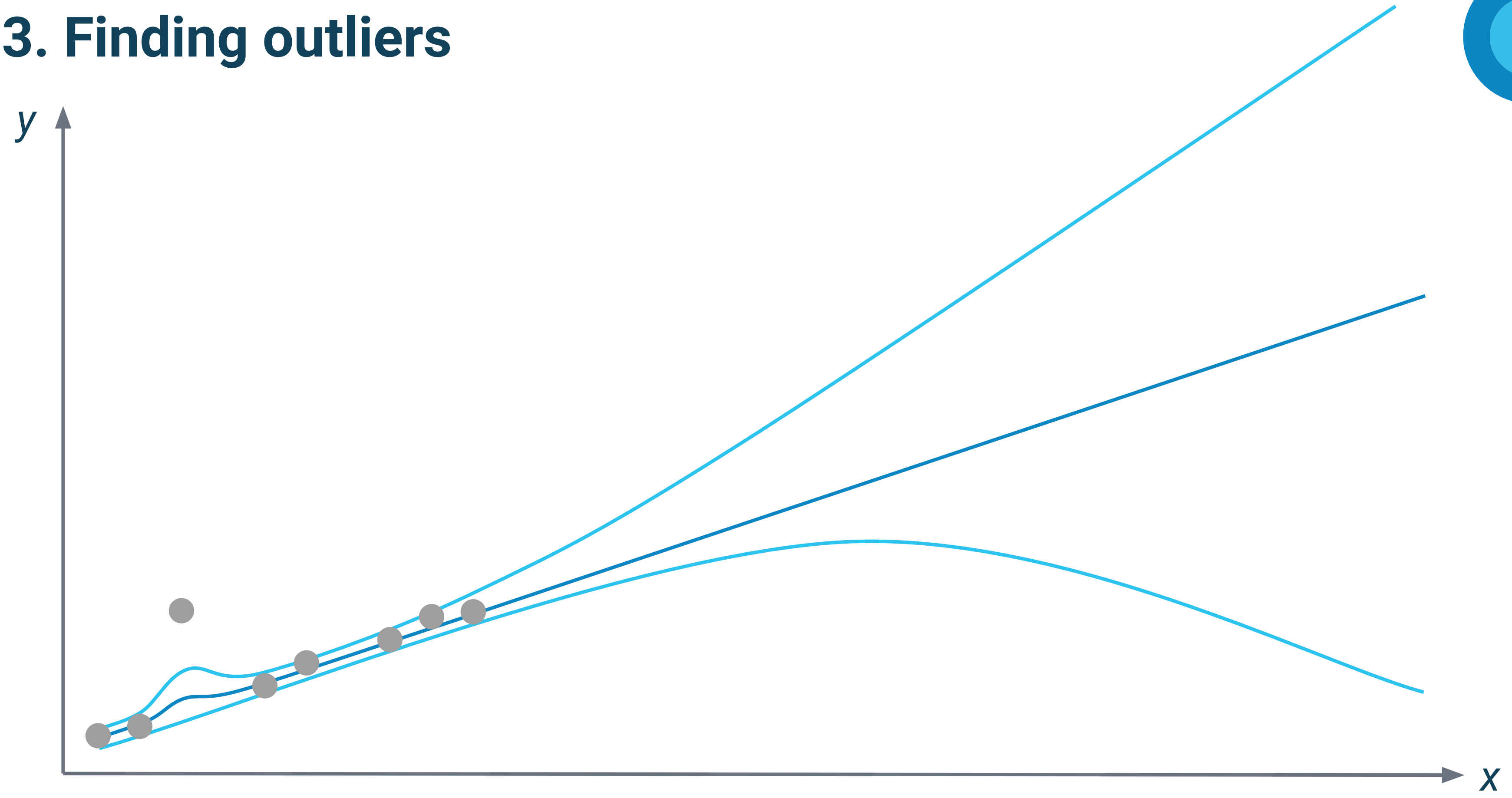


2. Choose value with most uncertainty

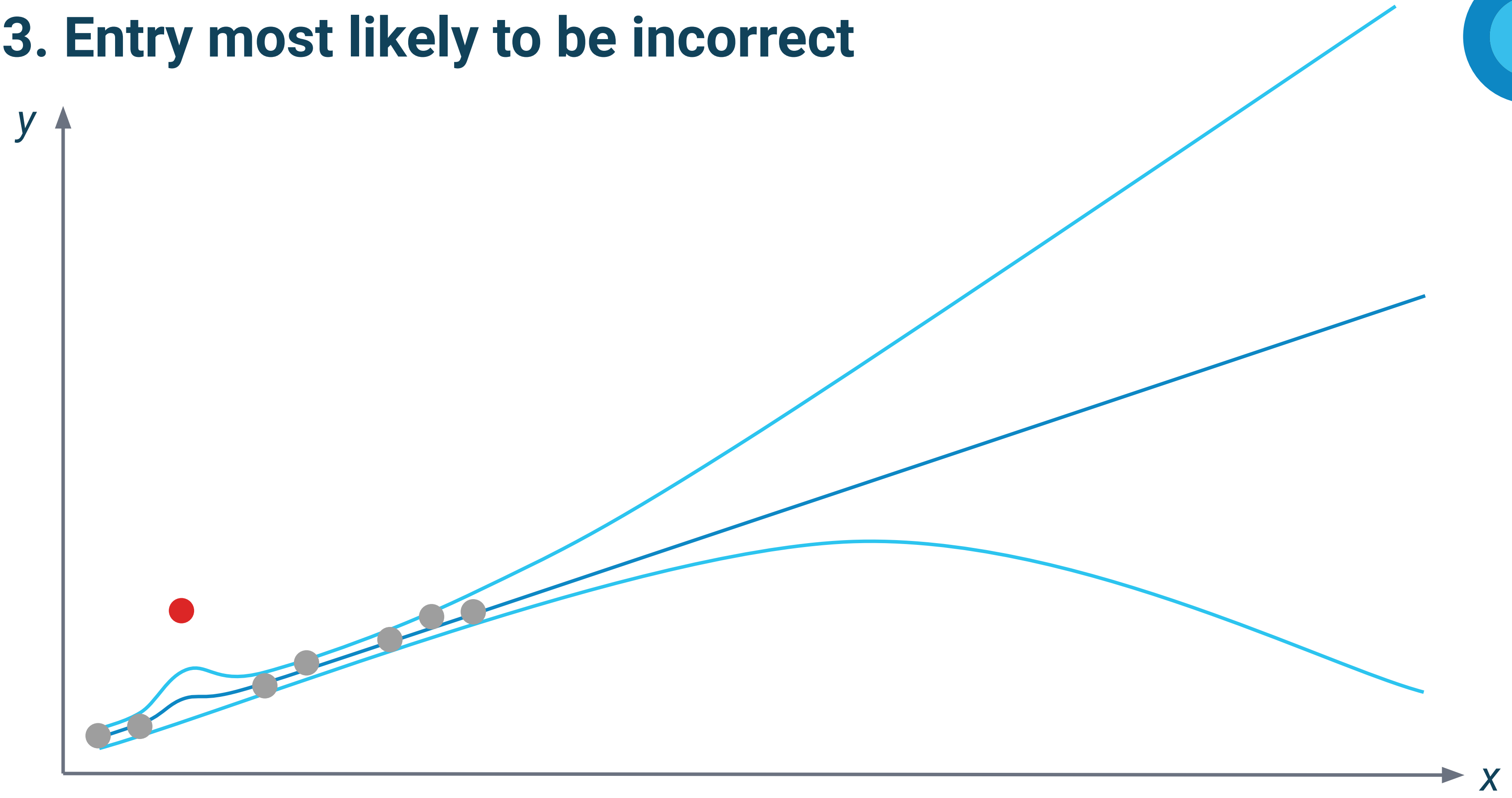


Whitehead, Chen, Daly & GJC, Johnson Matthey Technology Review **66**, 130 (2022)

