



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

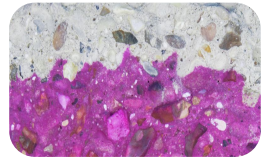
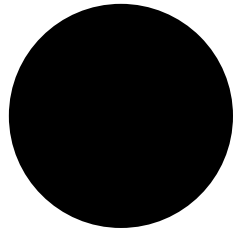
Exploit **uncertainties** to deliver most robust predictions to customers

Extract information from **noise** itself



Training a machine learning model

Machine learning



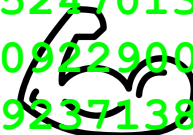
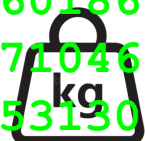
Train the machine learning



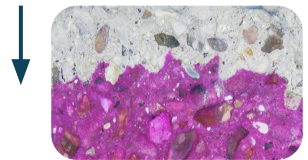
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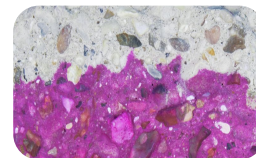
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Use the machine learning



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™

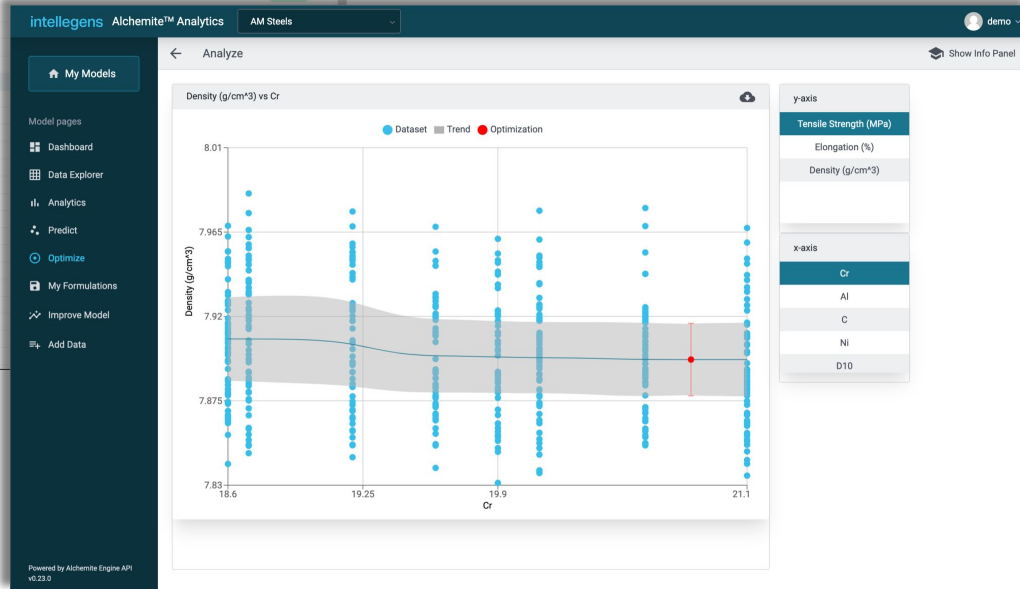


intelligens Alchemite™ Analytics Steels model demo

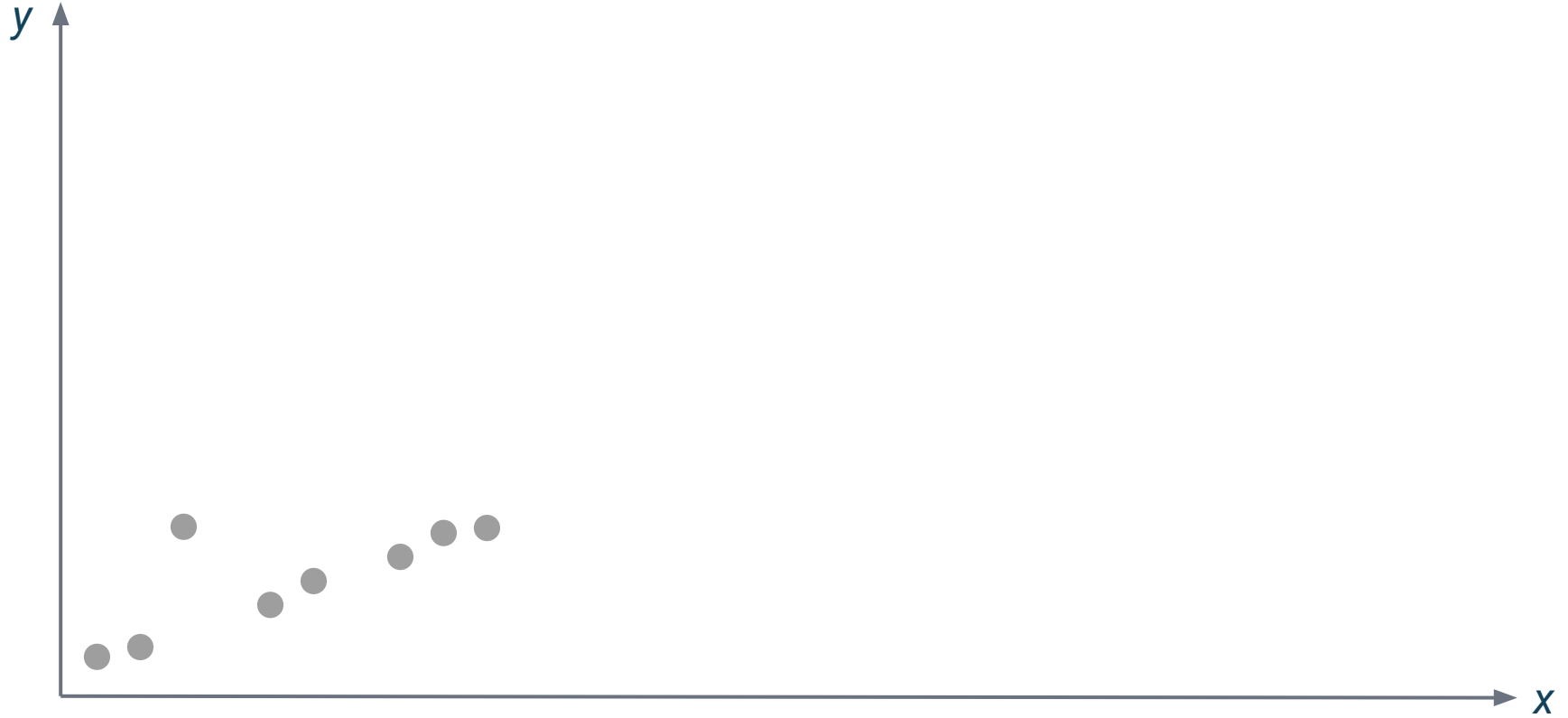
MY MODELS

Model pages: Dashboard, Data Explorer, Analytics, Predict, Optimize, My Formulations, Improve Model

