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Machine Learning in Lithium-Ion Battery Cell Production: A Comprehensive Mapping Study

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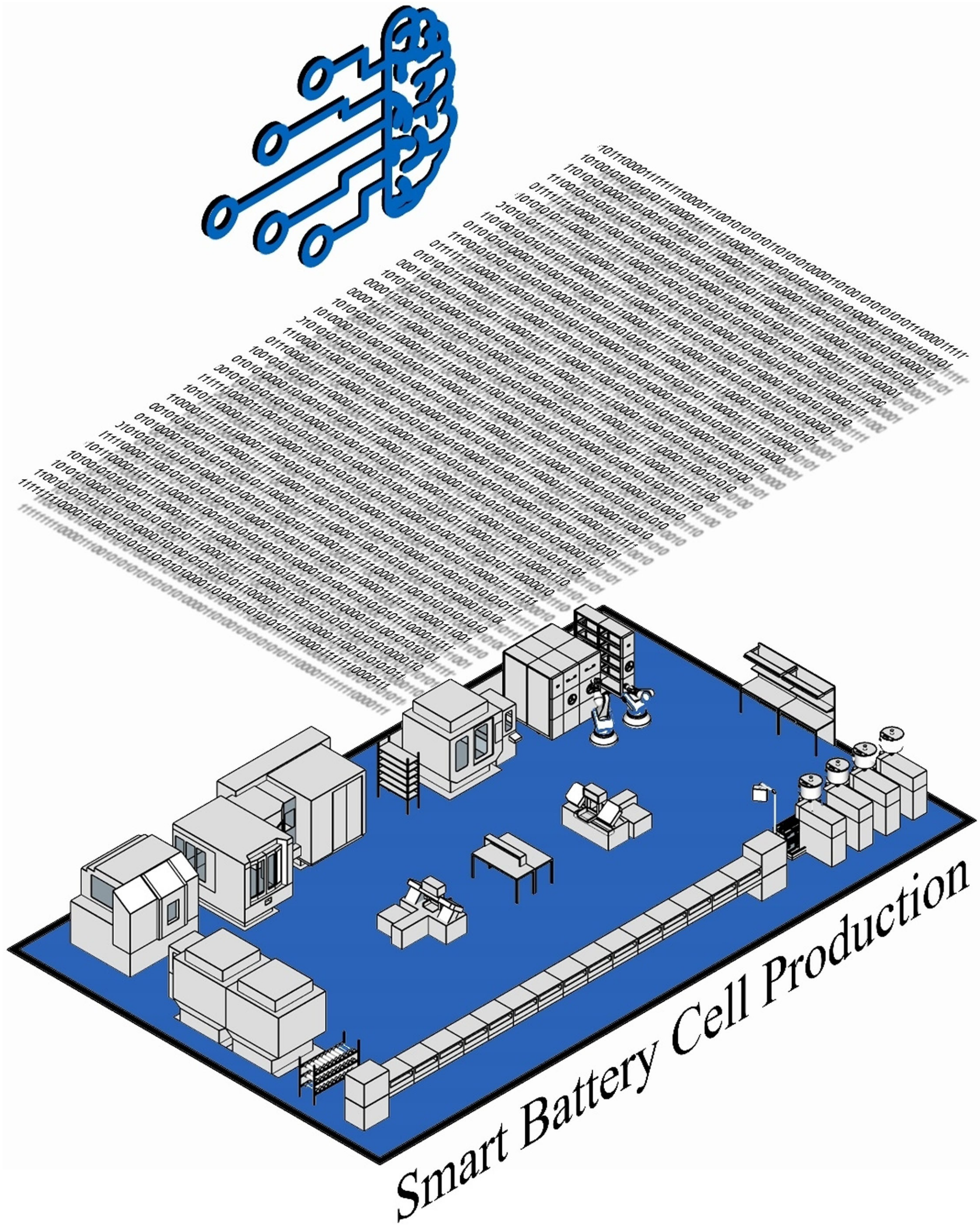

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With the global quest for improved sustainability, partially realized through the electrification of the transport and energy sectors, battery cell production has gained ever-increasing attention. An in-depth understanding of battery production processes and their interdependence is crucial for accelerating the commercialization of material developments, for example, at the volume predicted to underpin future electric vehicle production. Over the last five years, machine learning approaches have shown significant promise in understanding and optimizing the battery production processes. Based on a systematic mapping study, this comprehensive review details the state-of-the-art applications of machine learning within the domain of lithium-ion battery cell production and highlights the fundamental aspects, such as product and process parameters and adopted algorithms. The compiled findings derived from multi-perspective comparisons demonstrate the current capabilities and reveal future research opportunities in this field to further accelerate sustainable battery production.

1. Introduction

The lithium-ion battery (LIB) is taking on a prominent role in the transition to a more sustainable future by facilitating zero-emission mobility and revolutionizing the energy sector. LIB technology is still subject to continuous improvement to meet the industry's rising demands in terms of performance, costs, and quality.[1] Efforts are being made to optimize the entire battery value chain, which consists of different stages from material to cell production, battery pack, and recycling. Battery cell production is a crucial part of the value chain, accounting for 46 % of value-creation and macroeconomic opportunities by 2030.[2] The production process chain consists of multiple interconnected process steps with a large number of parameters that can influence the final cell characteristics. Due to the complexity of the processes with manifold interdependencies, the causality between the manufacturing parameters, environmental conditions, and product performance of both the final cell and its constituent components is still mostly unknown. For a cost-efficient quality-oriented optimization of the process chain, an in-depth understanding of the individual process steps, their interdependencies, and their impact on the cell properties is deemed to be absolutely imperative.[3] Given the high complexity of the process chain, along with advancements in digitalization and information technology, data-driven approaches have gained attention in battery research over recent years.[4,5]

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While the application of artificial intelligence (AI) and particularly machine learning (ML) as one of its significant branches has been profoundly analyzed and reviewed in the battery material domain[6,7] and the system-level operation,[8–10] the field of battery cell production has received comparatively less attention. The major achievements in the interdisciplinary field of ML and battery research, from material discovery to microstructure characterization and battery system design, have been reviewed by Ling.[11] The report highlights the availability of high-efficacy battery data as the primary challenge in this domain and describes mitigation strategies and the relevant existing studies to overcome this barrier.[11] In a book presenting examples of data-driven approaches across the battery lifespan, Liu et al.[12] dedicated a chapter to data-driven battery manufacturing management, including a summary of common ML tools and four use cases in electrode and cell manufacturing. Lombardo et al.[13] conducted an extensive review of ML-focused research activities in the battery community. The review provides a comprehensive overview of ML's working principles, followed by a summary of primary studies in material design, manufacturing, characterization, and battery diagnosis and prognosis. The study emphasizes that the battery community has not given equal attention to all fields, with manufacturing accounting for only 6 % of the 200 analyzed articles.[13]

An in-depth analysis of the ML applications in battery cell production is desired to foster and accelerate the adoption of ML in this field and assist the interested battery manufacturing community with the first steps towards smart, sustainable battery cell production. This article addresses this demand with a comprehensive assessment of existing ML-based analysis in battery cell production. Based on a systematic mapping study, relevant use cases are identified, and critical information is extracted and synthesized, with the aim to provide new insights into the state-of-the-art and deliver instructive guidance for future research. This research work is novel and unique as it categorizes and evaluates existing studies systematically based on various evaluation criteria such as production scale, cell type, process steps, and product and process parameters.

The remainder of this article is structured as follows. Section 2 provides a short introduction to the terminology used and outlines the methodology and criteria adopted to identify and analyze existing studies. Section 3 begins with an overview of the current use cases, followed by a meta-analysis of the studied processes and the variables involved in ML

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modeling. Additionally, the adopted algorithms and the evaluation metrics are reported. The various aspects presented in Section 3 are accompanied by critical analysis, while Section 4 elaborates on overarching future research perspectives, followed by concluding remarks in Section 5.