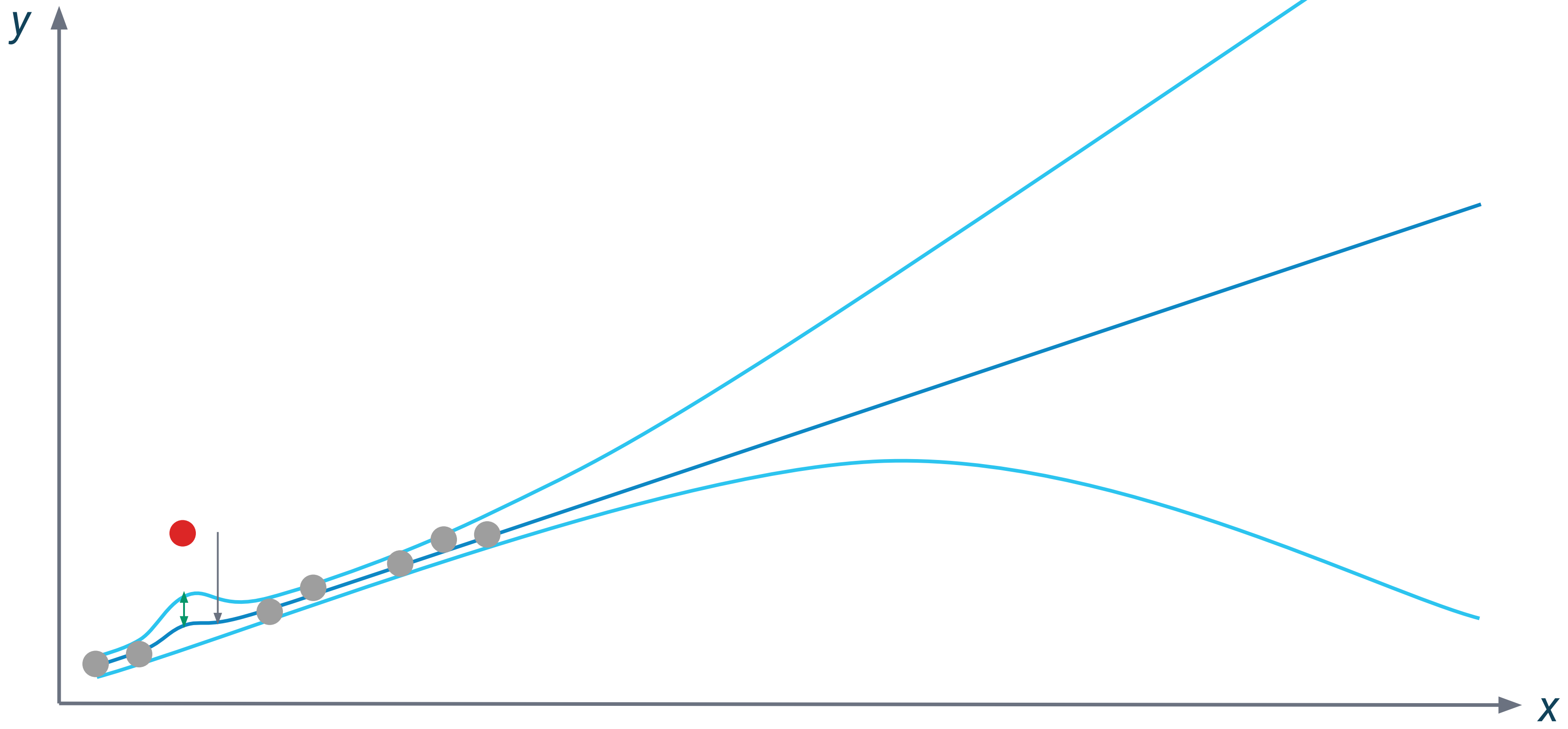
3. Finding outliers



3. Entry most likely to be incorrect



3. Entry most likely to be incorrect



Verpoort, MacDonald & GJC, Computational Materials Science **147**, 176 (2018)