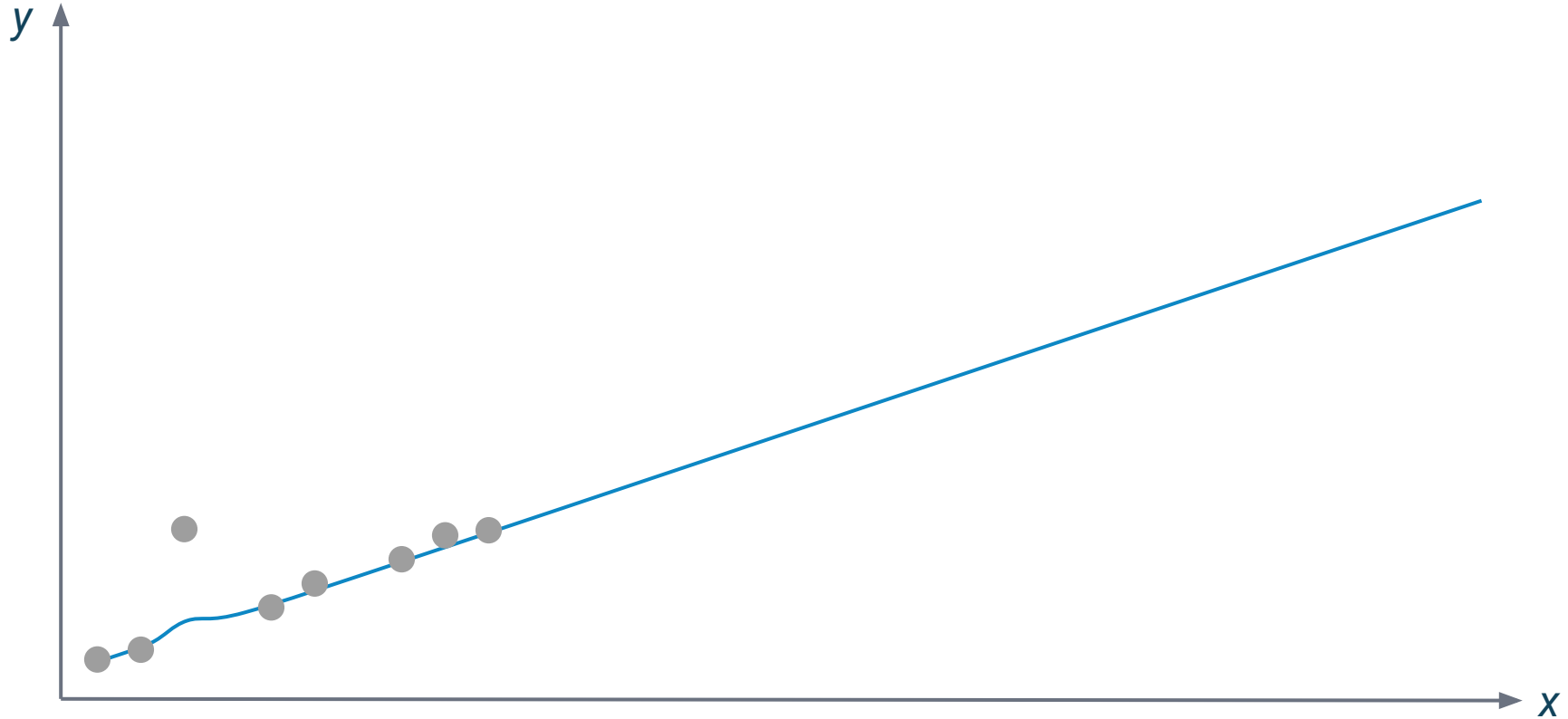
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material 636	0.1900	0.01000	0.01000	14.50	0.01000	5.000	13.50	0.05000	0	1093	1468	1998	12.00
material 634	0.1900	0.01000	0.01000	14.50	0.01000	5.000	13.50	0.05000	0	1093	1507⁺⁹⁹	1847	10.00
material 633	0.1900	0.01000	0.01000	14.50	0.01000	5.000	13.50	0.05000	0	1093	1481	1998	11.90⁺⁷⁸
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material 254	0.2100	0.4300	0.5000	12.53	1.180	2.060	15.95	0.03000	0				
material 230	0.2100	0.4300	0.5000	12.53	1.180	2.060	15.95	0.03000	0				
material 226	0.2100	0.4300	0.5000	12.53	1.180	2.060	15.95	0.03000	0				
material 286	0.2000	0.5100	0.5100	12.59	1.030	1.980	15.40	0.03000	0				
material 279	0.2000	0.5100	0.5100	12.59	1.030	1.980	15.40	0.03000	0				
material 757	0.07000	0.6000	0.3000	15.00	7.000	2.250	0.01000	1.200	0				
material 751	0.06000	2.090	0.3200	16.42	5.140	1.510	2.030	0.8800	0				
material 750	0.06000	2.090	0.3200	16.42	5.140	1.510	2.030	0.8800	0				
material 748	0.06000	2.090	0.3200	16.42	5.140	1.510	2.030	0.8800	0				
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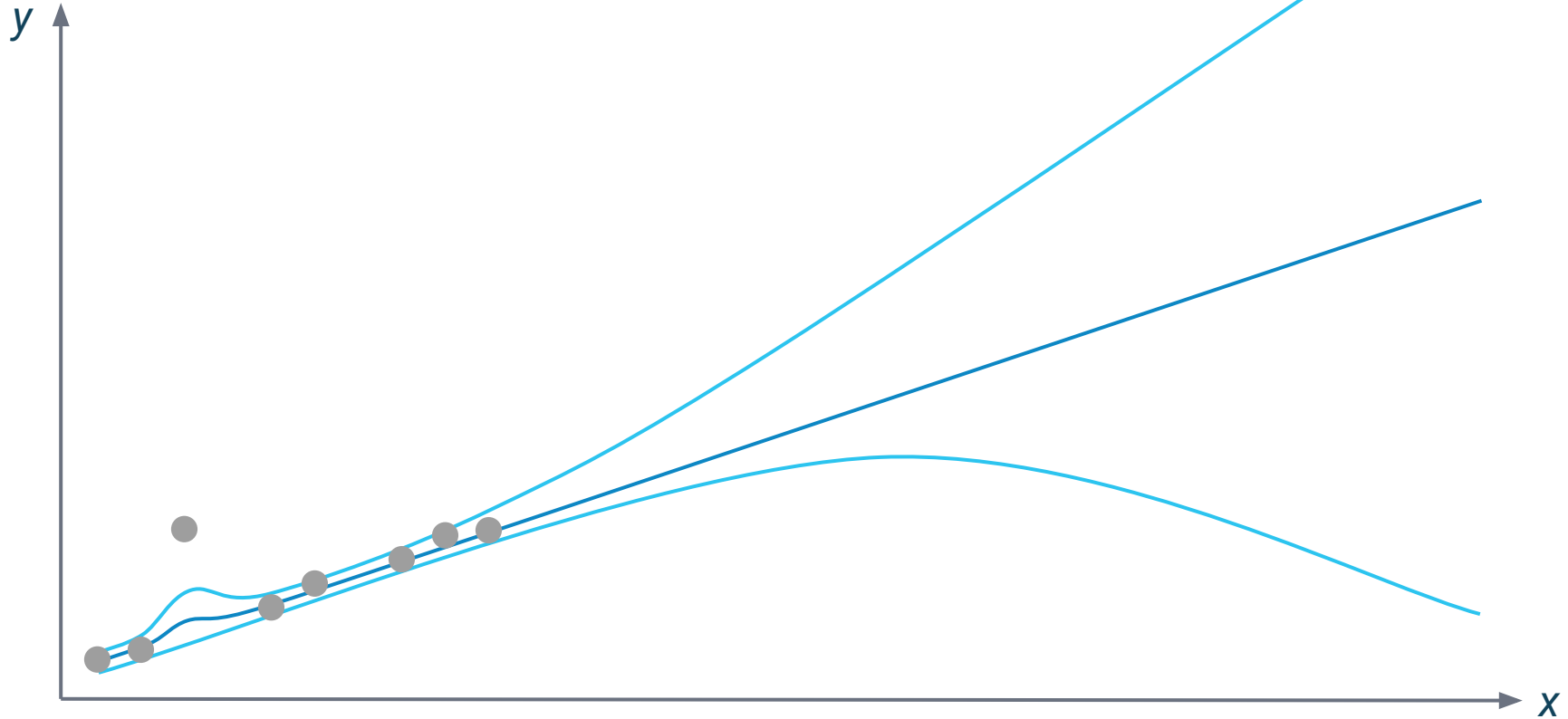
Training data