2. Terminology and Methodology

Concerning ML techniques, a distinction can be made between supervised, unsupervised and semi-supervised learning.[14] In supervised learning, the algorithm is presented with data points labelled as input and output variables. The ultimate objective is to develop a model that can predict or classify the output for previously unseen input variables. In case of unsupervised learning, the model aims to identify the underlying structure and pattern from the input variables. Semi-supervised approaches fall between the previously mentioned categories and are based on a combination of labelled and unlabelled data.[15] In statistical literature, input variables are often referred to as predictors or independent variables. The term feature in the ML domain is also used interchangeably with the input variable.[16] In particular, in the pattern recognition literature, the feature can be seen as a numeric representation of an aspect of the raw data.[17] From the production perspective, various process and product parameters can be used as input variables in ML modeling. Depending on the type of output variables, the supervised ML can be further divided into regression and classification. While the latter evaluates data in classes, the former quantitively predicts continuous output values.[16] With the common terms in the ML field briefly introduced, the adopted approach is presented in the following.

In contrast to a systematic literature review, which is guided by a specific research question that can be answered empirically, a mapping study can be used to examine a broader topic and categorize the primary research in a particular field.[18] To provide insights into the applications of ML in battery cell production, a systematic mapping study was undertaken based on the following five steps, according to Kitchenham et al.;[18] (i) definition of the research scope, (ii) searching the literature for primary studies, (iii) screening for inclusion, (iv) classifying the studies, (v) data extraction and aggregation.

The Scopus database was searched using the search strategy shown in Table 1. It should be noted that the indicative keywords employed during the search included but were not constrained to the ones shown in Table 1, as the review process is iterative in nature. In total, 215 publications were retrieved, examined, and shortlisted based on their title and abstract. In addition, for authors with more than five relevant articles, an author-specific search was conducted. As a result, 38 articles were identified as pertinent and subjected to a comprehensive analysis.

Parallel to the research scope, evaluation criteria were defined to classify and characterize the studies. These included the analyzed aspects and processes, investigated material, production scale, input and output variables of the ML model, adopted algorithms, evaluation metrics as well as the size of the dataset employed in the respective study. In the following, a brief description of the evaluation criteria is presented for completeness.

From the production perspective and analyzed aspects, a distinction was made between formulation, mixing, coating, drying, calendering, cell assembly and finalization, and cell characterization. The investigated electrode and the active material were also noted. In terms of scale, material research and development in battery production are primarily carried out on a lab scale using partially manual, discontinuous process stages, whereas production research is conducted on a pilot scale using semi to fully continuous and automatic processes. The manufacturing readiness level (MRL) as a systematic metric can be used to assess the maturity of a production system and processes.[19] The MRL for the lab scale is between 3 and 4, while the MRL for the pilot scale is between 5 and 6, with the ability to produce prototype components in a production-relevant environment. Furthermore, the amount of material employed to conduct experiments can be used as an indicator of the production scale. Based on the information provided, the studies were divided into lab and pilot scales. Additionally, from the product perspective, the cell type – coin, pouch, or prismatic cell – was considered for the studies investigating cell characteristics.

From the ML perspective, the product and process parameters that served as variables and the adopted algorithms were highlighted. It is beyond the scope of this article to provide details on the working principle of different ML algorithms; a detailed description can be found in a number of publications and handbooks such as Ref.[13,14,16,20–22]. In case of supervised learning, depending on the model type – regression or classification – different evaluation metrics are employed to assess the model's performance, robustness, and prediction capability. The reported evaluation metrics were also considered. Additionally, the sample size, which reflects the number of unique instances in each study, was analyzed. The results are presented in the following section.

Table 1. Search strategy for the mapping study.

Conceptualization	Operationalization
Keywords used in the query	(Lithium-Ion OR Batter* Production OR Electrode Production OR Electrode Manufacturing) and (Data-driven OR data mining OR machine learning OR Artificial Intelligence)
Field of search	Article title, abstract, keywords
Timeline	2018–October 2022

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3. Application of Machine Learning in Battery Cell Production

3.1. Overview

The 38 studies identified as relevant are listed in Table 2, categorized based on the type of study. The largest fraction of these studies (39%) used ML to predict cell characteristics based on product or process parameters in the production process chain. Among these, some studies initially developed models to predict intermediate product properties, followed by models for cell characteristics.[23–26] 26% of the studies have only focused on intermediate product parameters by analyzing single or multiple processes. Within this context, intermediate product properties include viscosity at specific shear rate, electrode mass loading, electrode thickness, and porosity. These studies generally revolved around the mixing, coating, and calendering process. One unique study showcased ML's potential for investigating and optimizing manufacturing energy demand.[27] 21% of the articles explored the utilization of simulation models coupled with ML. Among these, some studies combined experimental data with in silico methods and ML techniques to analyze the manufacturing process and its influence on mesoscale electrode properties.[28,29] Lombardo et al.[30] demonstrated the benefit of ML methods for the efficient parametrization of a simulation model. Shodiev et al.[31] developed an ML model to reproduce the electrolyte filling dynamics in three dimensions using simulation data. Studies involving deep-learning-based image processing have been listed separately (see Table 2). While most of these studies used images as input variables, Rohkohl et al.[32] demonstrated the application of deep learning to analyze data from eddy current measurement as an inline method for weld seam inspection, replicating computer tomography images.

The majority of the studies are based on supervised ML, aiming to predict or classify an output variable. Duquesnoy et al.[33] presented an approach combining unsupervised and supervised ML algorithms to predict the electrode properties and systematically cluster the produced electrodes concerning heterogeneity. Primo et al.[34] adopted an unsupervised ML algorithm in combination with advanced statistical methods to analyze the interdependencies in the calendering process.

The categorization of the analyzed articles serves to offer an overview of the possible use cases or methods applied in ML-based studies in battery cell production, following the systematic mapping study approach. It is worth noting that studies may be categorized differently depending on the overall research objective.

Figure 1 shows a breakdown of the analyzed studies from different perspectives. The majority of the studies explored the interdependencies between processes and cell characteristics. This is followed by process-specific studies analyzing the intermediate products. Around 60% of the studies analyzed processes in electrode manufacturing, followed by 24% investigating processes in cell assembly and finalization. Among the studies focusing on electrode manufacturing, 62% investigated cathodes, while 14% only concentrated on anodes. The remaining 24% studied both cathodes and anodes. In terms of active material, NMC (mainly 622 and 811) was the focus of 81% of these studies, while graphite was investigated as the primary anode material in 33% of the studies.

Most studies utilized data generated at the pilot scale, followed by simulation-based and lab-generated data. 18% of the studies were based on publicly available external datasets. While the majority of the data were generated on the pilot scale, around 53% of the studies analyzing the electrochemical cell characteristics were based on coin cells (in both half-cell and full-cell formats). This is in line with the fact that most studies only focused on electrode manufacturing. 40% of the studies evaluated cell performance on multilayer pouch cells, and one single study was conducted based on the data collected from prismatic cells.