Exploit uncertainty

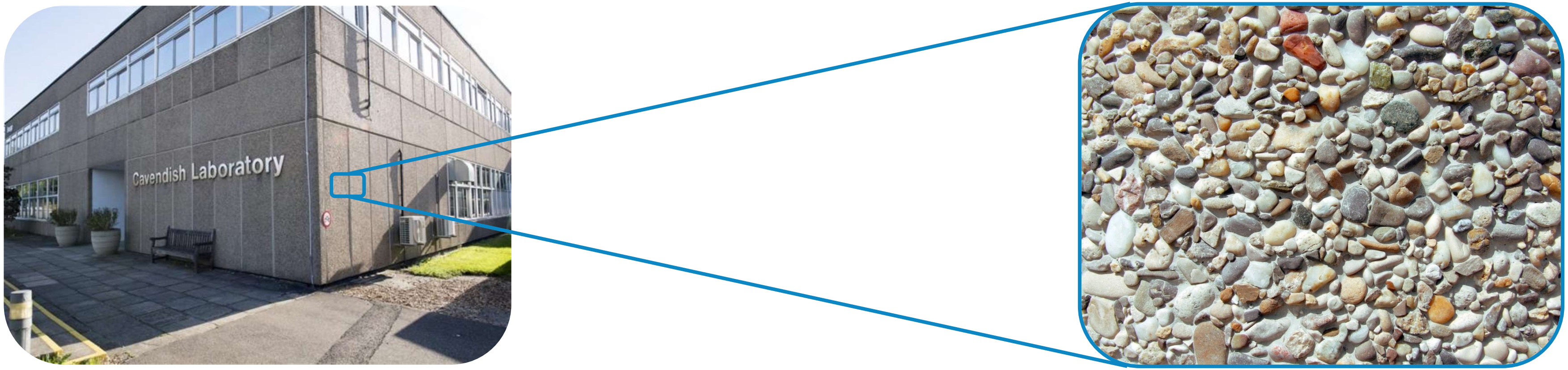
Bogdan Zviazhynski

Dr Gareth Conduit

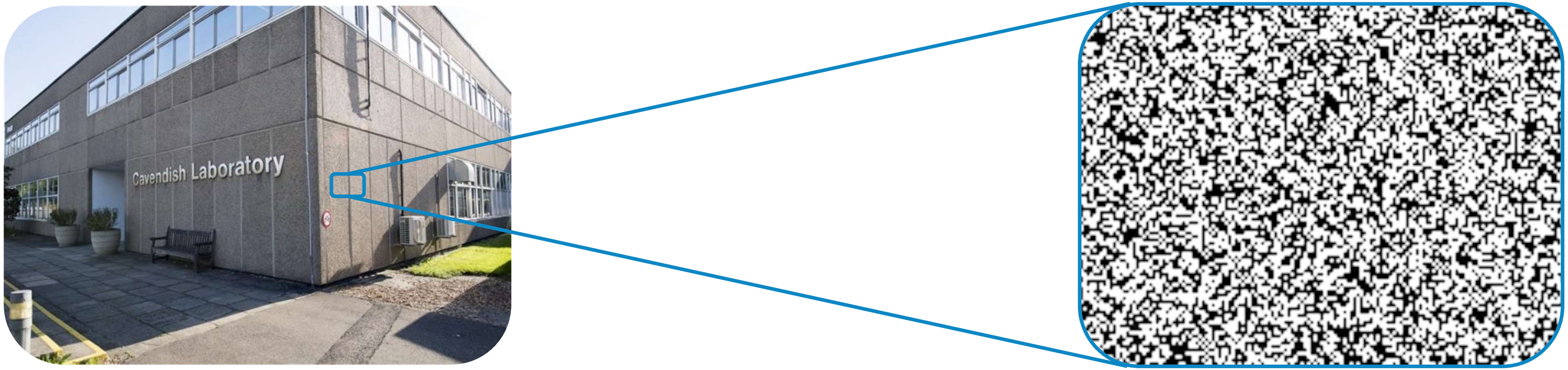
Cavendish Laboratory, University of Cambridge