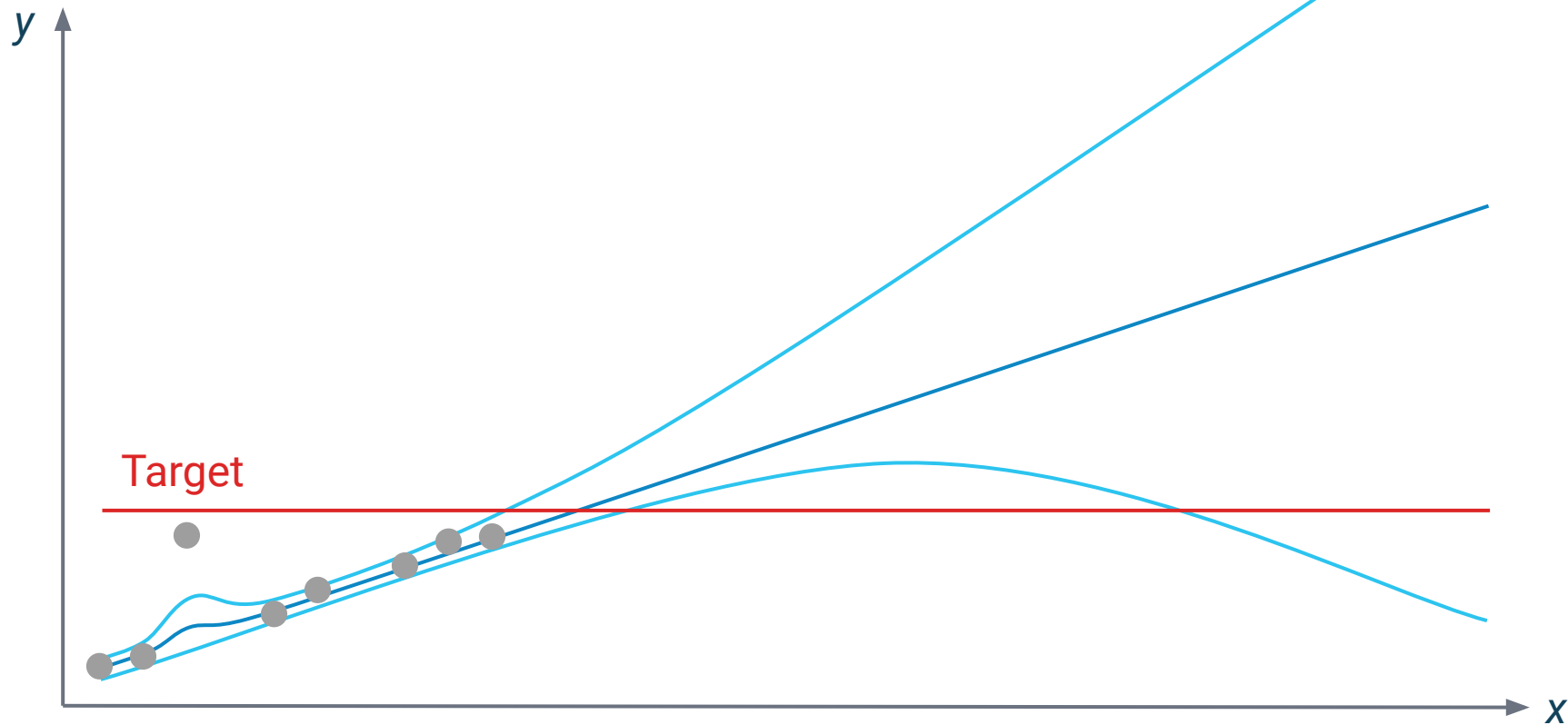
Machine learning model



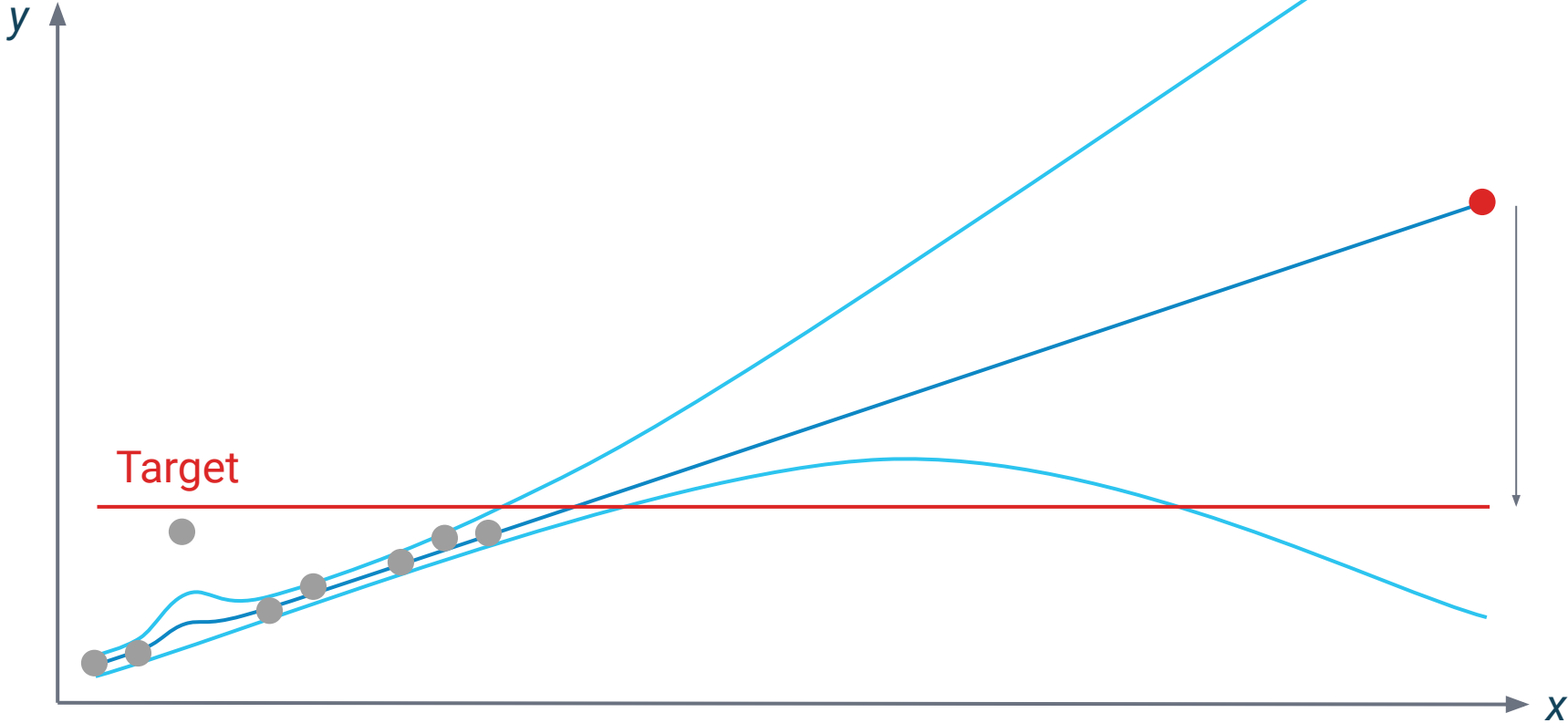
Uncertainty in the model



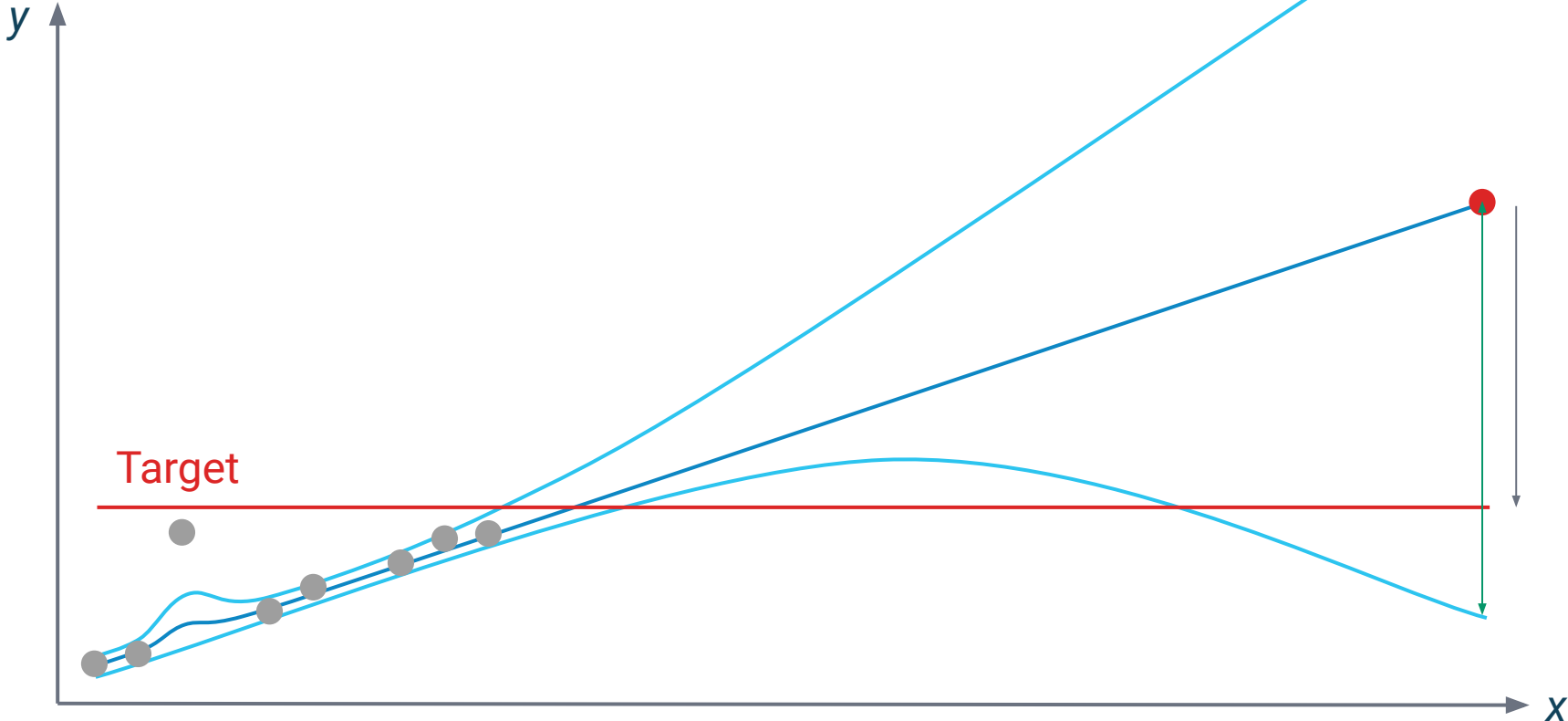
1. Target for the design



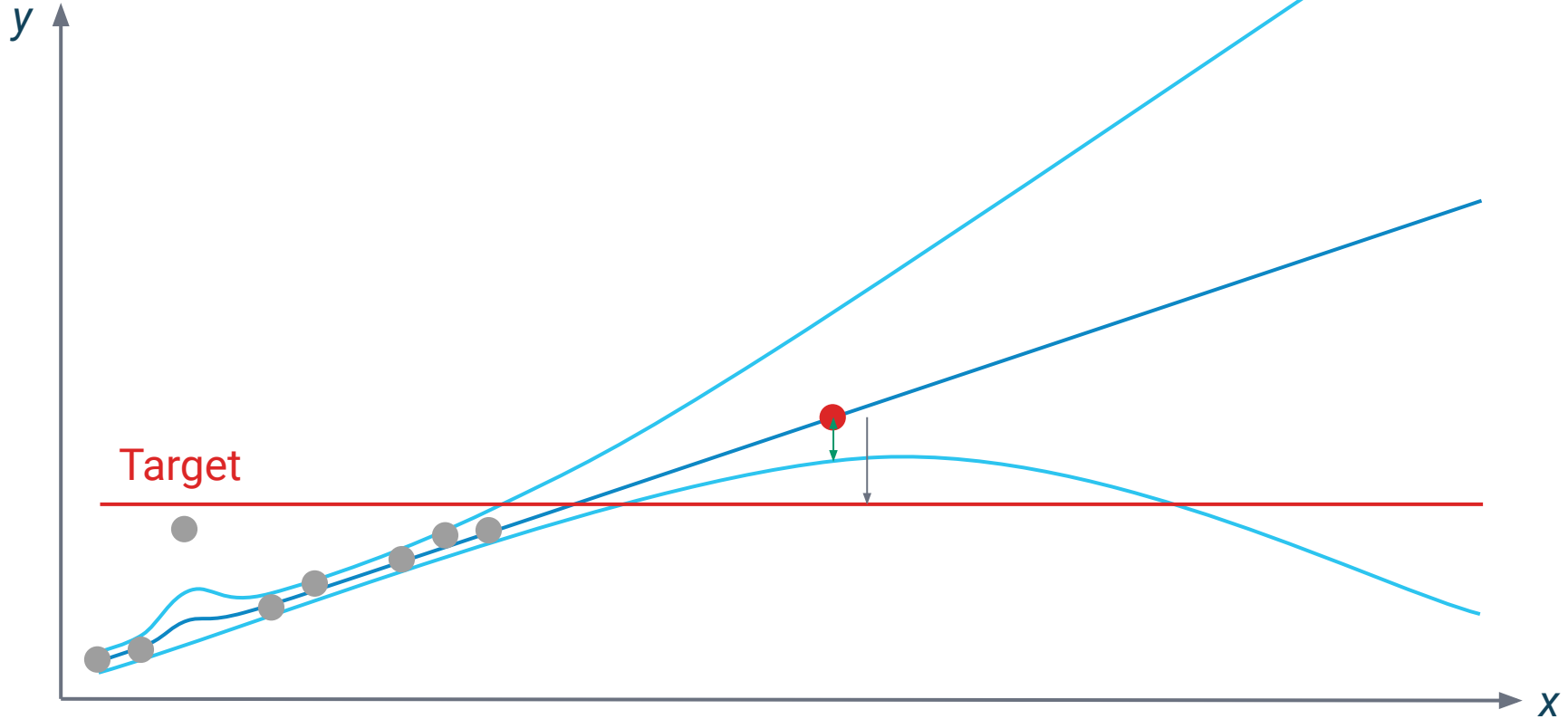
1. Choose formulation with best expected property