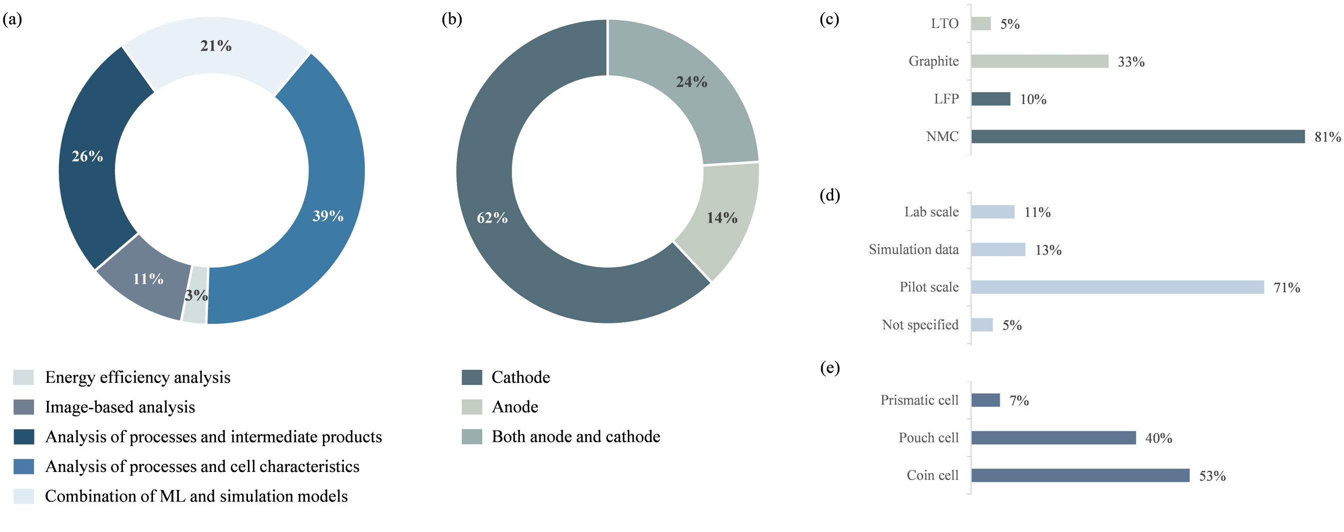

Figure 1. Breakdown of the analyzed articles categorized by a) type of the studies, b) type of the electrode analyzed in the electrode manufacturing, c) active material analyzed in studies focusing on electrode manufacturing, d) production scale and e) cell type.

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Table 2. Overview of the analyzed articles based on the type of study.

Type	Publication	Main objective	Ref.
Analysis of processes and cell characteristics	Drakopoulos et al., 2021	Analysis of the slurry formulation and electrode manufacturing parameters and their influence on the cell performance with a focus on the graphite-based anode	[23]
	Faraji Niri et al., 2021	Investigating the effects of coating control parameters on the electrode properties and cell characteristics using different ML models	[26]
	Faraji Niri et al., 2022a	Quantifying the effect of the N:P ratio on energy capacity and gravimetric capacity at different C-rates	[35]
	Faraji Niri et al., 2022b	Analysis of the calendering control variables on the cell impedance and capacity fading using explainable machine learning	[36]
	Faraji Niri et al., 2022c	Quantification of the contribution of coating control parameters to predict electrode and cell properties	[24]
	Faraji Niri et al., 2022d	Analysis of the slurry properties in combination with different coating parameters and their impact on final cell characteristics using explainable machine learning	[25]
	Kornas et al., 2019	Establishment of a framework to combine domain expert knowledge with data-driven approaches to analyze the cause-and-effect relations in the LIB production	[37]
	Liu et al., 2022a	Development of a framework based on interpretable machine learning to analyze the effects of coating parameters on the prediction of cell properties	[38]
	Schnell et al., 2019	Application of data mining approach to analyze interdependencies between parameters along the process chain and the final cell capacity	[39]
	Stock et al., 2022	Early classification of battery cycle life into two groups based on the formation and impedance data collected in different stages of cell finalization	[40]
	Thiede et al., 2019	Application of data mining approach to predict multi-criterial cell properties based on the parameters collected along the process chain	[41]
	Turetskyy et al., 2020a	Development of a holistic data-driven concept to acquire data along the LIB process chain and analyze the product and process interdependencies	[42]
	Turetskyy et al., 2020b	Establishment of a cyber-physical concept based on quality gates to predict the cell capacity using the intermediate product properties	[43]
	Turetskyy et al., 2021	Development of a multi-output approach for a battery production design to predict the final cell characteristics based on the intermediate product features	[44]
	Wang et al., 2022	Establishment of an interpretable machine learning framework to predict battery capacity under different C-rates based on the battery component properties	[45]
Energy efficiency	Thiede et al., 2020	Development of a systematic ML-based approach to analyze the energy efficiency potential in a manufacturing system based on a use case from LIB production	[27]
Analysis of processes and intermediate products	Cunha et al., 2020	Investigation of the interdependencies between slurry parameters and electrode properties	[46]
	Duquesnoy et al., 2021	Assessment of the impacts of electrode manufacturing parameters on the heterogeneity of NMC811 cathode	[33]
	Leithoff et al., 2021	Implementation of signal analysis and ML techniques to monitor the lamination process concerning missing or misaligned components	[47]
	Liu et al., 2021a	Development of a classification framework to analyze the effects of product parameters in the mixing and coating process on the electrode properties	[48]
	Liu et al., 2021b	Establishment of an interpretable ML-based framework to analyze the interdependencies between porosity and critical parameters in the mixing and coating process	[49]
	Liu et al., 2021c	Quantification of the importance of intermediate product and process parameters in mixing and coating processes and their influence on the electrode mass loading	[50]
	Liu et al., 2021d	Development of a classification framework based on a support vector machine using different kernels to predict the electrode mass loading	[51]
	Liu et al., 2022b	Classification of the electrode mass loading and porosity based on the slurry properties and coating process parameter	[52]
	Primo et al., 2021	Analysis of the calendering process parameters and their influence on the electrode properties, such as porosity and electronic conductivity	[34]
	Rohkohl et al., 2022a	Development of a data-driven concept to run virtual experiments and identify the desired product characteristics, with a use case on the extrusion process for slurry production	[53]
ML and simulation	Duquesnoy et al., 2020b	Analysis of calendering process on the electrode mesoscale properties using a combination of ML and simulation models	[29]
	Duquesnoy et al., 2022	Development of a data-driven framework for fast prediction of the results of a molecular dynamics simulation for slurry rheology	[54]
	Kim et al., 2022	Establishment of a synthetic-data-based framework for the classification and quantification of battery aging mode	[55]
	Lombardo et al., 2020	Comparison of data-driven and manual optimization approaches for the parametrization of a 3D simulation of the slurry	[30]
	Quartulli et al., 2021	Development of ML models based on data generated by simulations to predict the battery performance	[56]
	Takagishi et al., 2019	Establishment of a data-driven approach to design the mesoscale electrode properties using 3D virtual structures and ML technique	[28]
	Turetskyy et al., 2019	Introduction of a concept to combine a physical battery model and a data-driven feedforward network for end-of-line battery cell characterization	[57]

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Table 2. continued

Type	Publication	Main objective	Ref.
	Shodiev et al., 2021	Application of ML techniques to predict electrolyte infiltration using mesostructured of NMC cathode	[31]
Image-based analysis	Badmos et al., 2020	Identification of microstructural defects in battery electrodes based on microscopy images using a deep learning approach	[58]
	Faraji Niri et al., 2022e	Development of a framework to quantify electrode structural characteristics via 2D and 3D images using a deep learning approach	[59]
	Gayon-Lombardo et al., 2020	Evaluation of a method to generate synthetic 3D microstructures with a use case for the LIB cathode	[60]
	Rohkohl et al., 2022b	Application of ML techniques to analyze eddy current measurement data and evaluate the quality of the weld seam	[32]

To a certain degree, the identified studies coincide with the conventional use cases of the ML in the production domain,[61] such as quality control. Given the complexity of battery production, the majority of studies focus on establishing a foundation for process understanding by analyzing the interdependencies between process parameters and (intermediate) product properties. A possible next step in this field is enabling inline process control and optimization using ML-based process models and optimization techniques such as genetic algorithms.[62,63]

Considering the cost-intensive production and the high share of greenhouse gas emissions,[2] ML approaches can be used for a holistic sustainability assessment in battery production,[64] particularly from economic and environmental perspectives. Nonetheless, this aspect has not yet been fully explored in battery production. Thiede et al.[27] proposed a framework for analysis of the energy efficiency potentials in manufacturing processes. The application of the proposed framework was demonstrated based on the data collected from a battery pilot production line. Rohkohl et al.[53] developed a data-driven framework that enables the execution of virtual experiments to determine the appropriate set of process parameters, considering economic and ecological targets. For this purpose, a cost model is included in the framework.[53] The application of the proposed framework is demonstrated for the continuous mixing process using an extruder, focusing on the application of ML to predict the product characteristics based on the set process parameters. However, the cost model‘s implementation is considered as future work.