Concrete in construction

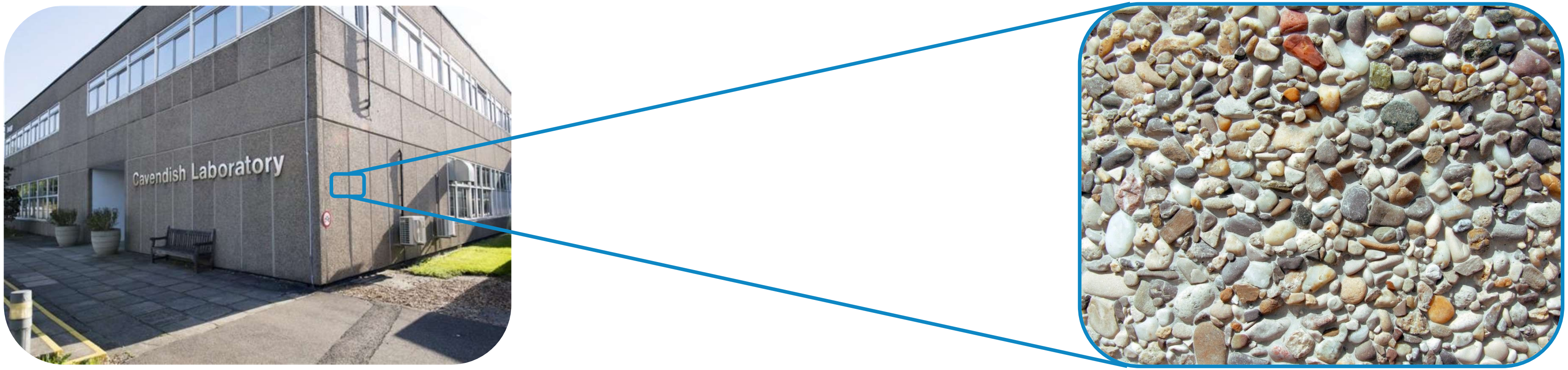
Cement & aggregate look like noise



Cement & aggregate look like noise

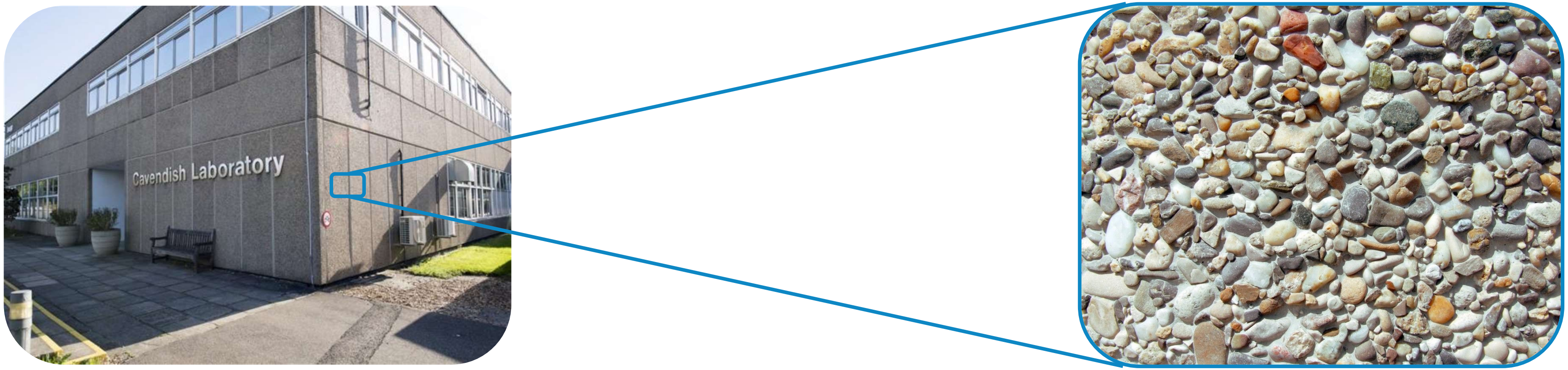


Mission



Design a concrete that is robust and environmentally friendly

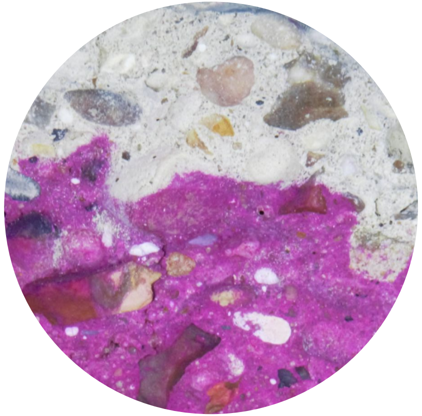
Mission



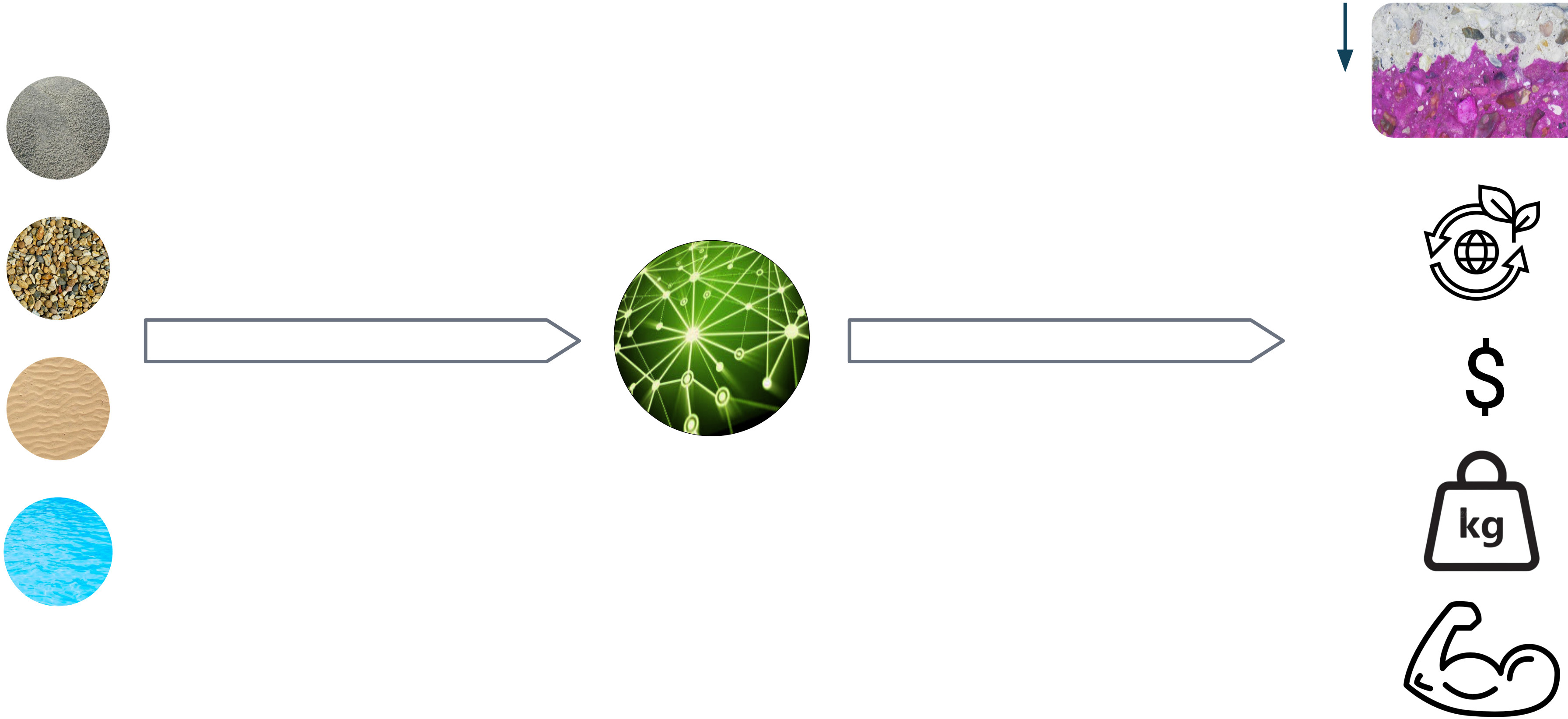
Design a concrete that is robust and environmentally friendly

