Novel deep neural network toolset for industrial formulations

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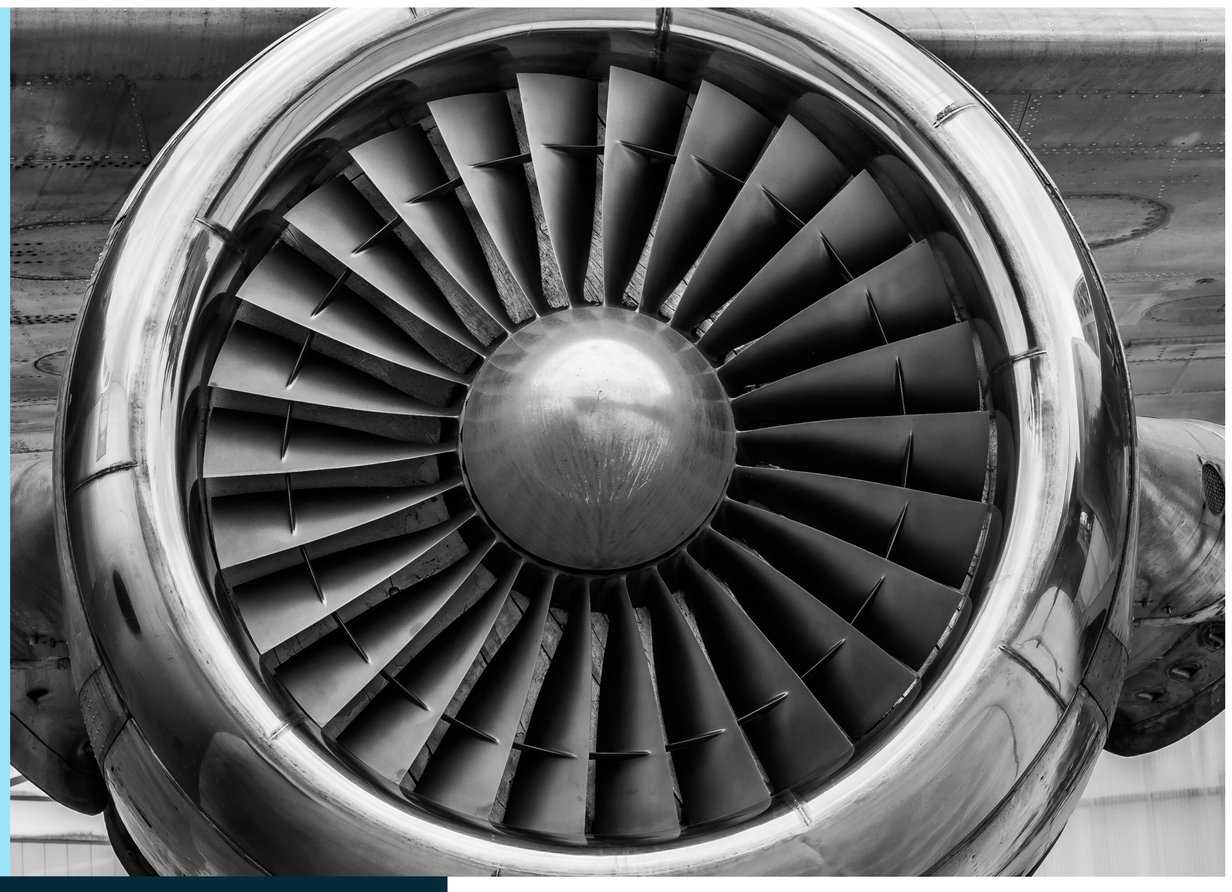
AI FOR INDUSTRIAL FORMULATIONS

At Intellegens we have developed a unique deep learning tool, Alchemite™, that can learn property-property relationships between all available parameters in sparse, unstructured, corrupt or even noisy datasets. Suitable for deployment across any kind of numeric dataset, our deep learning solutions are delivering ground-breaking results in industrial formulations such as drug discovery, advanced materials, chemicals, and predictive maintenance – enabling organisations to break through data analysis bottlenecks, reduce the amount of time and money spent on research, and support better, faster decision-making.



DEEP LEARNING TECHNOLOGY

Alchemite™ is a unique deep learning solution that accelerates innovation and production of industrial formulations. This cutting-edge technology is capable of extracting valuable knowledge hidden in your data and creates predictive models that reduce costs and speed-up the materials, chemicals and drugs design process.

Alchemite™ can computationally design new superalloys that are better suited to the target application, accurately predict activity against targets in drug discovery, improve battery management systems and optimize manufacturing supply chains.