Predictive maintenance is another promising use case in the production domain that has been overlooked in battery cell production, particularly in processes such as calendering, which are subject to wear over time. This shortcoming could be traced back to the fact that most of the studies are based on laboratory or pilot line productions with discontinuous operations, a limited amount of data, a lower level of digitalization and IT infrastructure compared to industrial mass production. The latter also hinders the application of methods such as process mining[65] and its integration in life cycle assessment.[66]

3.2. Processes, variables, and algorithms

A more detailed analysis based on the data pooled from the evaluated studies is presented in this section. Figure 2 provides an overview of the analyzed processes, including single-process investigations and studies considering correlations between at least two process steps. The electrode coating process is the most investigated step in the process chain, accounting for 39%, whereas the drying process is in the minority, accounting for only 5% of the research studies. While several studies focused on a single process step, 37% looked into cross-process effects. However, these effects have not been limited to consecutive process steps; for instance, there are studies examining coating and calendering processes. Around 35% of the cross-process studies are based on non-consecutive process analyses. Such studies are built on the assumption that the effects of the intervening process – for instance, the drying step – can be filtered out. Given the high interdependencies of the subsequent processes, neglecting the effects of an intervening stage while assessing cross-process effects is associated with some degree of indeterminacy.

Following the process analysis, the product and process parameters were examined closely in the next step. One of the major challenges in battery cell manufacturing is an in-depth understanding of the cause-and-effect relations along the process chain that are relevant in determining the quality of the final product.[37] Hence, Figure 3 underlines the influential parameters analyzed in association with cell characteristics using supervised ML. 40% of the studies investigated the discharge capacity at different C-rates, with the majority (83%) based on half-cell coin format and 17% on full-cell coin format. The cell capacity after formation was analyzed in 47% of the studies. The multilayer pouch cell is the primary cell format in this category, followed by prismatic and half-cell coin format, each accounting for 14%. One-third of the studies analyzed the battery's cycle life, with 60% focusing on pouch cell format and the remainder on half-cell coin. It should be mentioned that a set of studies investigated the capacity loss after a certain number of cycles as a representation of the cycle life.

The discharge capacity at different C-rates and the cycle life are the two cell characteristics that have been most studied in conjunction with a high number of multiple input variables (see Figure 3). The primary input variables that have been included in predicting the cell characteristics are the active

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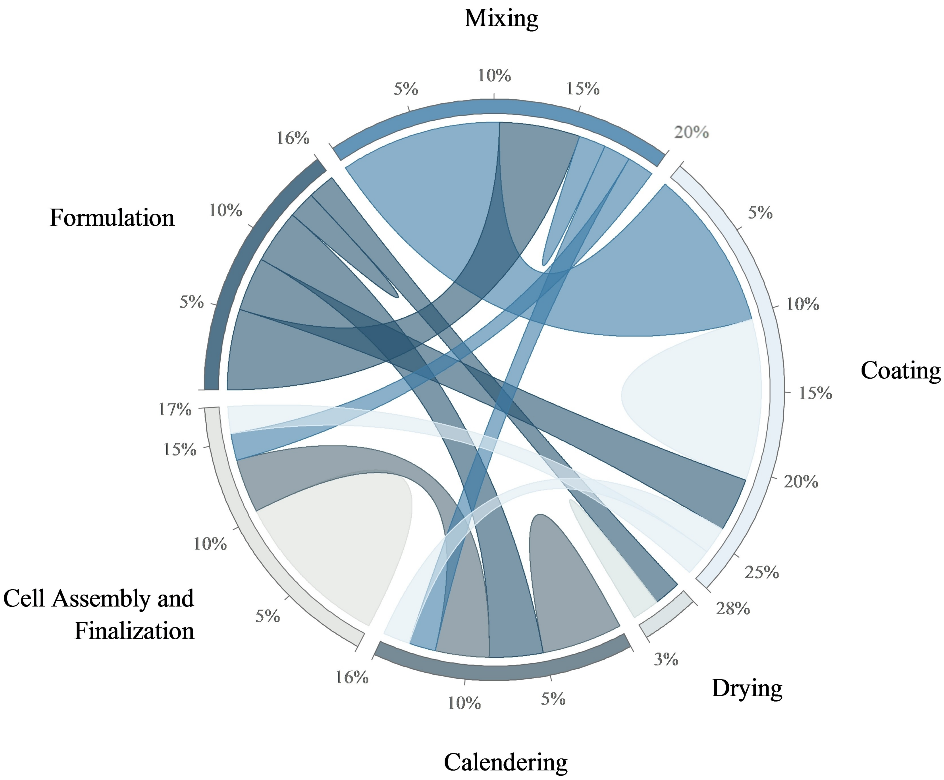

Figure 2. Overview of analyzed processes, including studies analyzing aspects between two process steps. The widths of the links are proportional to the number of studies. The percentages indicate the number of interdependencies related to one process step compared to the total number of interdependencies analyzed.

material weight, electrode thickness, and porosity. Although electrode thickness and porosity can be considered correlated, the variables were included as reported in the studies. A detailed list of input and output variables, not only limited to cell properties, can be found in the supplementary data.

Figure 4 explores the relationship between input variables, output variables, and adopted algorithms. To provide a concise overview, the focus has been given to the combination of input and output variables analyzed in at least two studies. The trend observed for the main input parameters in combination with the cell properties can also be confirmed in Figure 4. Additionally, variables such as solid content, coating ratio, coating gap, and slurry viscosity can be marked as frequently reported input variables in the modeling. Among the intermediate product properties, dry mass loading and porosity are the prominent output variables. In terms of algorithms, tree-based models, including ensemble tree models, and neural networks, predominantly Artificial Neural Networks (ANN), are the most commonly used modeling techniques. The former was deployed in approximately 68% of the studies and the latter in 50%. For image-centered studies, neural networks were the only model type employed due to the complex nature of image analysis.

While some detailed analyses have been carried out on intermediate products and cell characteristics using supervised ML, some aspects have not yet been thoroughly investigated or remain unaddressed. Considering the quality-relevant parameters in electrode manufacturing,[67] in the mixing process, the majority of the existing studies focus only on the product parameters of the slurry, leaving out the relevant process parameters, such as revolution speed. Rohkohl et al.[53] confirmed that experts identified 15 process parameters influencing the quality of the produced slurry in the extrusion process. However, these were not extensively analyzed and considered in the developed ML process model. As depicted in Figure 2, the drying process and its relevant parameters, such as the temperature profile[68] and the drying speed, have received comparatively limited attention. In terms of production technology, all ML-based studies involving the coating process address comma bar or doctor blade technology. As a result, other industry-relevant technologies, such as slot-die coating and its associated parameters,[69] or innovative approaches, such as solvent-reduced electrode production,[70] remain primarily unexplored. Concerning promising technologies, Leithoff et al.[47] showcased a unique study on applying ML models for inline process monitoring during the lamination process based on acoustic measurements. The environmental conditions, in conjunction with the manufacturing processes, have an impact on the electrochemical performance of the battery cell.[71] However, these factors have not been incorporated into the existing ML-based studies. In the cell assembly and finalization, the electrolyte filling process and the formation process are quality-critical steps that are regarded as bottlenecks in terms of throughput.[3,72] However, the existing ML-based studies do not thoroughly represent these processes. Shodiev et al.[31] presented a unique study demonstrating the use of ML to predict the degree of