Experimentally validate the concrete

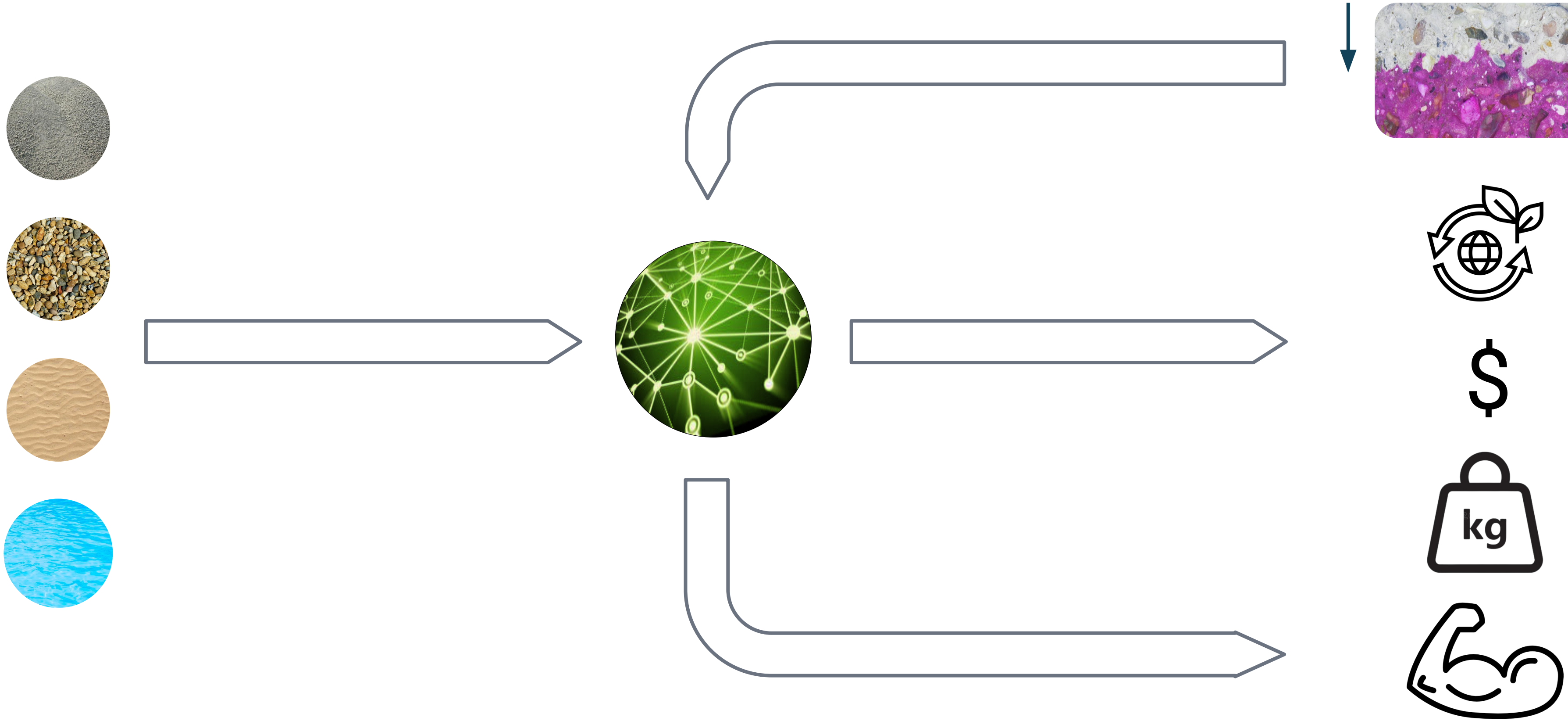
Carbonation



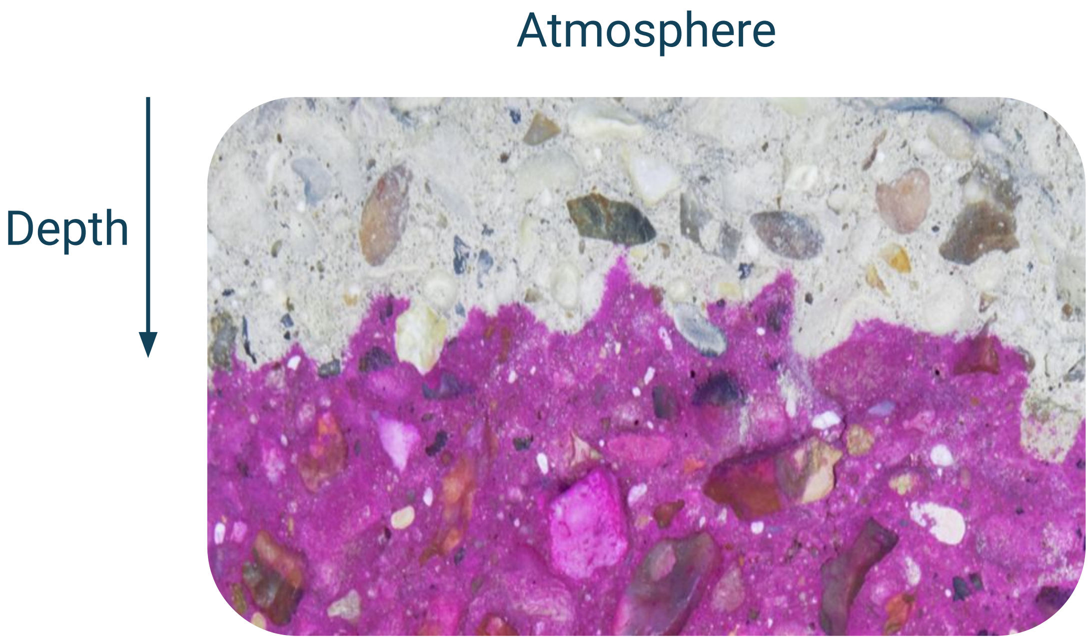
Machine learning



Carbonation depth to strength



Carbonation front

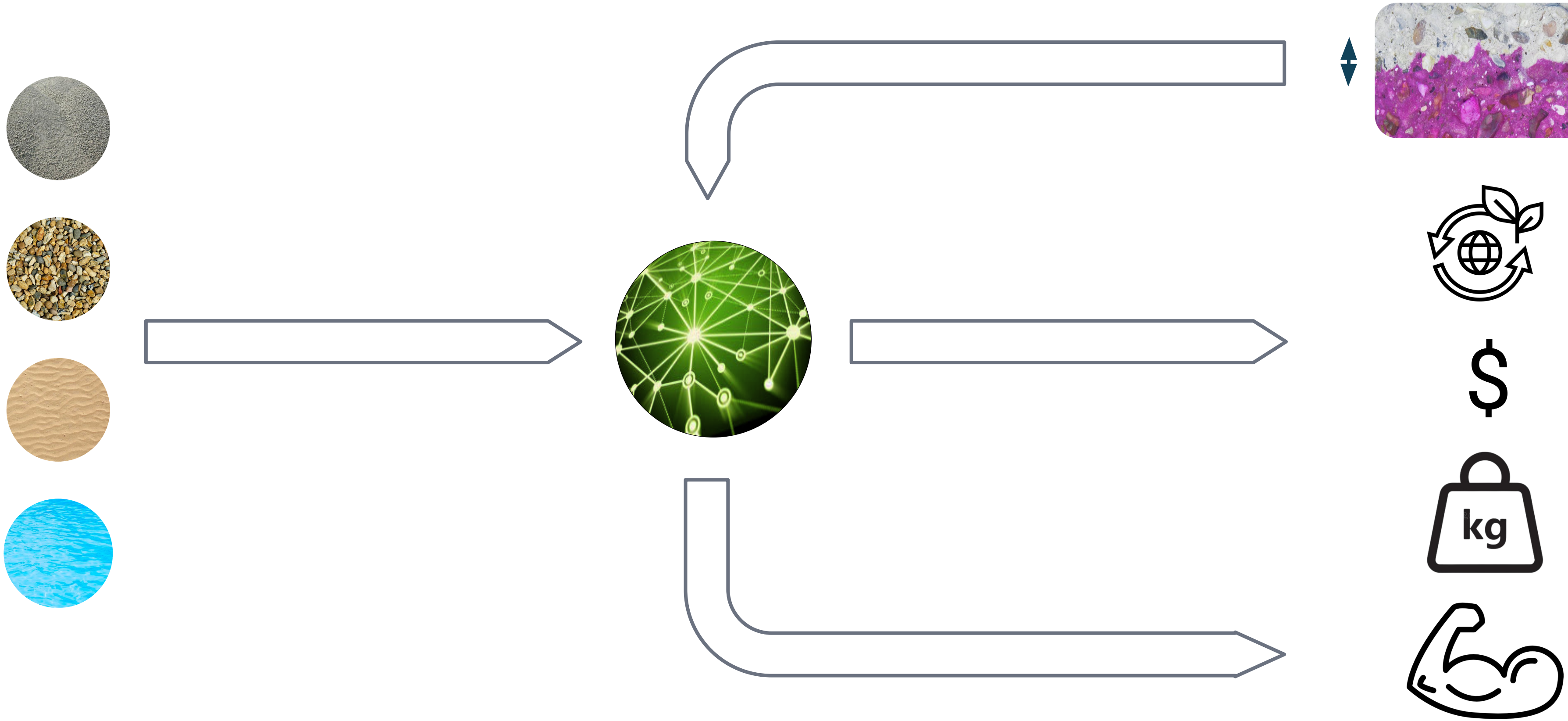


Uncertainty in the carbonation front

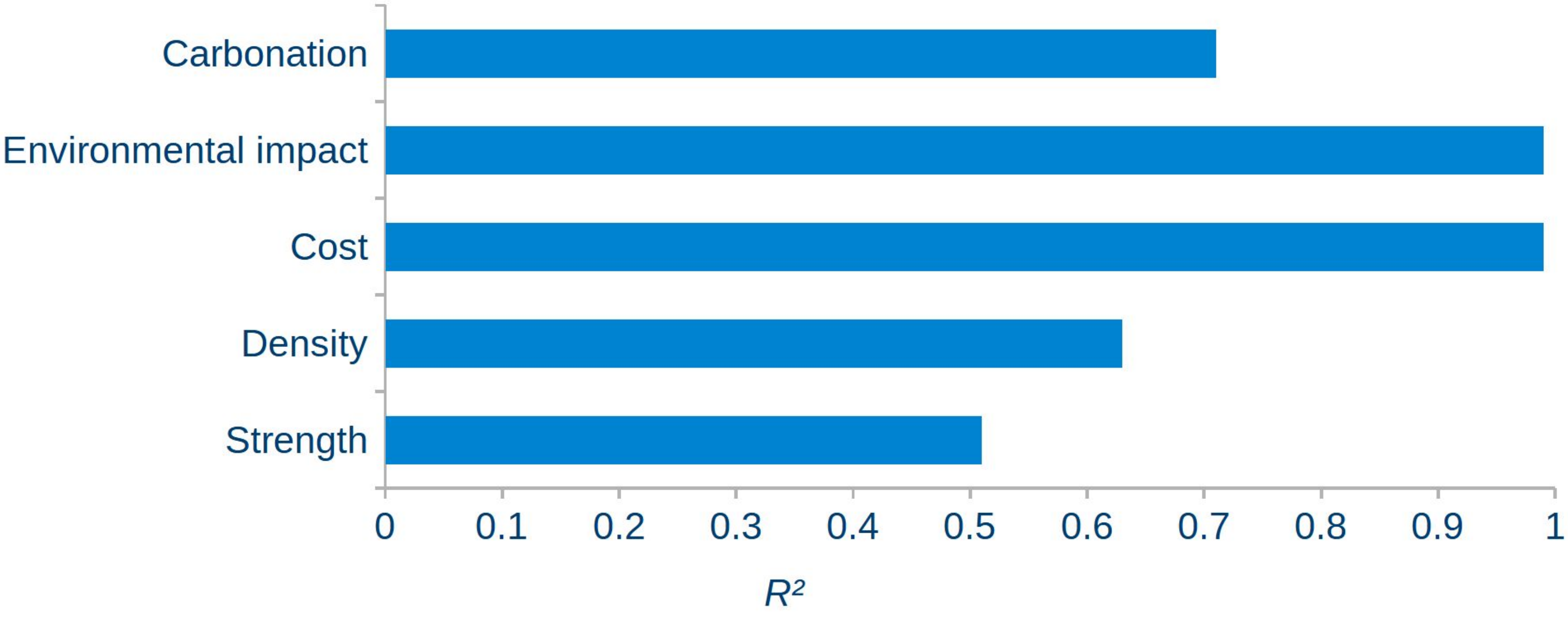
Atmosphere

Uncertainty

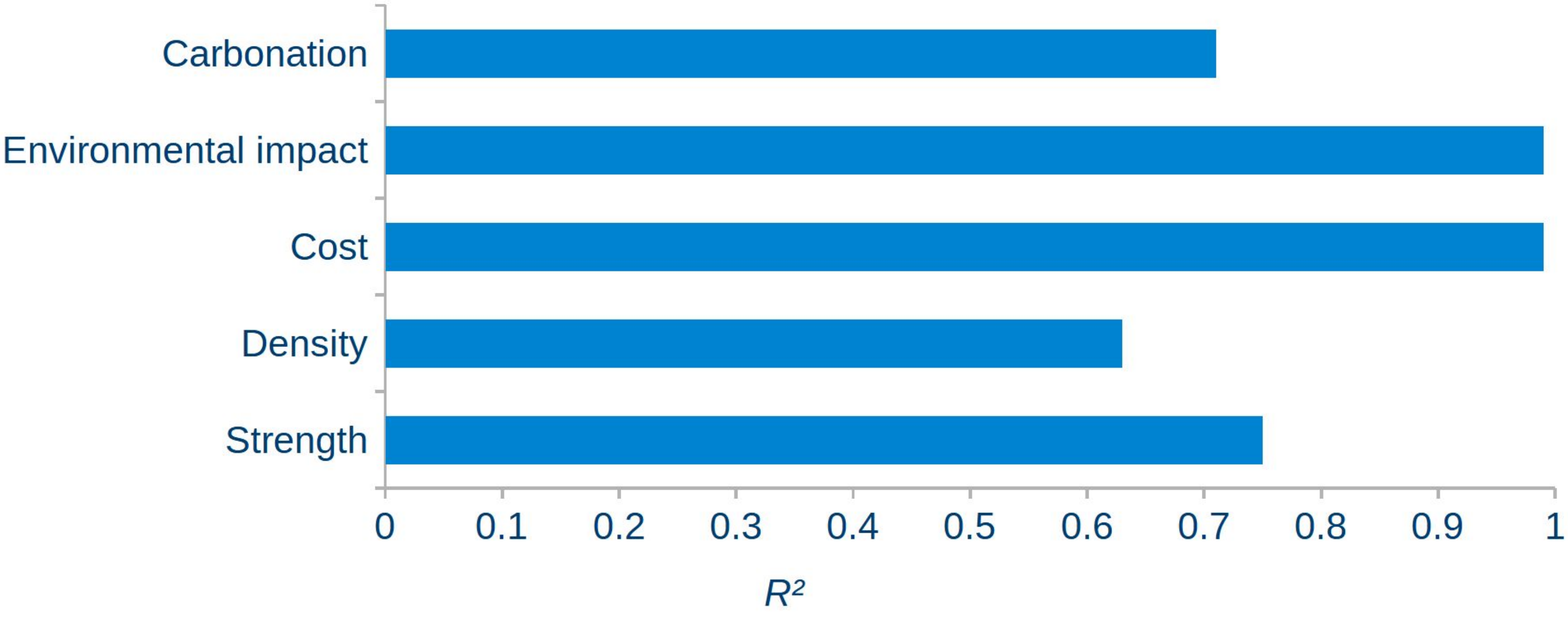
Carbonation depth uncertainty to strength



Original model accuracy



Model accuracy exploiting uncertainty



Concrete specification

First mix		Second mix