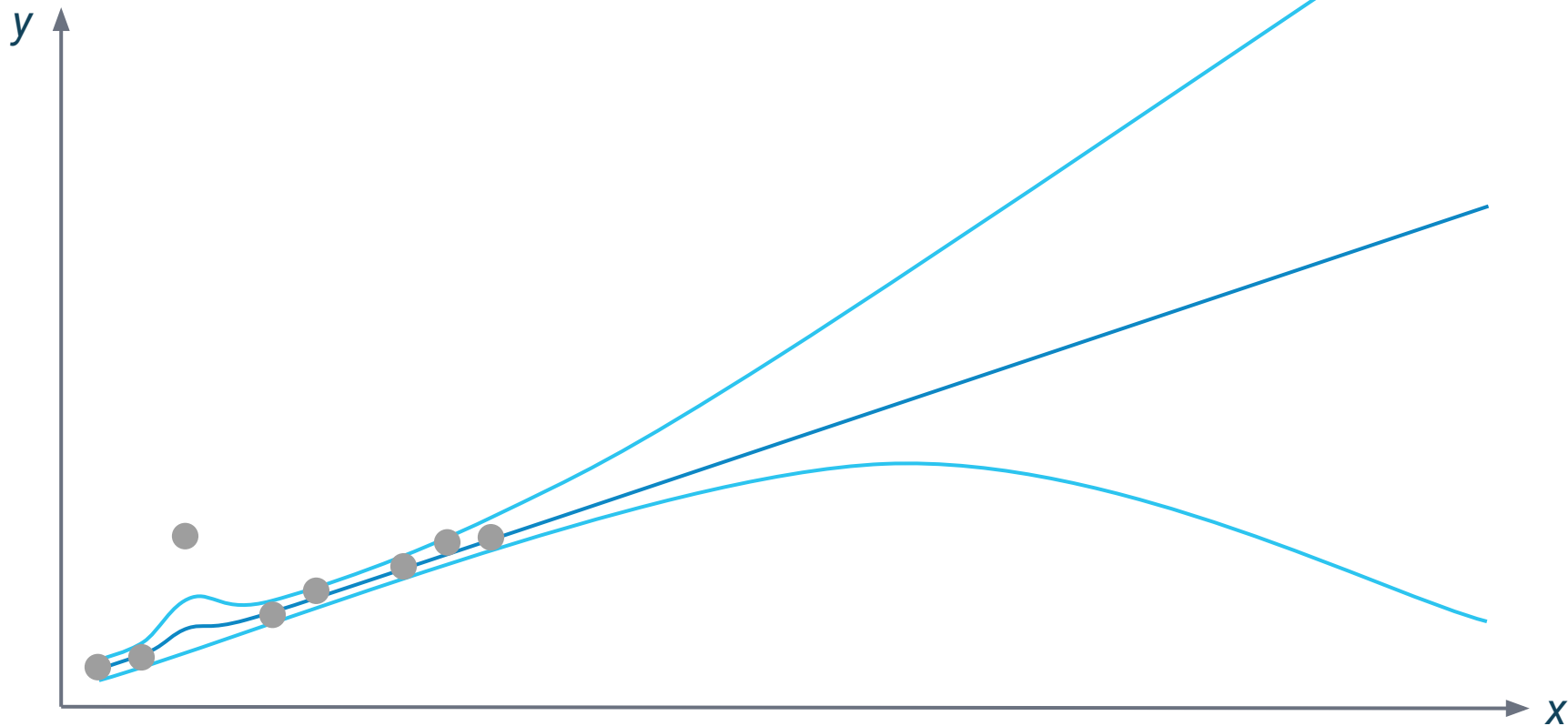
1. Choose formulation with best expected property