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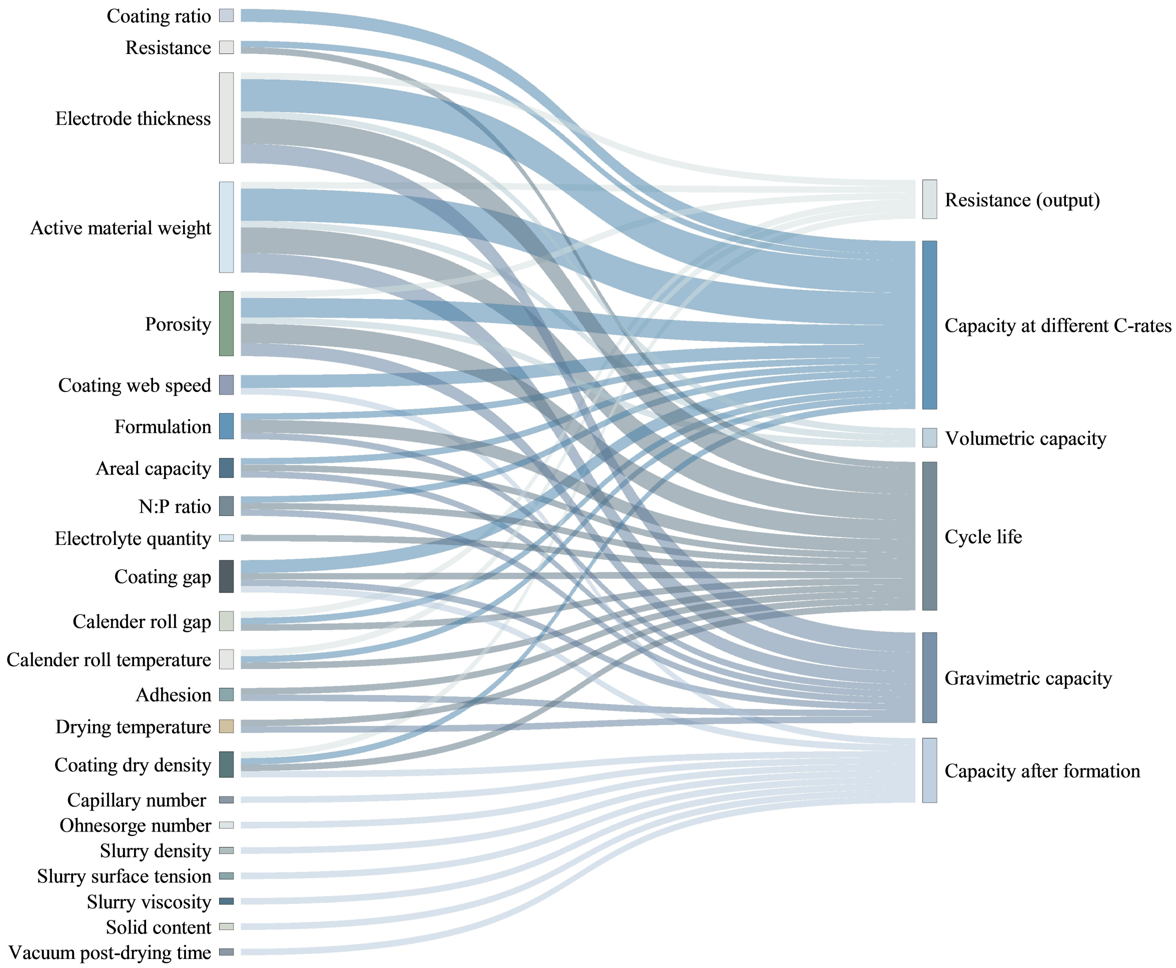

Figure 3. Sankey diagram with input variables for the ML modeling on the left side and the cell characteristics as output variables on the right side.

wetting based on a simulation model and electrode mesostructure.

After a comprehensive analysis of process steps and variables, the adopted algorithms are briefly reviewed in the following. There is often a trade-off between the performance and flexibility of an ML model and its explainability and interpretability,[73,74] with more complex models typically offering better performance and a closer representation of the studied system at the expense of reduced transparency and ease of understanding. Interpretability can be defined as the ability to present the cause-and-effect relationships within a system's input and output variables in understandable terms to a human being.[73,75] The selection of a model, with its level of interpretability and complexity, can be guided by the study's overall objective and the data characteristics. For example, Multivariate Linear Regression (MLR) is a white-box model with a high degree of interpretability.[16,73] The model is based on the assumption that there is an underpinning linear relationship between the input and output variables, or a linear model serves as a reasonable approximation of the studied system.[16] Although MLR has a higher degree of interpretability compared to more complex, black-box ML models, its interpretability might be hampered by effects such as multicollinearity,[76] a condition in which the input variables are highly correlated. The Variance Inflation Factor (VIF) is a common technique that can be used to identify multicollinearity among the input variables.[76] A high VIF value indicates a high level of multicollinearity. Typically a threshold of 10 is set as the highest acceptable value.[76] In more conservative cases, a VIF value of 5 is considered as acceptable.[74] If multicollinearity exists in the dataset and it is not possible to extend the dataset using methods such as design augmentation[77], alternative techniques such as Principal Component Analysis (PCA) can be used for dimensionality reduction and improved interpretability.[78] Despite the high transparency of the MLR, this algorithm has found relatively limited application in battery production (see Figure 5), which could be due to the high complexity of the process chain or the fact that these models require a certain degree of prior knowledge of the system.

Another main trade-off to consider when selecting ML algorithms is the one between bias and variance. Variance is the degree to which a model's predictions vary, depending on the changes in the training dataset. A model with high variance is prone to overfitting to the training data and may not generalize well to new, previously unseen data. A low-variance model, on the other hand, is more resistant to changes in the