⬇️ carbonation		✔ carbonation
✔ environmental impact		⬇️ environmental impact
✔ cost	$	✔ cost
✔ density	kg	✔ density
✔ strength		✔ strength

Concrete design

First mix		Second mix
10.5% cement		14.2% cement
48.4% gravel		48.9% gravel
32.6% sand		28.4% sand
8.5% water		8.5% water

Experimental validation

Jess Forsdyke

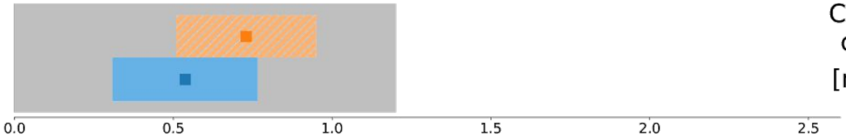
Professor Janet Lees

Civil Engineering, University of Cambridge

Concrete manufacture

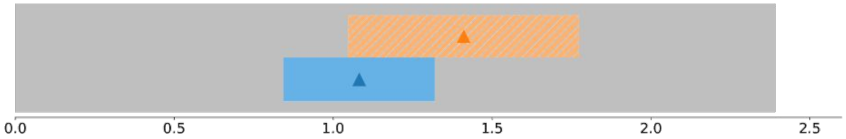
Experimental validation of carbonation coefficient

