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WHITE PAPER

Machine Learning for Battery Applications

Executive summary

The battery industry is growing dramatically, driven by the needs of electric vehicles, consumer devices, and energy storage for renewable sources. Any approach that delivers improved battery technology sooner, or that aids safety and efficiency, will attract significant interest. Machine Learning (ML) is one such method. But there are limitations on applying ML to battery R&D due the real-world data involved, the complexity of the problems being studied, and deployment challenges for ML tools.

In this white paper, we introduce the **Alchemite™** deep learning software, which has been developed to overcome these obstacles. We outline case studies of its use in three key areas across the battery value chain: **battery materials and formulations**, **battery pack design**, and **battery management systems**. The examples show how ML can help to maximise the performance of battery systems, cut experimental workload by up to 80%, minimise cost and environmental footprint, reduce defects, and increase efficiency through standardised processes.

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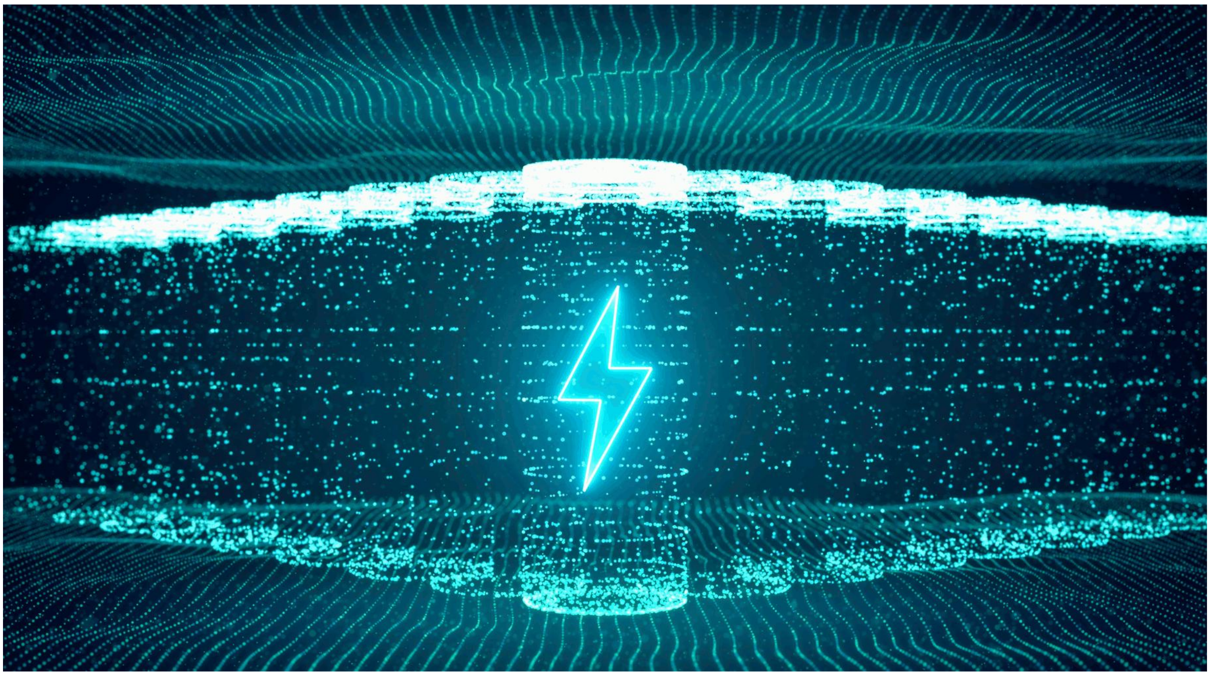
Introduction

Demand for, and government investment in, the electrification of transport has surged in recent years with increasing concerns about climate change and pollution. Similar drivers exist for energy storage to maximize usage of renewable energy sources. Consumers are looking for ever-longer battery lives from their devices. These are three key drivers ensuring that the stakes for the global battery market are consistently rising, with predictions that the electric vehicle (EV) battery market alone will be worth £150bn per year by 2028 [1].



The performance, cost, and safety of batteries determine the successful development of electric vehicles. Currently, Lithium-ion (Li-ion) batteries are the preferred choice for EVs due to their cycle life and energy density, followed by a range of other battery chemistries including Lithium-sulphur (Li-S), Sodium-ion (NIB), and Sodium-nickel chloride (Na-NiCl2) batteries. Further research into battery materials and chemistries will result in more complicated battery dynamics, with the potential for enhanced performance, alongside safety and efficiency as key concerns. Advanced battery management systems that can optimise and monitor safety are crucial for the electrification of vehicles.