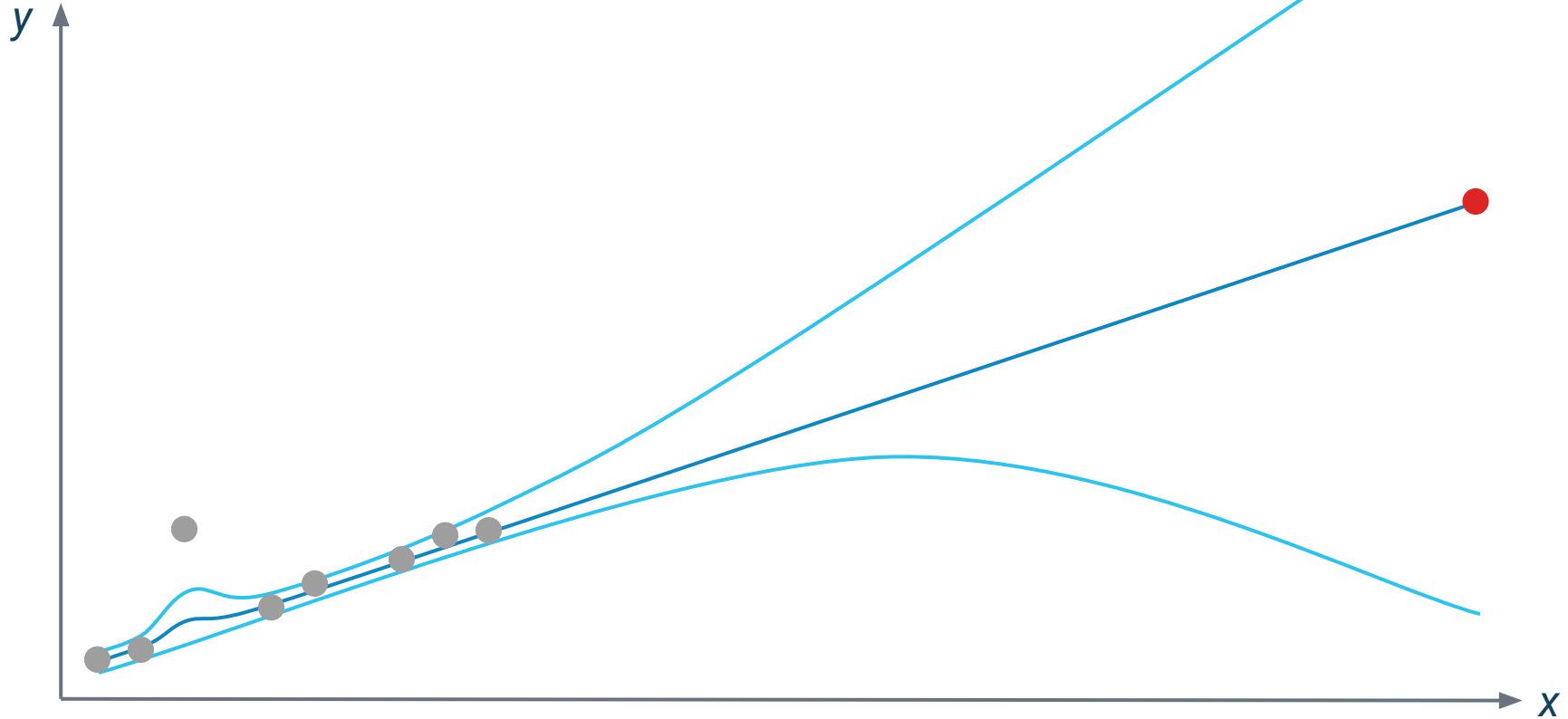
1. Formulation most probable to work



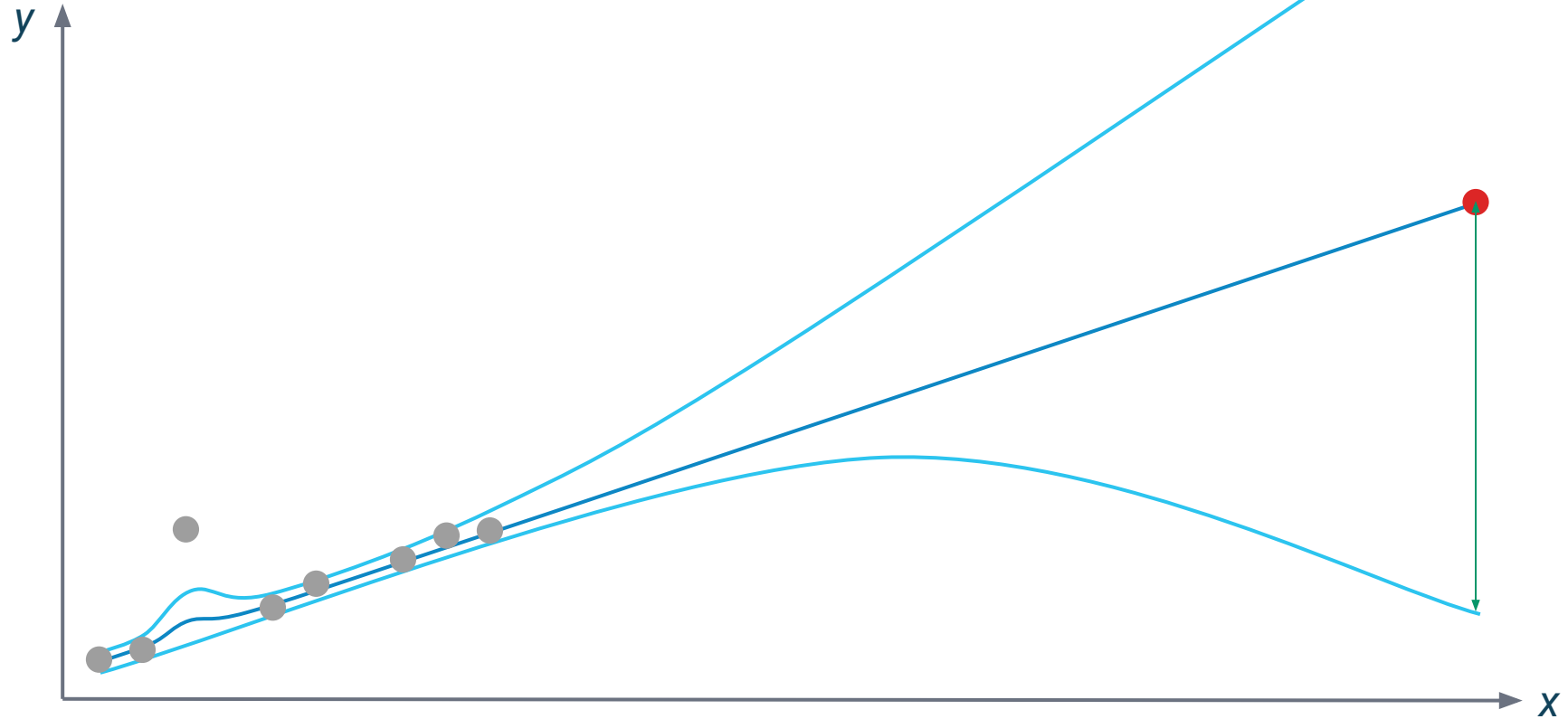
2. Design of experiment



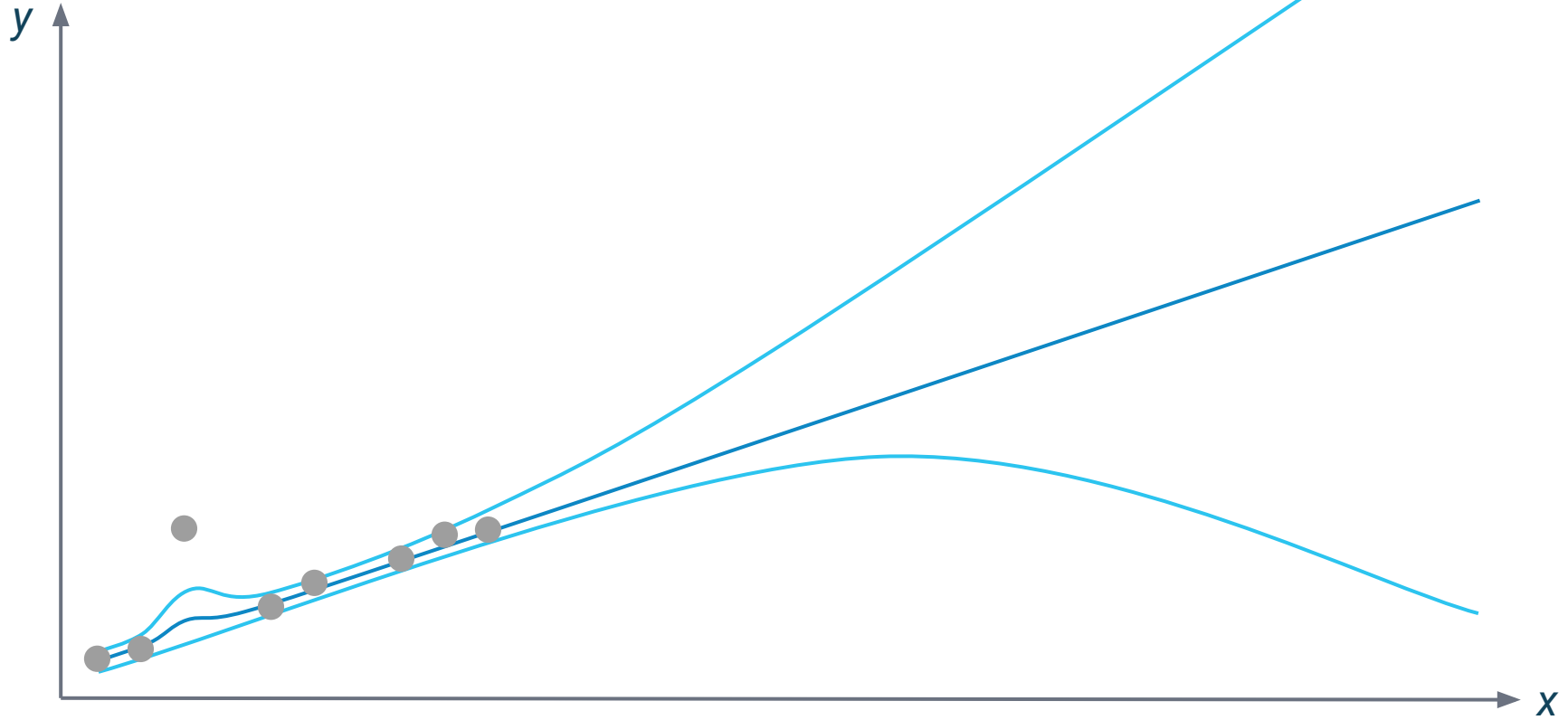
2. Choose value with most uncertainty



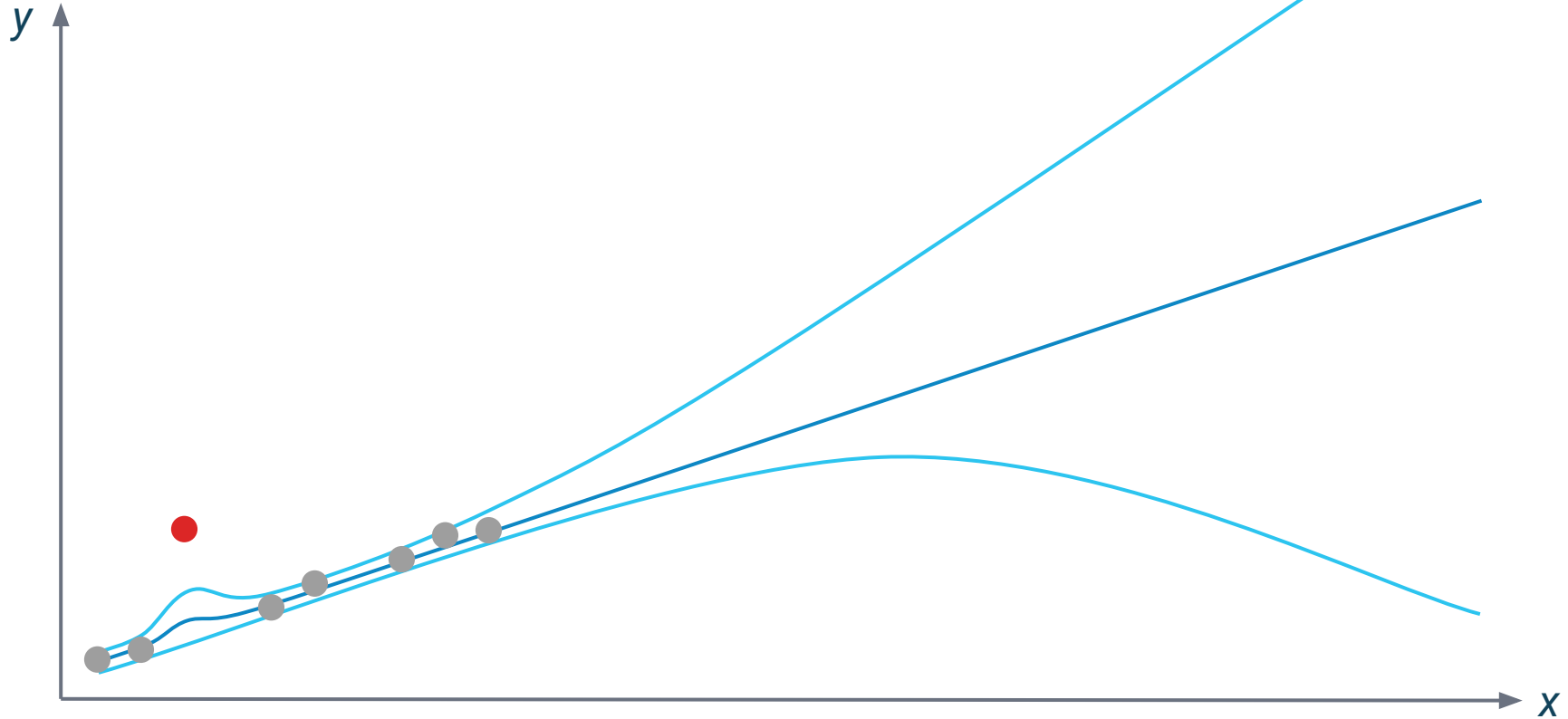
2. Choose value with most uncertainty



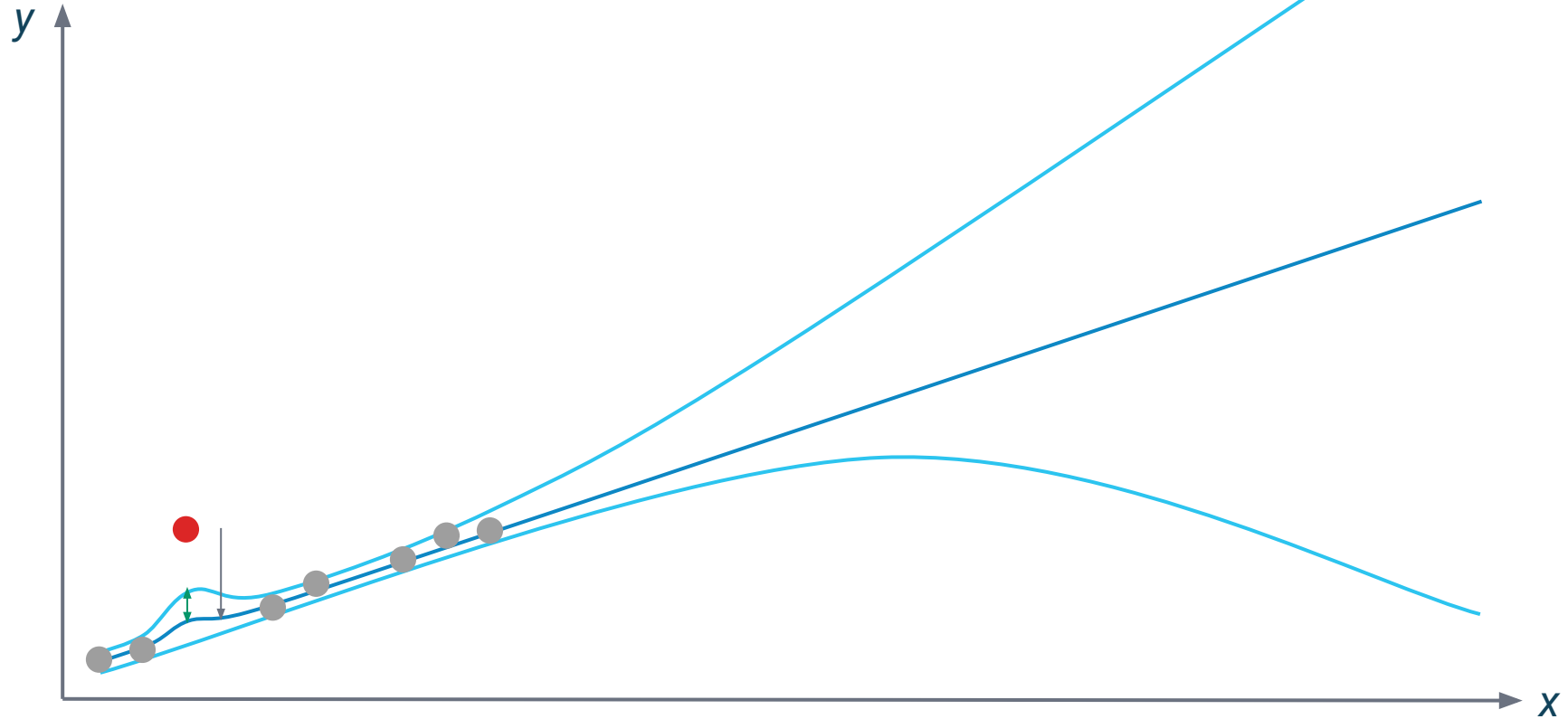
3. Finding outliers



3. Entry most likely to be incorrect



3. Entry most likely to be incorrect





Exploit uncertainty



Bogdan Zviazhynski



Dr Gareth Conduit

Cavendish Laboratory, University of Cambridge

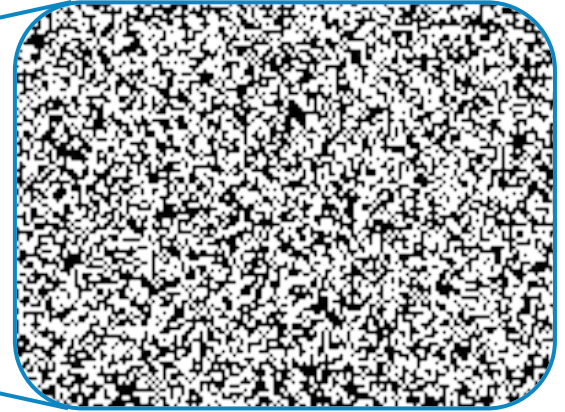
Concrete in construction



Cement & aggregate look like noise



Cement & aggregate look like noise