First mix



Carbonation coefficient $[\mathrm{mm\ day}^{-\frac{1}{2}}]$

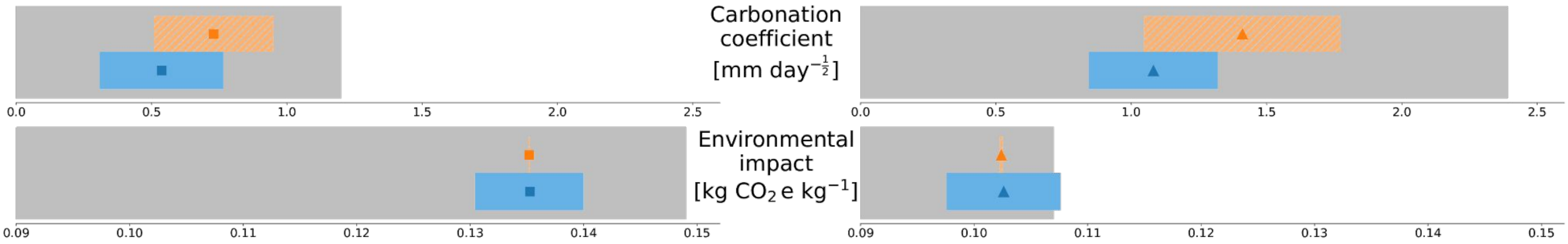
Second mix



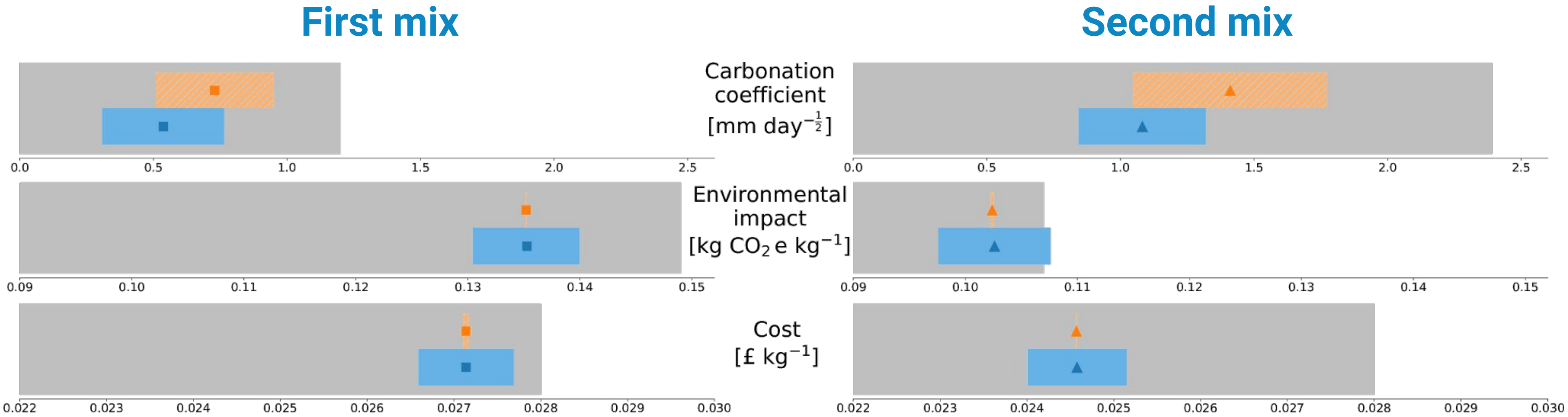
Experimental validation of environmental impact