Any approach or method that can deliver better battery technologies sooner, or make that technology operate safely and efficiently, will attract significant interest.

Machine learning is one such method.

Machine learning for battery R&D

Machine learning (ML) is a class of Artificial Intelligence (AI) methods that can 'train' models using available data and then apply those models for analysis, prediction, and decision-making without need for further programming.

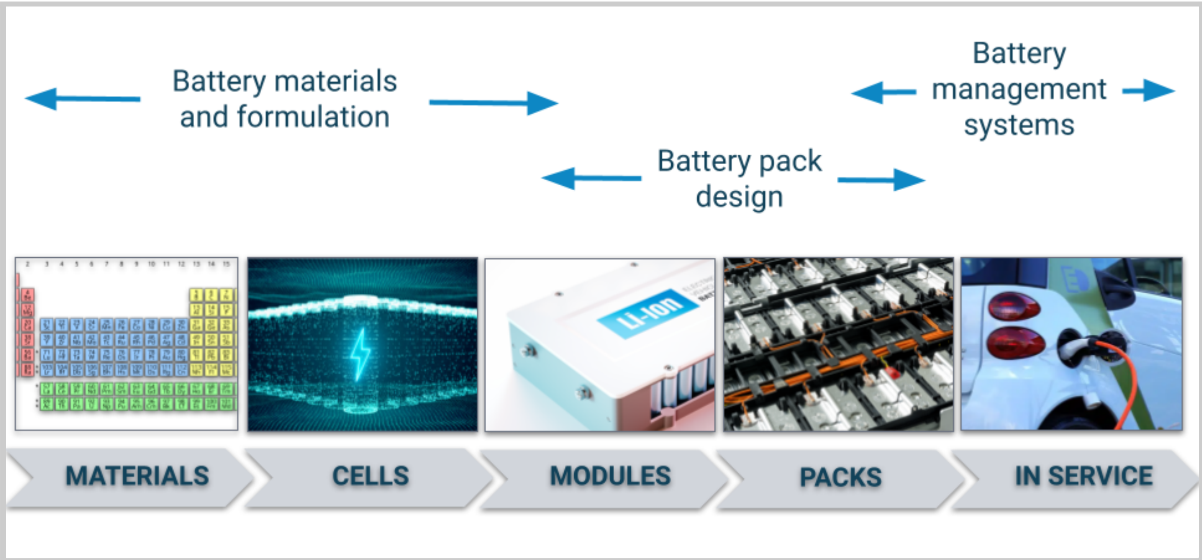


Figure 1. Identifying ML applications across the battery value chain.

Through its industry collaborations and conversations with customers, Intellegens has identified three key areas where ML can benefit organisations working on batteries:

1. **Battery materials and formulations** – finding new formulations and optimising the design and manufacturing of the cell is an experimentally-intensive, and thus time-consuming and expensive, process. ML can propose optimal formulations and guide experiments along the most productive pathways.

2. **Battery pack design** – it is necessary to trade off many factors (e.g., voltage, capacity, charge speed, heat transfer, dimensions…) to meet the specific needs of an application. ML is the ideal tool for such multi-parameter optimisation.

3. **Battery management systems** – understanding key metrics such as State of Charge (SOC) and State of Health (SOH), and predicting Remaining Useful Life (RUL) are valuable in the control systems that maximise battery performance in the field. ML can improve models to evaluate and predict these factors using data including output from sensors monitoring in-service batteries.

ML challenges

Before sharing ML case studies for these three application areas, it is worth noting some of the key challenges that need to be overcome in applying ML, and how they are met.

Sparse data

Real-world experimental or process data is often sparse (i.e., not all of the possible values in the dataset are populated). Consider two examples. Battery formulation teams usually investigate novel systems for which data will inevitably be incomplete and it is too time-consuming and expensive to conduct experiments to measure every property value for every conceivable formulation. Battery pack design often compares cells from different suppliers who are unlikely to measure exactly the same performance factors in exactly the same way. Thus, the combined dataset describing cells of interest will be sparse.

Real-world experimental or process data is often sparse and this causes conventional ML methods to fail

The problem with these scenarios is that the first step in ML is to train a model using a subset of the available data, and conventional ML methods fail when asked to work with sparse training data.