Mission



Design a concrete that is **robust** and **environmentally friendly**

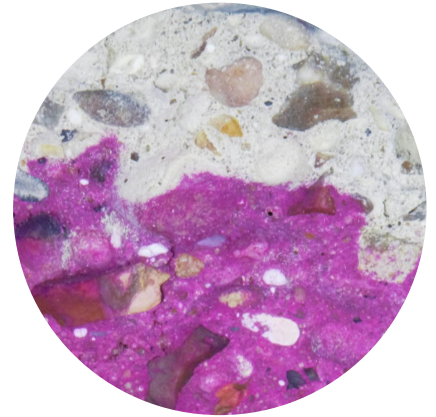
Mission



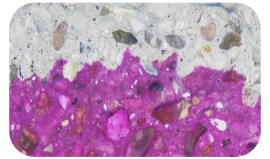
Design a concrete that is **robust** and **environmentally friendly**

Experimentally validate the concrete

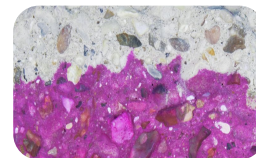
Carbonation



Machine learning



Carbonation depth to strength



Carbonation front



Atmosphere

Depth



Uncertainty in the carbonation front

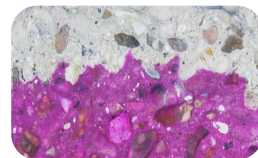


Atmosphere

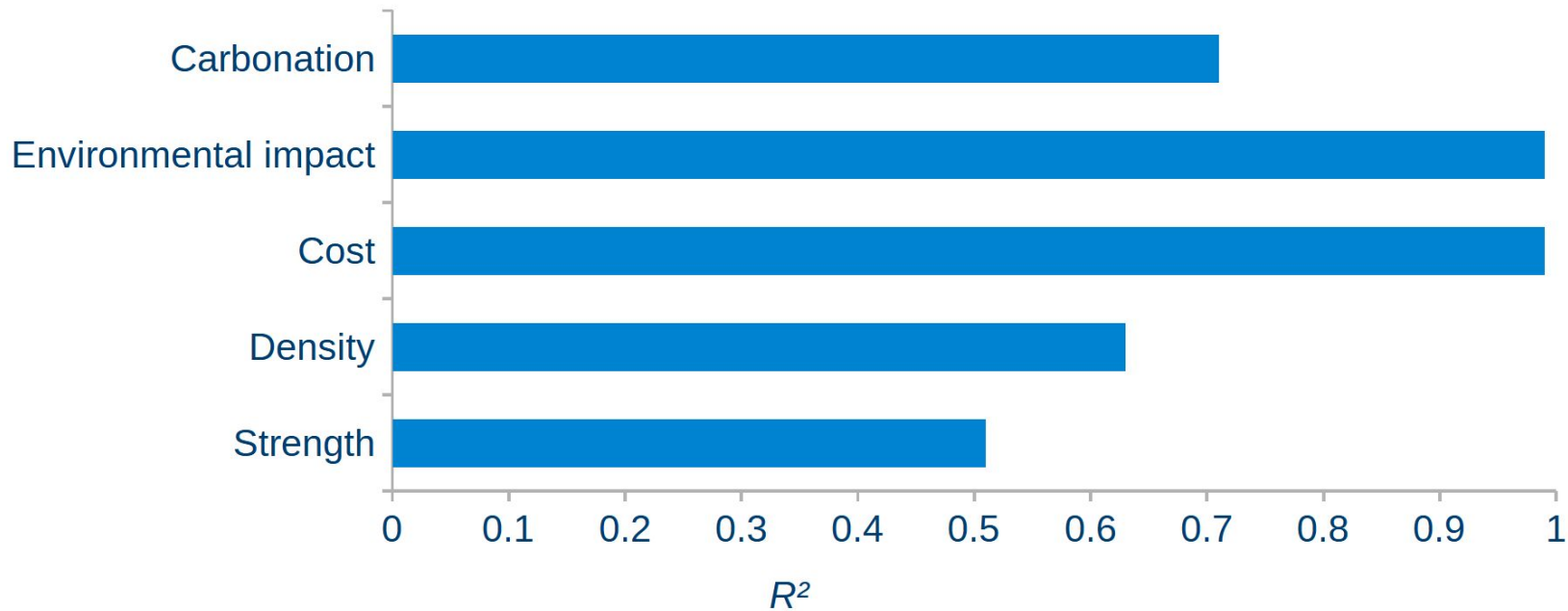
Uncertainty \updownarrow



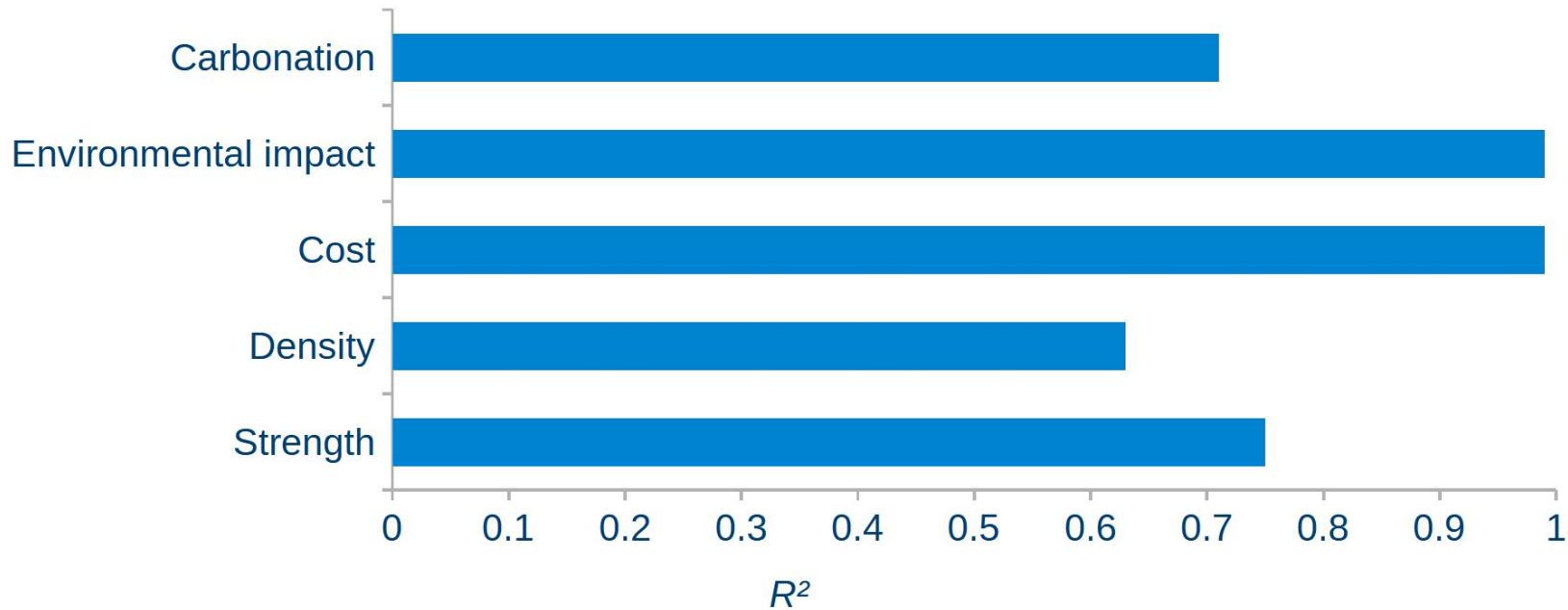
Carbonation depth uncertainty to strength