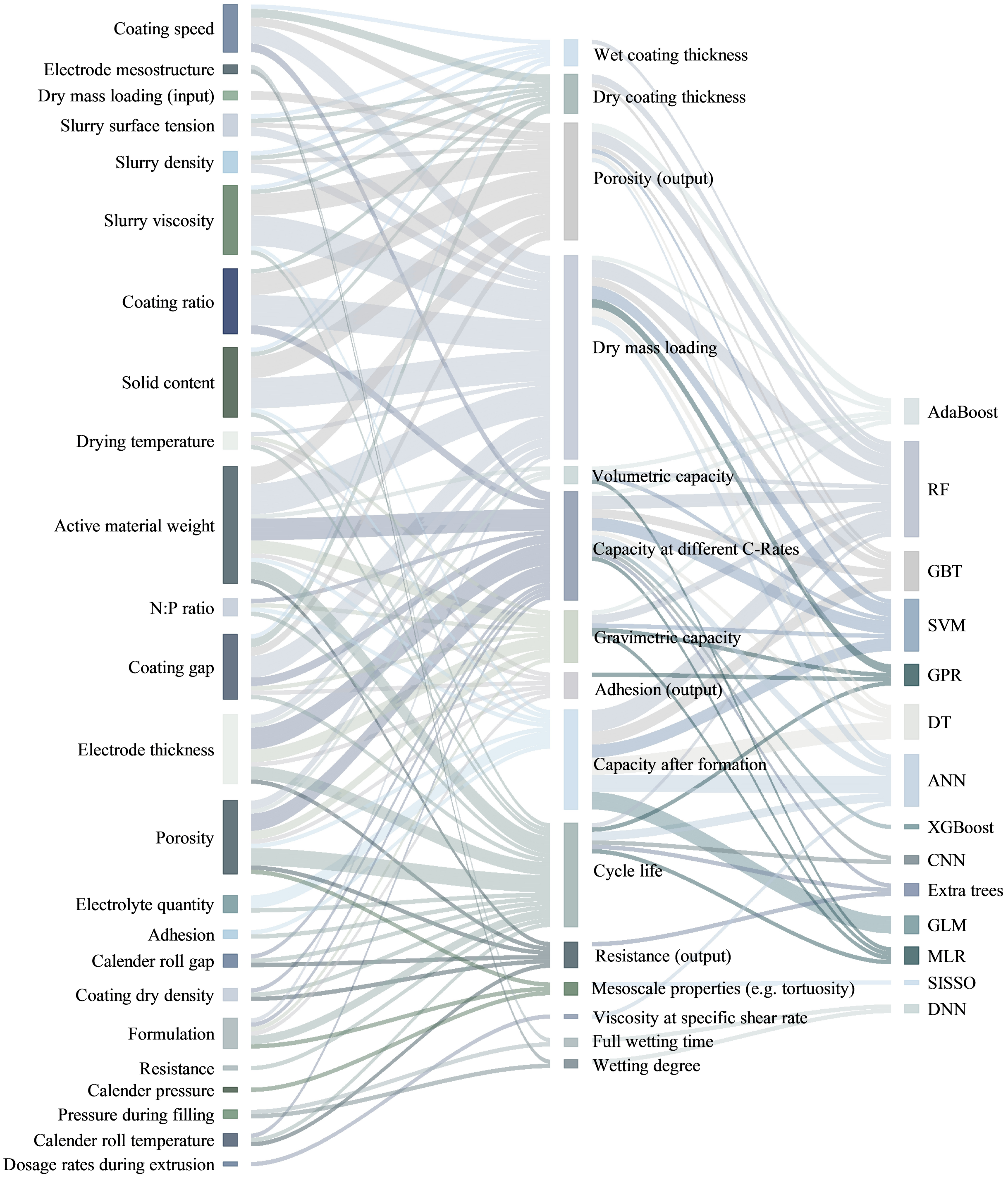

Figure 4. Sankey diagram illustrating the relationship between major input variables (left), major output variables (middle) and adopted algorithms (right).

training dataset and may generalize better to new data.[74] Bias is defined as the error that is introduced by approximating and simplifying the analyzed system. For example, linear regression is based on an oversimplified assumption of a linear relationship between the input variables and the output, which may not be entirely accurate for real-world complex systems.[74] Hence, using linear regression may introduce some degree of bias in estimating the output variable. The ultimate objective is to have ML models with low bias and relatively low variance. The Mean Squared Error (MSE) can be used to find a trade-off between these two factors.[74] The trade-off between bias and variance should also be considered in the validation approach.[16] While the leave-one-out approach may result in low bias, it might lead to high variance. To balance these two factors, *k*-fold cross-validation can be adopted.[16] The learning curve can be used to estimate the impact of the size of the training dataset on the model's performance. Empirically, k

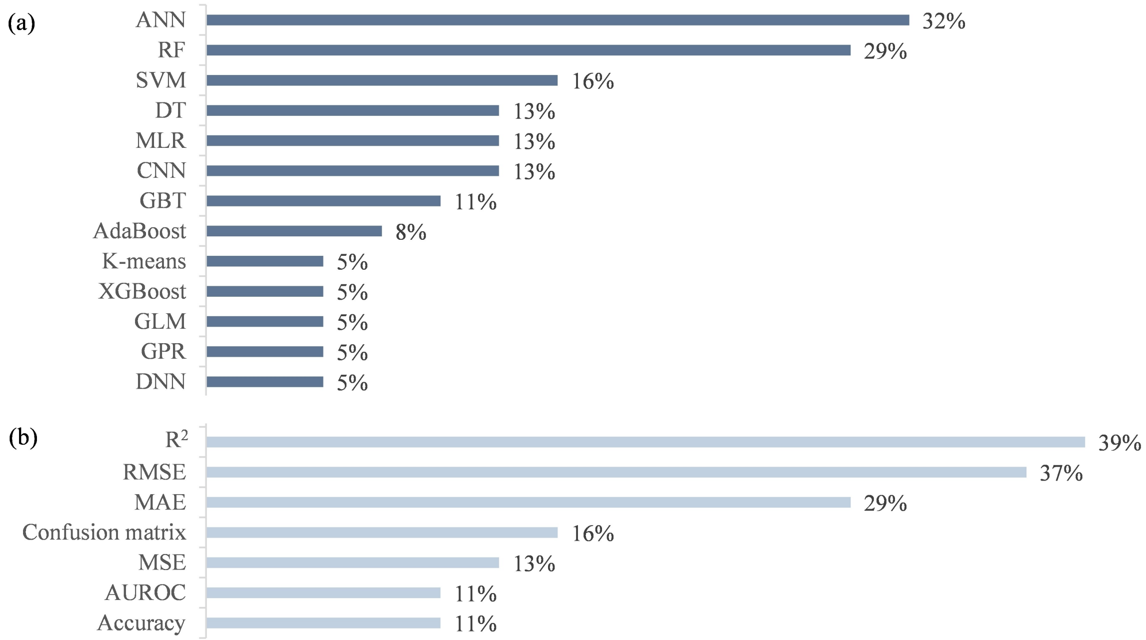

Figure 5. Percentage distribution of a) the most prevalent algorithms and b) the commonly used evaluation metrics in the analyzed articles.

values of 5 or 10 are shown to be suitable, considering also the computational resources required.[16]

In contrast to MLR, ANN, as a comparatively less interpretable ML algorithm, is one of the most frequently used techniques in battery cell production (see Figure 5). ANN is a nonlinear technique inspired by the oversimplified neural network structure of the brain.[21,79] By simulating interconnected nodes known as artificial neurons or units, ANNs attempt to mimic how neurons in the brain process and transmit information.[80] The neurons are organized into layers and can process complex patterns and relationships in data. Although ANN is recognized as a powerful technique capable of learning complex interdependencies within a system, this strength can also be a downfall. ANN models, especially those with complex architectures and limited datasets, have a tendency to overfit the training data, which can compromise their ability to generalize well to previously unseen data.[81] Another disadvantage of ANN is the large amount of data required. In addition to the volume of data needed, the data must also be suitably diverse to facilitate the model's training. This latter requirement is often a challenge when intending to analyze large-scale production due to the cost and limited flexibility of the equipment employed.

Similar to ANN, Random Forest (RF) is one of the most used algorithms in the analyzed studies in battery cell production. RF is a robust ML algorithm based on an ensemble of decision trees with some desirable characteristics such as high accuracy, robustness to outliers, and lower variance.[74,82] Given its ability to reduce overfitting and lower variance, RF can be considered a favorable choice over ANN in some cases.

Assessing the performance of unsupervised ML models can be challenging as, unlike supervised ML, there is no established ground truth that can be served as a benchmark for the model's performance. An overview of possible approaches in this regard can be found in Ref. [83–85]. In case of supervised ML, the model performance can be evaluated based on the model type; for classification problems, metrics such as accuracy can be used, whereas Root Mean Squared Error (RMSE), R^2, or Mean Absolute Error (MAE) are adopted in regression studies. A brief definition of different evaluation metrics can be found in Joshi[86] and Liu et al.[12] Figure 5 provides an overview of the adopted algorithms and the evaluation metrics used in at least two studies. It should be noted that 44% of the studies used more than one algorithm for modeling, and 50% included more than one metric for the model evaluation. Given that different evaluation metrics can offer distinct perspectives on the performance of the model, it is appropriate to use different metrics for a comprehensive evaluation of a model.[87,88] Considering aspects such as variance, bias, performance, and complexity, it is also advantageous to compare different ML algorithms on the same dataset to determine the most suitable model for the specific use case and its requirements.