Complex, high-dimensional data

Many of the problems studied will be high-dimensional – i.e., they have many inputs and outputs. Reducing dimensionality to focus the study risks missing less obvious factors that could prove to be important. Data can also be complicated. For example, there is often a need in battery R&D to work with time series data. ML is ideal for delivering insights from multi-dimensional problems, but it can be computationally expensive to do this on large, complex datasets, requiring significant data pre-processing and model setup.

Complex problems can be computationally expensive and the process of making ML operable is a stumbling block

The 'ML Ops' challenge

Deploying ML for use in scientific and engineering teams that are not data science experts can be difficult, both because these teams are unsure how to manipulate the available data so that their standard ML tool can handle it, and because many ML tools require skills such as coding or scripting. 'ML Ops' – the process of making ML operable – is a frequent stumbling block.

The Alchemite™ solution

The following case studies have been undertaken using the Alchemite™ deep learning software from Intellegens [2].

Originating at the University of Cambridge and now available from and continually developed by Intellegens, Alchemite™ overcomes these problems with:

- A unique algorithm that can train ML models on the available data, **no matter how sparse or noisy**. Alchemite™ uses underlying correlations to predict missing values and generate complete models for any numerical dataset.

- Accurate **uncertainty quantification** based on nonparametric probability distributions, informing users about how much confidence to place in a prediction from the ML model. This enables rational decision-making.

- A **light CPU/memory footprint** that makes Alchemite™ fast for large datasets and high-dimensional problems.

- Delivery within an easy-to-use **web platform**. Alchemite™ overcomes the ML Ops challenge by generating a model quickly from any dataset, enabling the user to inspect results and refine the model using an intuitive web browser user interface.

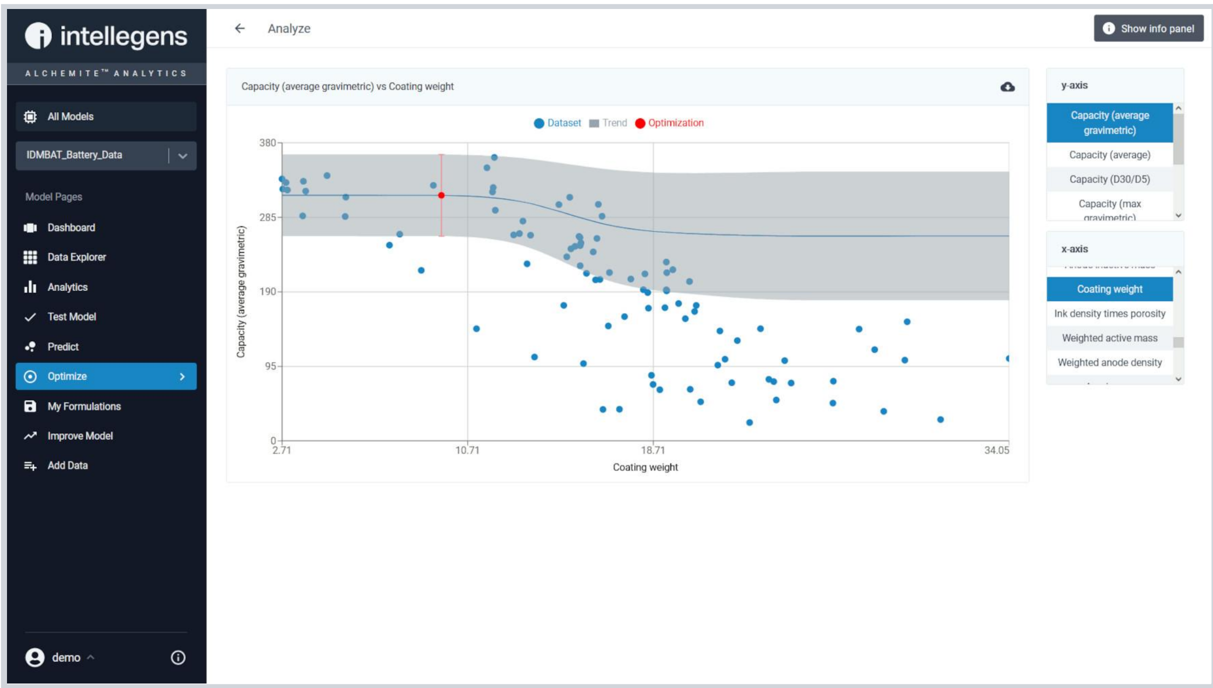


Figure 2. Alchemite web browser user interface.

Alchemite™ case studies

In three example projects, Alchemite™ has been successfully applied to battery design.