Original model accuracy



Model accuracy exploiting uncertainty



Concrete specification



First mix

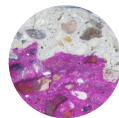
 carbonation

 environmental impact

 cost

 density

 strength



Second mix

 carbonation

 environmental impact

 cost

 density

 strength

Concrete design



First mix

10.5% cement



48.4% gravel



32.6% sand



8.5% water



Second mix

14.2% cement

48.9% gravel

28.4% sand

8.5% water



Experimental validation



Jess Forsdyke



Professor Janet Lees

Civil Engineering, University of Cambridge

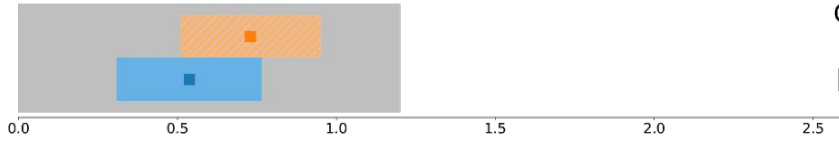
Concrete manufacture



Experimental validation of carbonation coefficient

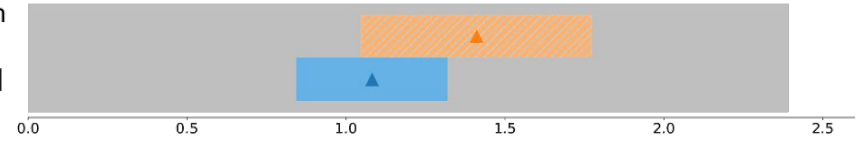


First mix



Carbonation coefficient
[mm day^{-1/2}]

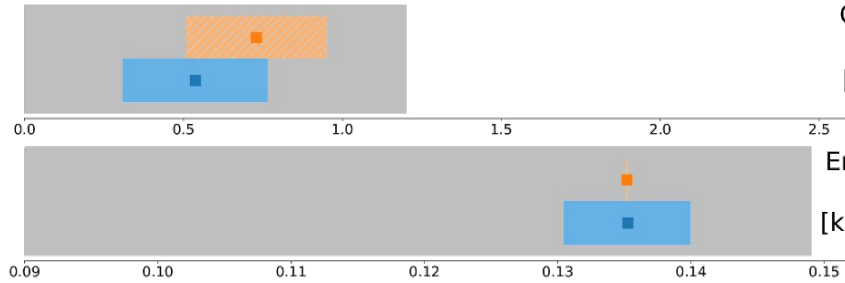
Second mix



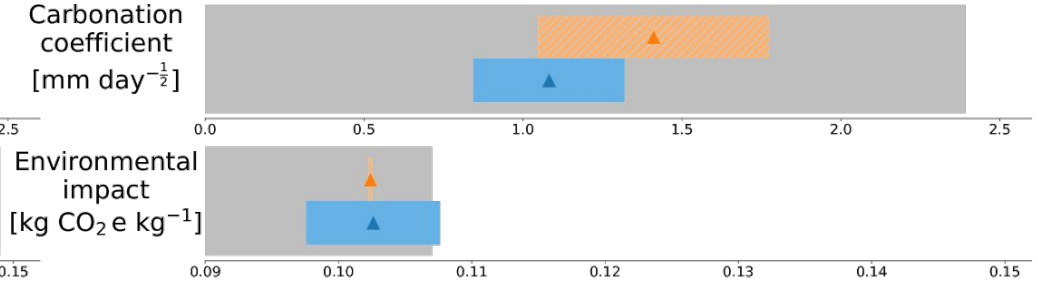
Experimental validation of environmental impact