ALCHEMITE™ FEATURES

Alchemite™ is a platform with a suite of tools that use AI to optimize development and processes. It is capable of handling incomplete data sets in both training and predicting.

- Reduction of material costs by minimizing expensive properties
- Maximization of target physical property identification
- Acceleration of discovery and validation
- Standardization of workflows
- Reduction of environmental impact

ADVANCED MATERIALS

SUPERALLOYS. Our deep learning software has been developed to target multiple parameters from compositions and treatments processes to cost and environmental impact. Alchemite™ was used to propose a new nickel-base superalloy that would fulfill eleven different physical criteria.

Results. The tool predicted that the new nickel-base polycrystalline alloy offered an ideal compromise between its properties for disc applications. Seven of these properties were experimentally verified, demonstrating that it has better yield stress and oxidation resistance than commercially available alternatives. Alchemite™ reduced costs by $10 million and accelerated the discovery and validation process from 20 to 2 years.

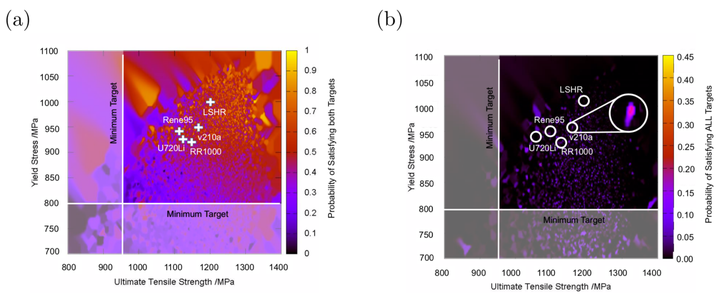


Figure 1. (a) A relief plot of simultaneously satisfying two targets, a minimum yield stress target of 850 MPa at 750°C and a minimum ultimate stress target of 950 MPa at 750°C. (b) A relief plot of simultaneously satisfying all targets for the material, plotted with respect to yield stress and ultimate tensile stress targets.

CHEMICALS

LUBRICANTS are used to protect surfaces from wear, reduce friction, transfer heat, and ensure the smooth functioning of mechanical devices. Predicting physical properties of alkanes and understanding the relationship between lubricant performance and alkane structure facilitates the development of computationally-derived optimal base oils.

Results. The results reproduced by Alchemite™ were significantly more accurate and consistent than those reproduced by other methods. By combining sparse experimental data with molecular dynamics simulations to predict physical properties of alkanes, Alchemite™ identified and sped up the identification of alkanes to be used for lubricant base oils with superior physical properties.

BATTERIES. It is estimated that around 50% of the value of future vehicles will be associated to the battery and the systems that support it. The development of new battery technologies is slow, taking many years to both in terms of new technologies and , more importantly, the substantial manufacturing challenges needed to be scale up production.

Results. Secured Battery Faraday Challenge (Innovate UK) grant to use artificial intelligence to reduce fabrication and development costs while improving key battery metrics. Intellegens is providing deep learning predictive models (Alchemite™) for process parameter prediction.

DRUG DISCOVERY

BIOACTIVITY ASSAY DATA. Conventional machine learning approaches require complete, clean data whereas Alchemite™ is proven to work on large, sparse bioactivity data sources, typical of those found in public and commercial databases.

Results. Our novel deep neural network imputation technique was able to predict bioactivity from incomplete bioactivity data. It improved the quality of predictions by using correlations between both different bioactivity assays and also between molecular descriptors and bioactivities, which resulted in an important improvement in the accuracy of prediction over other conventional QSAR models, even those that implement deep learning.

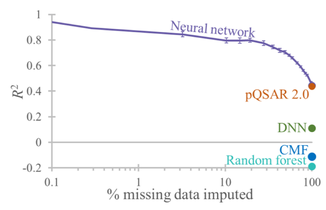


Figure 2. The coefficient of determination for predicting the activity of the clustered Kinase data set with percentage of data predicted. The magenta line shows that the accuracy of the neural network predictions increases when focussing on the most confident predictions, at the expense of imputing only a proportion of the missing data. This confirms that the reported confidences in the predictions correlate strongly with their accuracy.

PAPERS

1.Conduit, B.D., Jones, N.G., Stone, H.J., & Conduit, G.J. 2017. Design of nickel-base superalloy using a neural network. Materials & Design, 131, 358-365. 2. Santak, P. & Conduit, G. 2019. Predicting physical properties of alkanes with neural networks. Fluid Phase Equilibria, 501, 112259. 3. Whitehead, T.M. Irwin, B.W.J. Hunt, P., Segall, M.D., & Conduit, G.J. 2019. Journal of Chemical Information and Modeling, 59 (3), 1197-1204.