1. Battery materials and formulations

A collaboration involving **Intellegens**, the Energy Materials Group at the **University of Birmingham**, **Ansys**, and the **Faraday Institution** applied Alchemite™ machine learning to understand and optimise formulation and manufacturing parameters for Lithium-ion battery applications. Such optimisation is crucial to enabling higher energy density and longevity in this key class of battery systems, which are essential to electric vehicles.

The electrode was manufactured and showed excellent lifecycle and capacity, as predicted

Based on a dataset of formulations, manufacturing protocols, and performance properties captured in a purpose-built materials database system, a machine learning model was built, validated, and applied to predict the optimal electrode formulation and manufacturing processes. The electrode was manufactured and showed excellent lifecycle and capacity, as predicted [3].

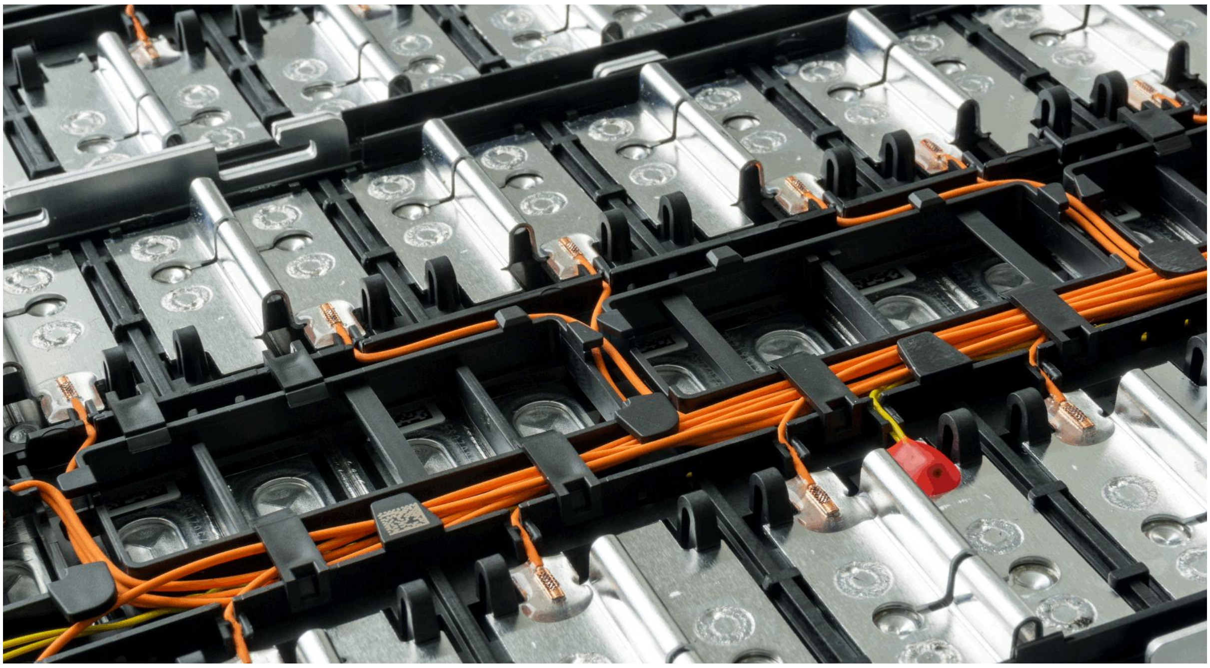
This work was completed with supporting funding from the Faraday Battery Challenge.

2. Battery pack design

> **Development teams can home-in on optimal pack designs faster, reducing the number of prototypes**

Alchemite™ is being used to generate models that capture howpack design impacts on performance. One example is the MAT2BAT battery design project [3] which explores how material selection, cell form factor, battery pack layout, and choice of thermal management system affect key performance metrics such as energy/power density, cost, embodied energy, and recyclability.

Because data for such studies is compiled from multiple, inconsistent sources throughout a supply chain it often contains gaps. Alchemite™ imputes this sparse data to determine which inputs drive the key outputs. Development teams can home-in on optimal pack designs faster, reducing the need for costly prototyping or time-consuming multi-physics modelling.



3. Battery Management Systems

Efficient operation of batteries requires effective Battery Management Systems. These need to determine the state-of-charge (SOC) and state-of-health (SOH) of batteries – metrics that enable them to, for example, estimate driving range for an electric vehicle. In addition, reliable prediction of remaining useful life (RUL) allow batteries to be used to their maximum life expectancy before replacement or disposal. Knowledge of the RUL for spent electric vehicle batteries could also enable their redeployment in less demanding, second life applications such as stationary grid storage.

