intellegens

CASE STUDY

Machine learning for virtual experiments – ink formulation

Executive summary

Empirical analysis is typically the most resource-intensive part of the R&D process – so much so that, in recent years, virtual experiments have become a topic of major interest. These allow researchers to use existing empirical data to predict and validate experimental outcomes, and are particularly useful when lab access is limited, as during the COVID-19 pandemic. Domino Printing Sciences used Alchemite™ advanced machine learning to leverage historical data, obtaining several novel ink formulations, some of which were later validated via physical experimentation. Domino was able to:

- **Optimise formulations** by maximising insight from carefully chosen experiments
- **Make more efficient use of lab capacity,** by reducing the number of experiments
- **Decrease time-to-market**, cutting experimental timescales from months to minutes.

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Challenge

The traditional ink development process requires the formulation and testing of a large number of designs to find an optimum formulation.

Domino is renowned for designing and manufacturing reliable and well-understood inks and, as such, has well-characterised historical data. Domino wanted to use this data to inform the replacement of ingredients that were no longer suited or available. However, as the data was gathered over varied projects, different properties have been measured for different formulations, limiting the value of most data analysis techniques—including many of those based on machine learning.

Intellegens aimed to build advanced machine learning models to propose new inks that matched, or exceeded design targets for existing formulations.

Limited lab access during the COVID-19 pandemic hampered activities that rely on empirical analysis, so it became even more essential to maximise value from newly acquired as well as historical data.

Solution

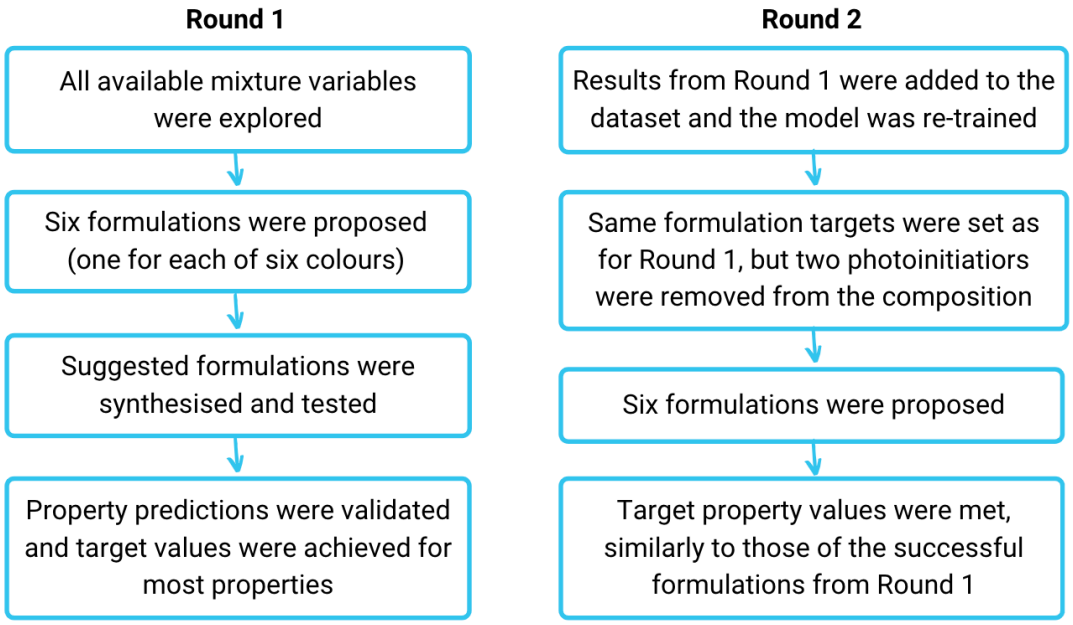
Intellegens' unique machine learning technology, Alchemite™, created a comprehensive model across multiple ink colours and compositions for 28 formulation properties.

The historical data available was sparse, but nevertheless the model exhibited a high coefficient of determination

Alchemite™'s flexibility allowed the assignment of different relative weights for each target property. Despite the sparse data, the model exhibited a high coefficient of determination (accuracy), with 75% of the properties being modelled accurately or highly accurately. The model successfully established relationships between design variables (mixture compositions) and formulation properties.

Outcome

Two rounds of formulation design were performed with Alchemite™:



Alchemite™ leveraged Domino's historical data and reduced the ink formulation timescale from months to minutes

Six conventional ink formulations were proposed as a result of Round 1. The property predictions were validated experimentally and they were found to be highly accurate. During model training, Alchemite™ had identified that one of the key target properties was likely to be negatively impacted by the desired removal of one of the components. This highlighted the ability to recognise important relationships between variables preemptively, which enabled Alchemite™ to mitigate the impact on the target property in Round 2.

A design of experiments campaign, driven by Alchemite™, could be used to ensure that the model has the data that will be most valuable in suggesting future formulations whose target properties can be predicted with a good level of accuracy.

"We were impressed with the ability of Alchemite™ to identify novel formulations quickly and accurately. This enabled us to make the most of limited lab resources and continue innovating during the COVID-19 lockdown."
Dr Andrew Clifton, Director of Marking Materials and Test Engineering Team at Domino.

Future opportunities

This case study demonstrates that Alchemite™ machine learning can be used to revolutionise the way that new inks are designed. It also establishes the system's potential as a solid platform to accelerate the design of any industrial formulation.

Three key opportunities offered by machine learning are:

1. The underlying model can be improved continually by including more historical data and/or new experimental results from quicker, lower cost experiments.
2. Alchemite™ predictions can be used in a design of experiments campaign, to suggest the next experimental measurements to take to most improve the model's predictions.
3. Alchemite™ can be integrated with Domino's robotic equipment in order to automatically formulate and test compositions based on the model's predictions.

About Domino

Founded in 1978, Domino has established a global reputation for the development and manufacture of coding, marking, and printing technologies, as well as its worldwide aftermarket products and customer services. Domino's continued growth is underpinned by an unrivalled commitment to product development. In 2017, Domino was honoured with its sixth Queen's Award – the UK's most prestigious awards for business performance.

About Intellegens

Intellegens has developed a unique deep learning engine, Alchemite™ for training neural networks from the sparse and noisy data typical of real-world science and business challenges. The technique was first developed at the University of Cambridge where it has been used to develop aerospace alloys, guide the design of new drugs, and design next-generation battery technology. The tool is now being used to solve a wide range of industrial customer problems, optimising products and processes, saving time and cost in discovery and development, and enabling breakthrough insights.

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