First mix



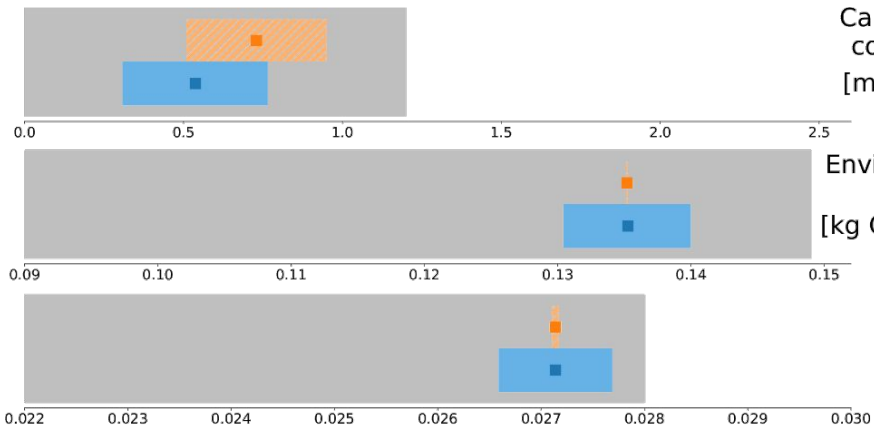
Second mix



Experimental validation of cost



First mix

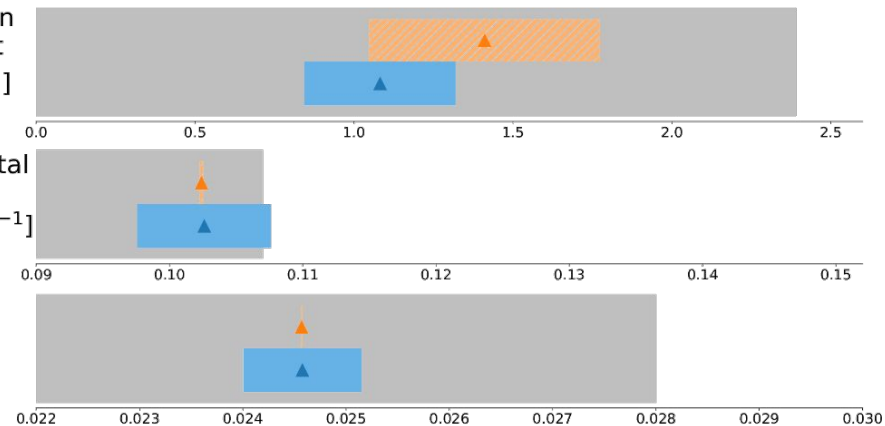


Carbonation coefficient
 $[\text{mm day}^{-\frac{1}{2}}]$

Environmental impact
 $[\text{kg CO}_2\text{e kg}^{-1}]$

Cost
 $[\text{£ kg}^{-1}]$

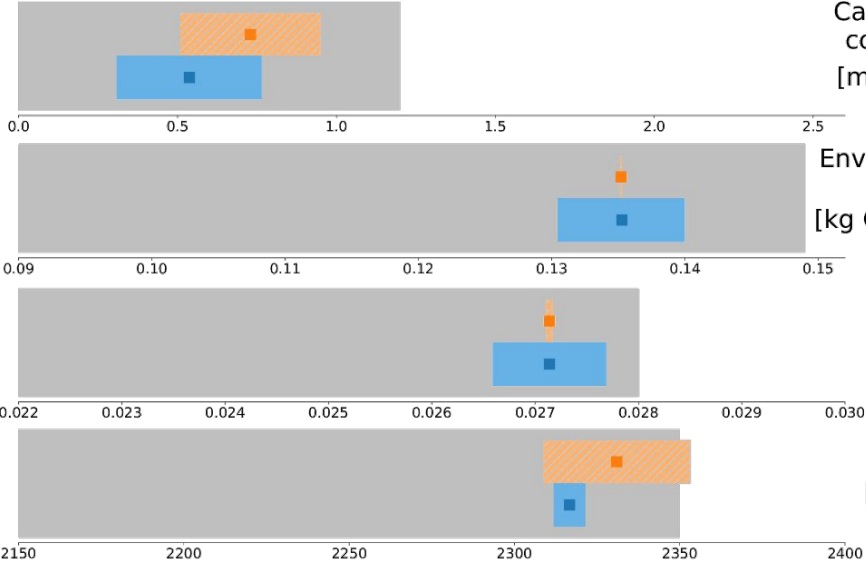
Second mix



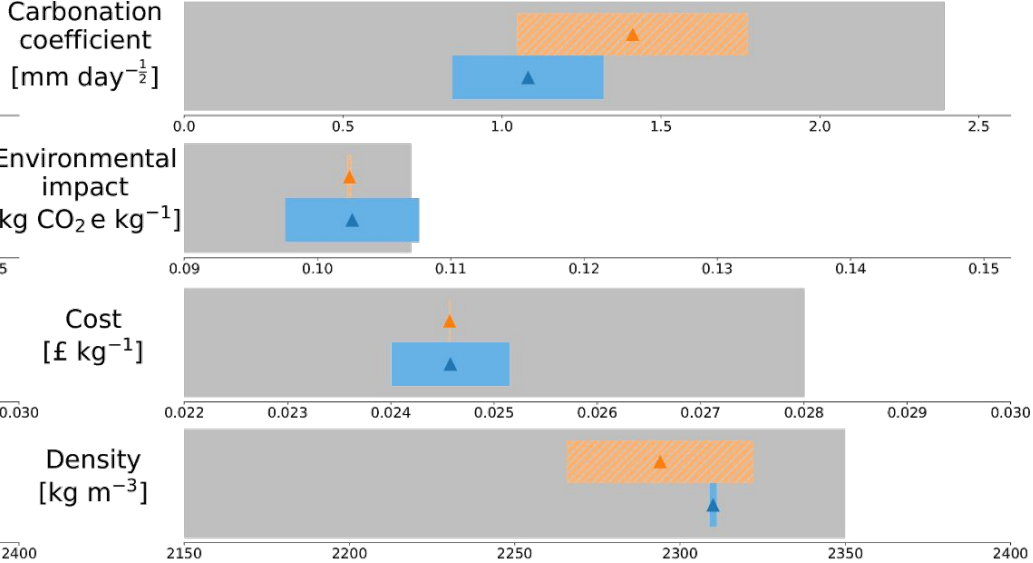
Experimental validation of density



First mix



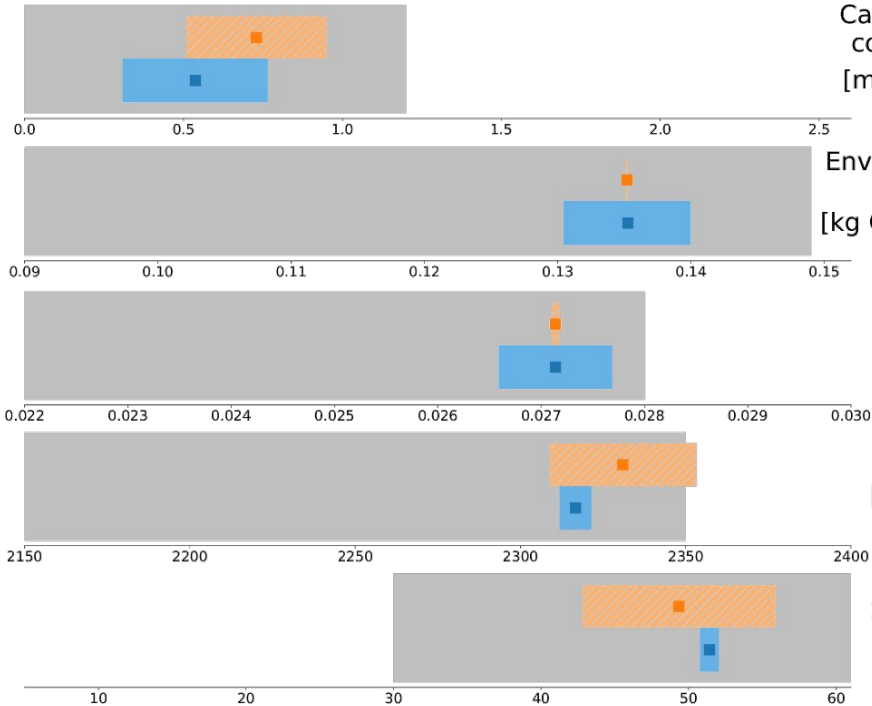
Second mix



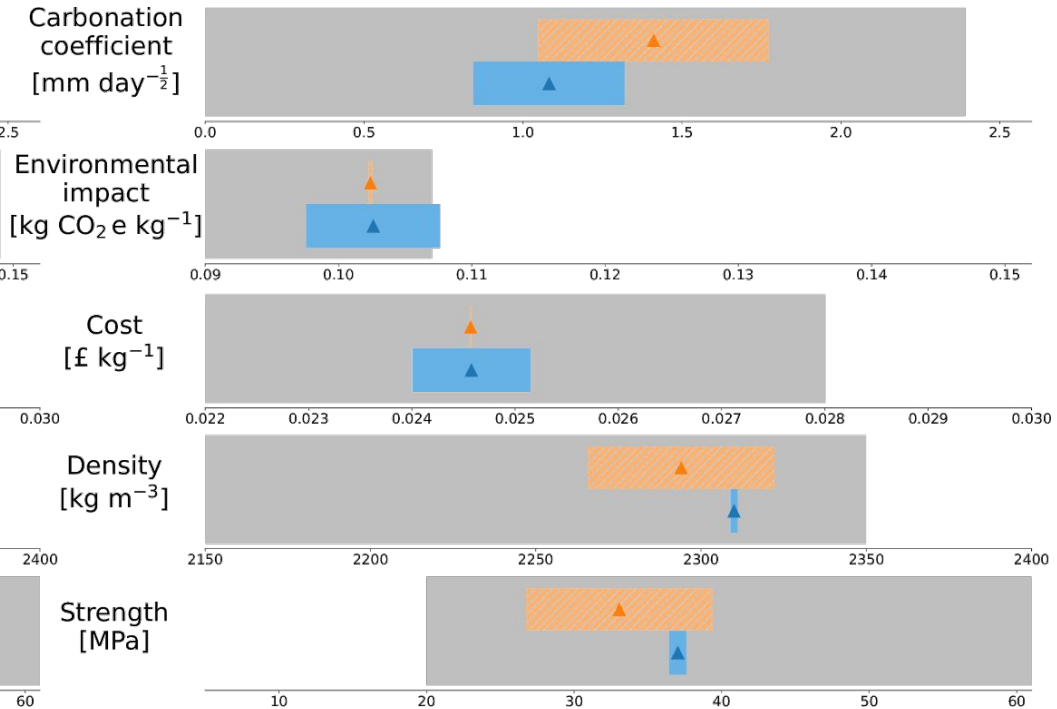
Experimental validation of strength



First mix



Second mix



Summary

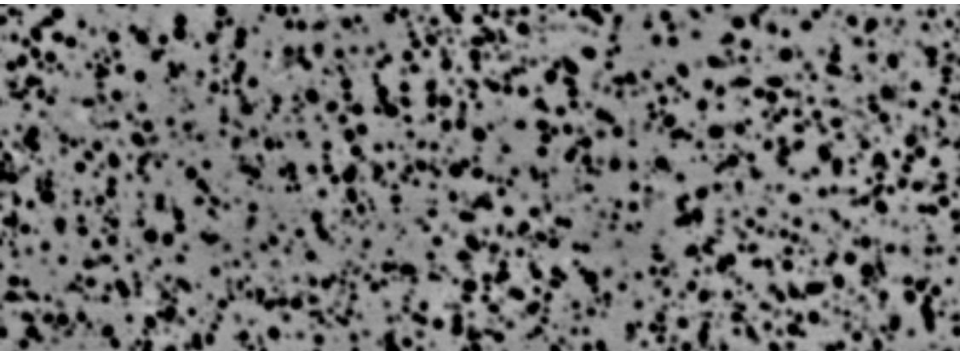


Extract information from **uncertainty** to design two verified concrete mixes

Summary



Extract information from **uncertainty** to design two verified concrete mixes

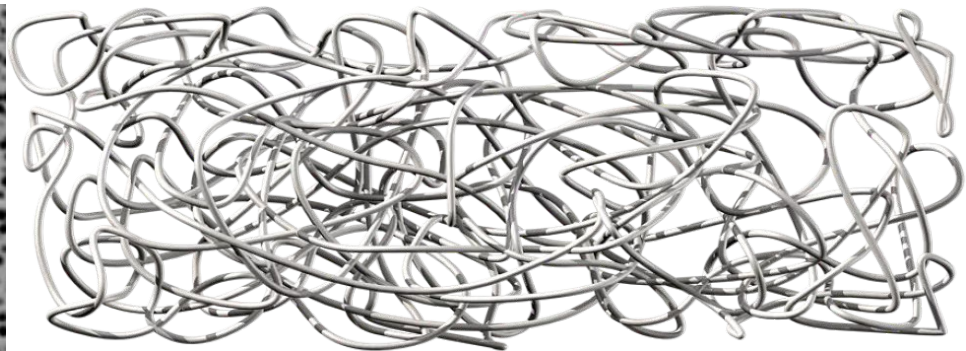
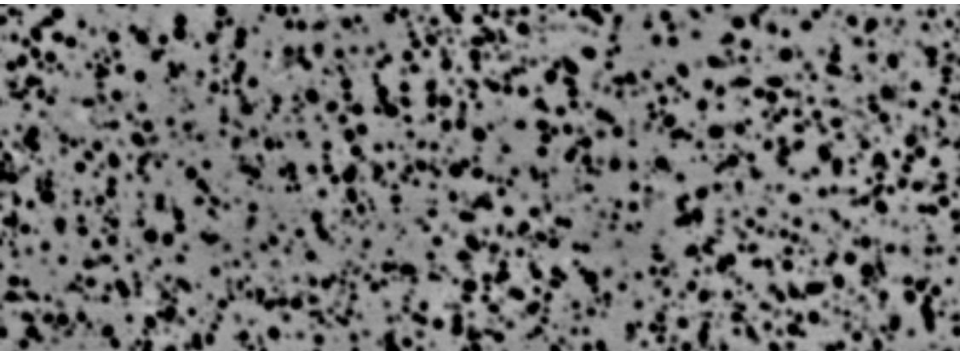


Alloy **microstructure** has information hidden in the noise

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

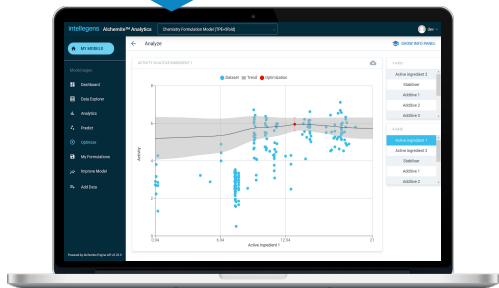


Alchemite™ product

Alchemite™ product family



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



←
*Option to
deploy
models*

Data scientists
Add to your ML toolkit



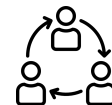
*Optional
connectors*



Lab systems



*Software &
scripts*



*Sharing &
collaboration*

Alchemite™ Analytics

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

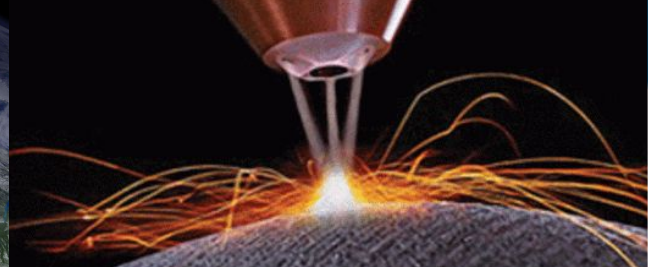
Alchemite™ Engine

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

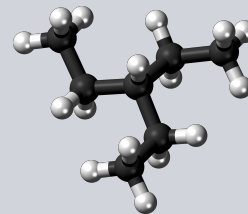
<https://doi.org/10.1038/s42256-020-0156-7>

Check for updates

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

Man-Fai Ng¹, Jin Zhao², Qingyu Yan², Gareth J. Conduit² and Zhi Wei Seh^{1,4}

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)

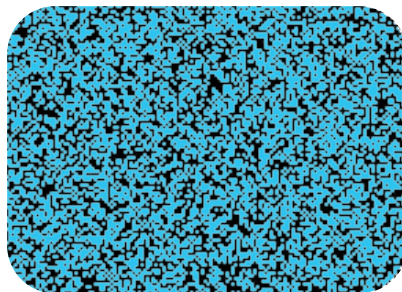


Applied machine learning

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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