Ideally, we want to predict SOC, SOH, and RUL based on easily-measurable properties in a live battery system, such as number of charge/discharge cycles, current flow, voltage, temperature, and battery type. Physics models that make these predictions are complex and need to trade-off accuracy against computational efficiency in order to be practical for use in battery management.

A recent study [5] by the Intellegens CTO in collaboration with the University of Cambridge, Institute of Materials Research and Engineering (A*STAR), and Nanyang Technological University examined the possibility of using Alchemite™ machine learning (figure 3). It used an ML model, trained using available data from simulation and high-throughput experimentation, to predict SOC, SOH, and RUL for lithium-ion battery systems. This opens up new possibilities for a data-driven approach to battery management systems.

This work suggests new possibilities for a data-driven approach to Battery Management Systems

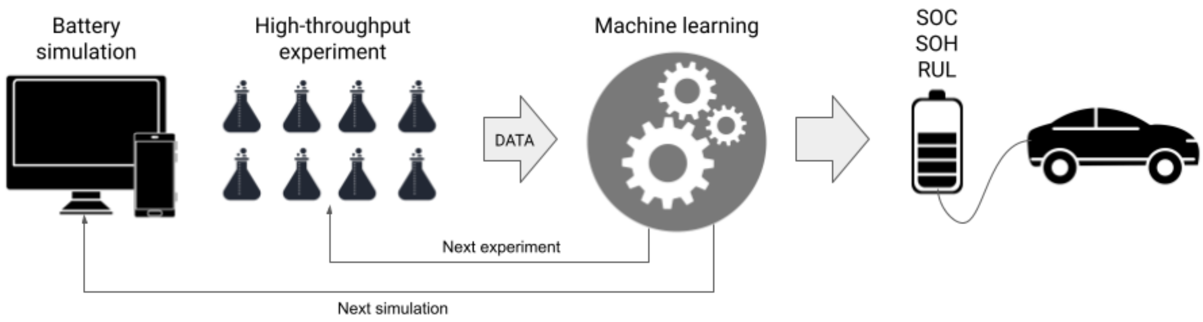


Figure 3. Potential use of machine learning in Battery Management.

Conclusion - benefits of Alchemite™ for batteries

We have seen how Alchemite™ deep learning can be applied in three key application areas for batteries. What benefits can this bring to battery development teams?

1. Maximise performance throughout the battery value chain

Machine learning can propose concepts for materials, formulations, and cells that would not be found via experimental approaches and scientific intuition alone. ML also helps to optimise battery packs and its potential to revolutionise battery management.

2. Accelerate development with up to 80% less experiment and prototyping

Alchemite™ enables you to explore formulation space more efficiently than traditional design of experiments approaches. It can propose optimal solutions, giving you a starting point for experiment closer to the desired outcome. Alchemite™ can also guide experimental programs by suggesting which test to do next in order to gain the greatest improvement in your model of a system for the least effort. Such approaches can reduce experimental workloads by up to 80% [6]. Similarly, you can reduce the number of prototypes needed during battery cell, module, and pack development and scale-up.

Machine learning approaches can reduce experimental workloads by up to 80%

3. Minimise cost and environmental impact

Machine learning can factor in all available data: not only chemical properties, engineering properties, and processing parameters, but also factors such as production costs and environmental impact. A holistic approach to achieving overall project objectives is built in from the start of the design process.

4. Reduce defects for lower business risk

Machine learning can reduce the number of defective cells by identifying which combinations of formulation and processing parameters increase defect rates. The ability for an ML model to continually learn from new data means that ML could be built into an on-going quality control process. Fewer product failures means a safer product, reduced business risk, and more satisfied customers.

Fewer product failures and standardised processes mean lower business risk and more satisfied customers

5. Standardise processes enterprise-wide

Systematic use of ML enables teams to apply the same process for each new project, capturing the results in ML models that can then be refined and applied in future projects. This ensures consistency and reduces risk due to variations in interpretation.

About Intellegens

Intellegens provides unique deep learning software, Alchemite™. Our focus is on making it easy to apply machine learning to accelerate innovation in materials, chemicals, manufacturing, and beyond. Alchemite™ can train neural network models from real-world, sparse, noisy data. The method originated at the University of Cambridge and development is on-going at Intellegens. Successful applications include industrial R&D and process improvements in superalloys, additive manufacturing, chemical processes, formulated products, batteries, and drug discovery.

References

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