The mapping study included an in-depth investigation of the publications in terms of the number of input variables and sample size. While some studies were based on the Design of Experiments (DoE) or explicitly described the design space, others used historical data collected across the process chain from various production runs with limited information concerning the coherence of the design space and the unique data points. The latter could be of interest regarding handling big data; however, such studies are characterized by certain issues of spuriousness and statistical biases.[89] Hence, only studies with the reported sample size indicating unique instances in the dataset, such as the number of cells built, including the replicates, were considered and analyzed further. Additionally, studies based on simulation data, deep learning approaches, and unsupervised ML were excluded, leading to a total of 40% of the publications.

Figure 6 outlines the combination of the number of input variables and the sample size reported for different algorithms. Upon initial review, the figure does not reveal any distinctive patterns or overarching rules concerning the analyzed aspects, conveying that a trial-and-error approach is often adopted. For small datasets with a limited number of variables, MLR can be considered as a suitable choice. However, if there are many input variables, it is possible to employ dimensionality reduction techniques such as PCA or adopt regularization methods to prevent overfitting.[86] A relatively larger dataset allows the utilization of more complex algorithms such as ANN or RF.

In case of less complex regression models, the 1:10 rule is a common guideline in the statistical literature, indicating the sample size required for a single-variable problem. However, for use cases with multiple variables, this rule might not apply as additional factors, such as the complexity of the analyzed system and the dependencies between the variables, should be considered.[86] Various studies tried to establish similar guidelines for more complex models such as ANN.[90–92] It should be noted that such guidelines can be seen as heuristic approaches. Aside from performance, interpretability, sample size, and dimensionality, additional factors such as acceptable error margin, training time and computational capacity, model tuning effort, and robustness to outliers can be considered in the selection of ML algorithms. These various factors impede efforts to develop a detailed guiding principle for selecting an algorithm in battery cell production. Nonetheless, the compiled findings can serve as a reference point for interested researchers, elucidating the current capabilities and potential and revealing future research opportunities.

4. Research Perspectives

The presented mapping study with different use cases in battery cell production – from in-depth process analysis to prediction of cell characteristics and energy-efficient production – demonstrates the potential of ML technology in battery cell production. To fully exploit this technology's potential and facilitate its application, certain challenges still need to be addressed.

Keppeler et al. have highlighted the role of manufacturing pilot lines as a bridge between fundamental research and industrial production of LIB.[93] The same is granted regarding the ML application for LIB's product and process optimization. While the DoE can assist in increasing the effectiveness of ML development,[94] implementing such methods on a mass-production scale for data generation is impractical due to the high costs and effort involved. Hence, pilot lines can be strategically used to investigate factor variability and analyze the interactions at relatively lower costs. The significance of ML-focused production research at the pilot scale can certainly not be neglected. Nevertheless, some aspects demand greater attention from the research community; these are highlighted below and serve as the foundation for further work.

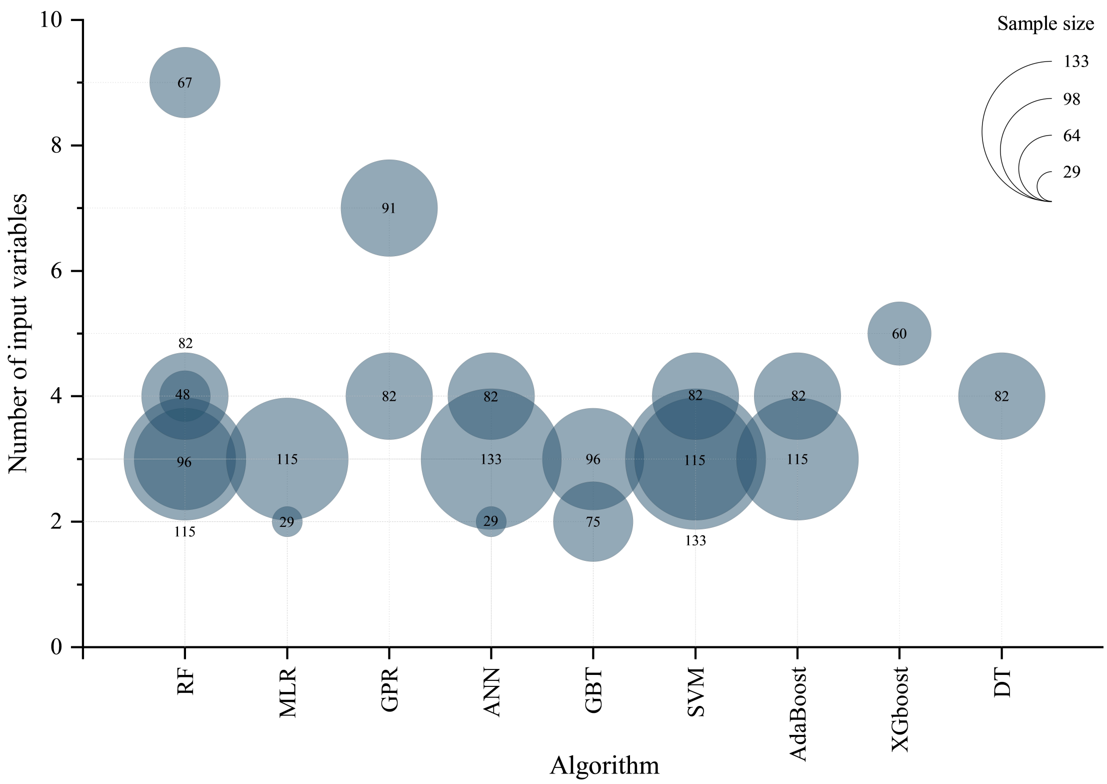

Figure 6. Bubble chart displaying the adopted algorithms, number of input variables and sample size for a collection of analyzed studies. The diameter of the circles indicates the sample size, with the sample size additionally noted.

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Due to the level of information discovered throughout the mapping study, some of the analyzed articles can be regarded merely as a proof-of-concept, demonstrating the potential of data-driven approaches in battery cell production. Although such exemplary academic implementations are beneficial, they are not sufficient to accelerate the realization of smart battery cell production on an industrial scale. Various researchers have tried to address this issue and provide high-level guidelines in the engineering field. For example, Banna et al.[95] have highlighted that little attention has been paid to the practical implementation of research-based ML techniques. To tackle this issue, they promoted best practices in the documentation and publication of the model in a way that others can easily use to build upon or reproduce their results.[95] Some major software companies, such as Google[96] or Microsoft,[97] have synthesized best practices in the large-scale development of data-driven applications. From the information system research community, Kühl et al.[98] confirmed the same challenge. Even with full access to data, the researchers cannot evaluate or replicate the results due to the inconsistency in the documentation and reporting of ML studies.[98] They proposed a "Machine Learning Report Card" as a solution to capture critical decisions and problem characteristics in the development of the ML model and to guide researchers toward rigorous, comprehensive analysis and extension. While the article focuses on supervised ML, the findings can also be adapted for unsupervised ML. The report focuses on general ML studies and consists of four main sections (i) model initiation, including information regarding data quality, data preprocessing, sampling, and data distribution, (ii) model development, which entails training and testing for supervised ML, (iii) performance estimation and (iv) model deployment. Such studies highlight the necessity of close cooperation between ML and domain, i.e., production experts.[98]

The above-mentioned inconsistencies in reporting have also been observed during the conducted mapping study, leading to a certain degree of uncertainty. For example, a key aspect that needs to be reported is whether a data point is a replication or a unique run. While the former considers, for example, three coin cells for each specific set of parameters, the latter is based on only one for each particular set of parameters. Both approaches have their advantages and can be considered in the modeling, with the former improving the model's robustness and the latter widening the scope of the model. However, the lack of information on this aspect makes it difficult to gauge the distribution and quality of the data.

Some initiatives have been launched to democratize the required tools, such as ontology, for scaling up ML models in battery production.[5,99] The democratization of such tools, combined with a standard protocol for the documentation and reporting of the necessary information throughout the entire procedure, is essential for both researchers and practitioners to build upon the valuable findings and accelerate ML application in LIB development and manufacturing.