First mix

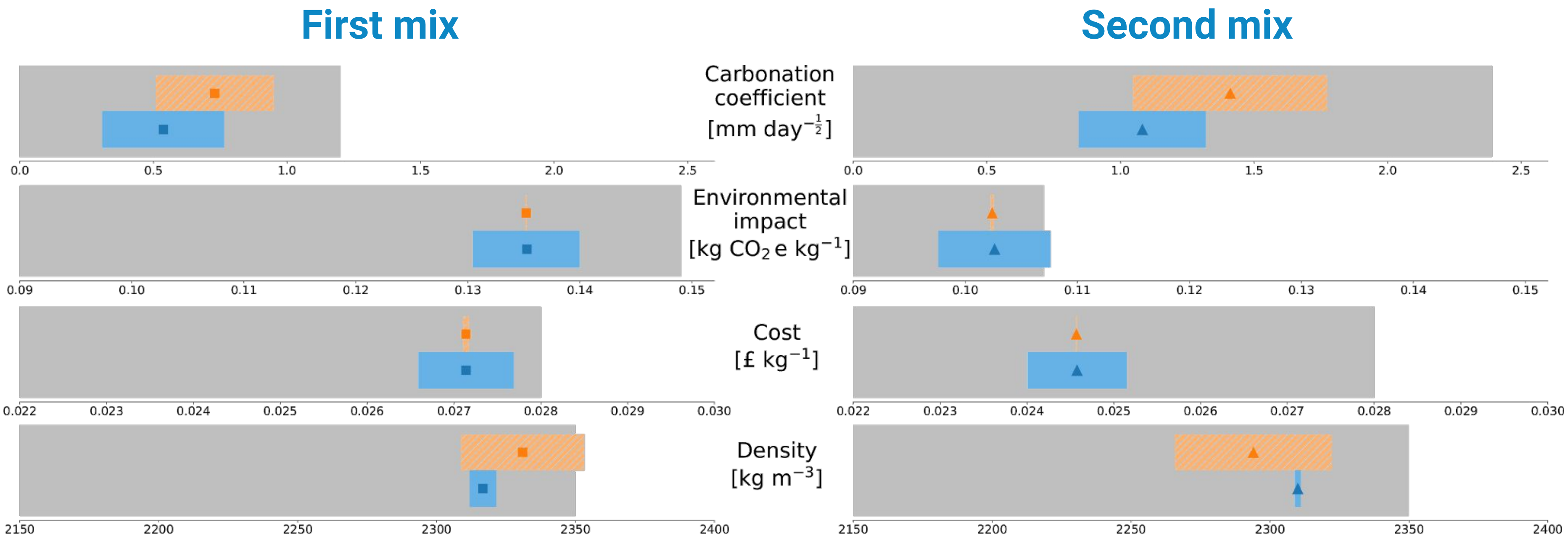
Second mix



Experimental validation of cost



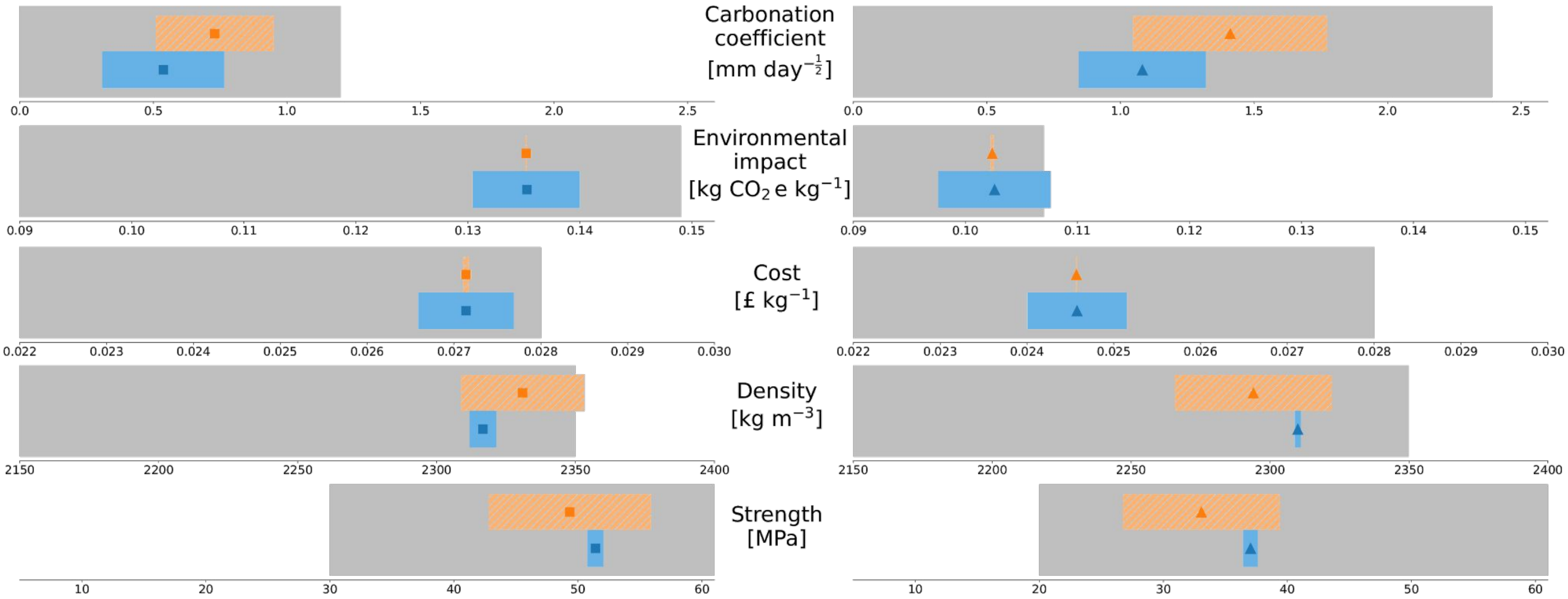
Experimental validation of density



Experimental validation of strength

First mix

Second mix



Summary

Extract information from uncertainty to design two verified concrete mixes

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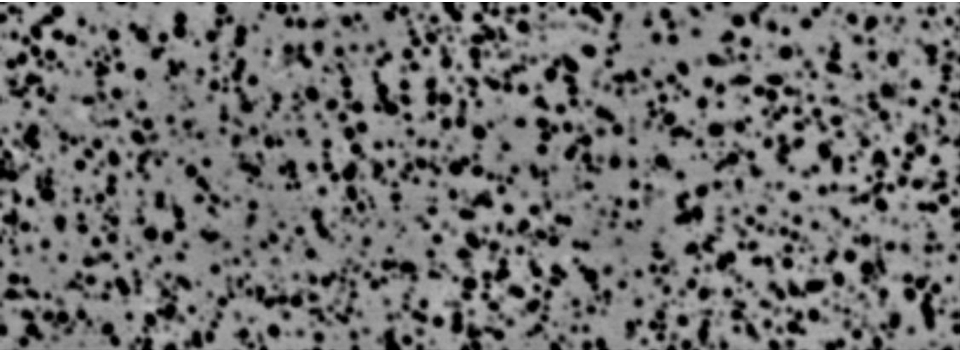
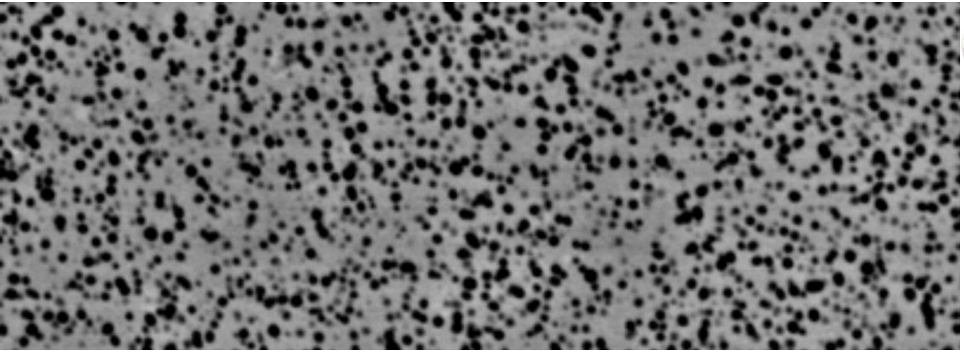
Extract information from uncertainty to design two verified concrete mixes

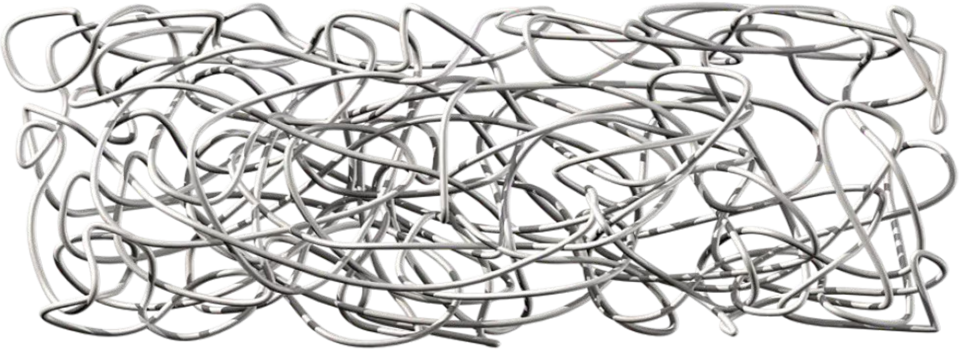


Alloy microstructure has information hidden in the noise

Summary

Extract information from uncertainty to design two verified concrete mixes





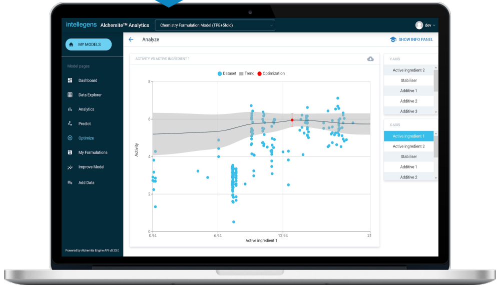
Alloy microstructure has information hidden in the noise

Rubber and plastic tangled polymer chains govern properties

Alchemite™ product

Alchemite™ product family

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



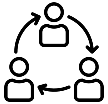
Option to deploy models

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

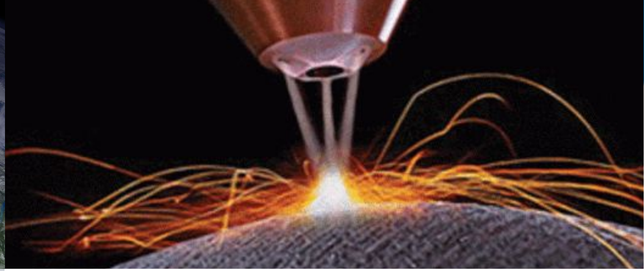
Alchemite™ Engine

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

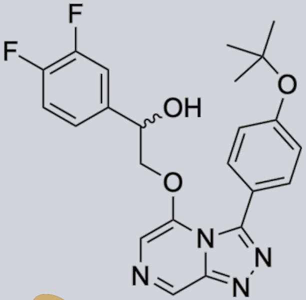
Alchemite™ Success

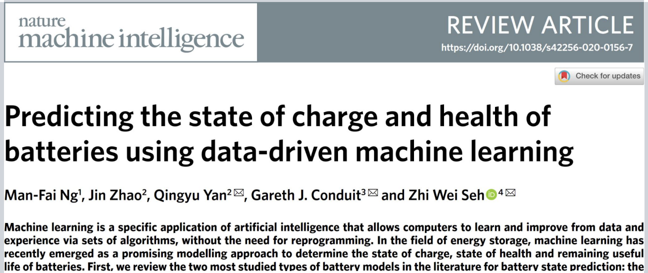
Access Intellegens deep learning expertise

Advice to your data science team or full project management



Heat exchanger
& shape memory
alloy applications





nature machine intelligence

REVIEW ARTICLE

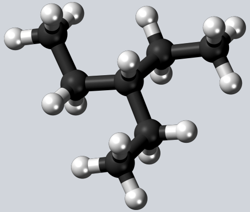
https://doi.org/10.1038/s42256-020-0156-7

Check for updates

Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng[1], Jin Zhao[2], Qingyu Yan[2]✉, Gareth J. Conduit[3]✉ and Zhi Wei Seh[4]✉

Machine learning is a specific application of artificial intelligence that allows computers to learn and improve from data and experience via sets of algorithms, without the need for reprogramming. In the field of energy storage, machine learning has recently emerged as a promising modelling approach to determine the state of charge, state of health and remaining useful life of batteries. First, we review the two most studied types of battery models in the literature for battery state prediction: the



Nature Machine Intelligence
2, 161 (2020)

Fluid Phase Equilibria
501, 112259 (2019)

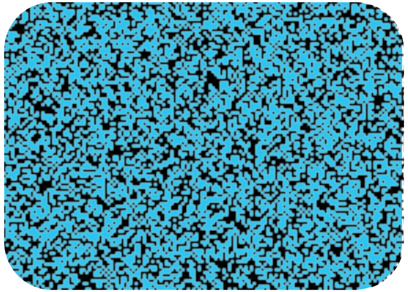
Journal of Chemical Physics
153, 014102 (2020)

Alchemite™ summary

Applied machine learning

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

Extract more value from real-world, sparse, noisy data



Extract unseen information out of noise itself

Save time and cost with up to 90% fewer experiments

Next steps

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