An in-depth understanding of the LIB as a complex multi-scale system requires multiscale characterization techniques and modeling, ranging from micro to meso and macro level.[100] Based on the available inline characterization techniques, a coupling of ML models and in silico approaches is required to bridge the scales and derive holistic optimizations along the process chain. Some examples of this field are the studies presented by Gayon-Lombardo et al.[60] and Duquesnoy et al.[29] Advances in this field of research, combined with close collaboration with system-level modeling, can highlight new vistas in battery optimization research.

To accelerate the efficient embedding of ML technology into LIB mass production for low-latency inline monitoring and optimization, the interpretability issue needs to be addressed. The emergence of opaque and complex decision-making systems such as DNN illustrates this imperative amply. In response to the need for trustworthy, robust, and powerful models for complex real-world applications, the field of eXplainable Artificial Intelligence (XAI) has been revived.[101] With the help of XAI, it is possible to pinpoint how the decisions and predictions of the system are derived, turning black-box to glass-box models. Various methods can be used for this purpose.[73] Faraji Niri et al.[25,35] have showcased the benefits of Accumulated Local Effects (ALE) and Shapley Additive Explanations (SHAP) as XAI methods in LIB production. Such methods have not yet been well established within battery production research, indicating an untapped potential that needs to be explored.

5. Conclusions

In conclusion, the presented mapping study has highlighted the current capabilities for the application of ML in LIB cell production. This article goes beyond a literature review by extracting and synthesizing the findings, outlining the current focal points in the state-of-the-art, and pinpointing aspects such as processes, product and process parameters that have received relatively less attention within the literature. These include, for example, the drying process in electrode manufacturing or the electrolyte filling and formation in cell assembly and finalization. The multi-perspective comparison serves as a rigorous starting point for researchers interested in this field. Furthermore, certain over-arching challenges, such as documentation and interpretability of the ML models, have been identified, which should be addressed to accelerate ML's application in large-scale LIB production. ML models can be used to enhance the efficiency and efficacy of manufacturing processes. A holistic integration of data-driven applications in battery cell production, as a critical phase in the value chain, will drive a paradigm shift in battery optimization and the scale-up of novel material generations.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

Nomenclature

AI Artificial Intelligence;

ALE	Accumulated Local Effects;
ANN	Artificial Neural Network;
AUROC	Area Under the Receiver Operating Characteristic;
CNN	Convolutional Neural Network;
DNN	Deep Neural Network;
DoE	Design of Experiments;
DT	Decision Tree;
GBT	Gradient Boosting-based Tree;
GLM	Generalized Linear Model;
GNB	Gaussian Naive Bayes;
GPR	Gaussian Process Regression;
KNN	K-Nearest Neighbors;
LARS	Least Angle Regression;
LFP	Lithium Ferro Phosphate;
LIB	Lithium-Ion Battery;
LTO	Lithium Titanium Oxide;
MAE	Mean Absolute Error;
ML	Machine Learning;
MLR	Multivariate Linear Regression;
MRL	Manufacturing Rediness Level;
MSE	Mean Squared Error;
NMC	Nickel Manganese Cobalt;
PCA	Principal Component Analysis;
RF	Random Forest;
RMSE	Root Mean Square Error;
SHAP	Shapley Additive Explanations;
SISSO	Sure Independence Screening and Sparsifying Operator;
SVM	Support Vector Machine;
XAI	eXplainable Artificial Intelligence.

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Conflict of Interests

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

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[1] E. Ayerbe, M. Berecibar, S. Clark, A. A. Franco, J. Ruhland, *Adv. Energy Mater.* **2022**, *12*, 2102696.
[2] World Economic Forum, A Vision for a Sustainable Battery Value Chain in 2030. Unlocking the Full Potential to Power Sustainable Development and Climate Change Mitigation, **2019**.
[3] A. Kwade, W. Haselrieder, R. Leithoff, A. Modlinger, F. Dietrich, K. Droeder, *Nat. Energy* **2018**, *3*, 290–300.
[4] A. Mistry, A. A. Franco, S. J. Cooper, S. A. Roberts, V. Viswanathan, *ACS Energy Lett.* **2021**, *6*, 1422–1431.
[5] F. M. Zanotto, D. Z. Dominguez, E. Ayerbe, I. Boyano, C. Burmeister, M. Duquesnoy, M. Eisentraeger, J. F. Montaño, A. Gallo-Bueno, L. Gold et al, *Batteries & Supercaps* **2022**, *5*, e202200224.
[6] Y. Liu, B. Guo, X. Zou, Y. Li, S. Shi, *Energy Storage Mater.* **2020**, *31*, 434–450.
[7] X. Chen, X. Liu, X. Shen, Q. Zhang, *Angew. Chem. Int. Ed.* **2021**, *60*, 24354–24366.
[8] S. Wang, S. Jin, D. Deng, C. Fernandez, *Front. Mech. Eng.* **2021**, *7*.
[9] A. Samanta, S. Chowdhuri, S. S. Williamson, *Electronics* **2021**, *10*, 1309.
[10] L. Zhang, Z. Shen, S. M. Sajadi, A. S. Prabuwono, M. Z. Mahmoud, G. Cheraghian, T. El Din, M. El Sayed, *Engineering Analysis with Boundary Elements* **2022**, *141*, 1–16.
[11] C. Ling, *NPJ Comput. Mater.* **2022**, *8*, 1–22.
[12] K. Liu, Y. Wang, X. Lai, Data Science-Based Full-Lifespan Management of Lithium-Ion Battery. Manufacturing, Operation and Reutilization, Springer International Publishing AG, Cham, **2022**.
[13] T. Lombardo, M. Duquesnoy, H. El-Bouysidy, F. Årén, A. Gallo-Bueno, P. B. Jørgensen, A. Bhowmik, A. Demortière, E. Ayerbe, F. Alcaide et al, *Chem. Rev.* **2022**, *122*, 10899–10969.
[14] S. J. Russell, P. Norvig, *Artificial intelligence. A modern approach*, Pearson India Education Services Pvt. Ltd, Noida, India, **2018**.
[15] J. E. van Engelen, H. H. Hoos, *Mach. Learn.* **2020**, *109*, 373–440.
[16] T. Hastie, R. Tibshirani, J. H. Friedman, *The elements of statistical learning. Data mining, inference, and prediction*, Springer, New York, NY, **2017**.
[17] A. Zheng, A. Casari, Feature engineering for machine learning. Principles and techniques for data scientists, O'Reilly, Beijing, **2018**.
[18] B. A. Kitchenham, D. Budgen, O. P. Brereton in *Electronic Workshops in Computing*, BCS Learning & Development, **2010**.
[19] OSD Manufacturing Technology Program, *Manufacturing Readiness Level (MRL) Deskbook*, **2011**.
[20] S. B. Kotsiantis, *Informatica, Vol. 31, No. 3* **2007**, pp. 249–268.
[21] M. Kuhn, K. Johnson, *Applied predictive modeling*, Springer, New York, **2016**.
[22] K. P. Murphy, *Machine learning. A probabilistic perspective*, MIT Press, Cambridge, MA, **2021**.
[23] S. X. Drakopoulos, A. Gholamipour-Shirazi, P. MacDonald, R. C. Parini, C. D. Reynolds, D. L. Burnett, B. Pye, K. B. O'Regan, G. Wang, T. M. Whitehead et al, *Cell Rep. Phys. Sci.* **2021**, *2*, 100683.
[24] M. Faraji-Niri, K. Liu, G. Apachitei, L. A. Román-Ramírez, M. Lain, D. Widanage, J. Marco, *Energy and AI* **2022**, *7*, 100129.
[25] M. Faraji-Niri, C. Reynolds, L. A. A. Román Ramírez, E. Kendrick, J. Marco, *Energy Storage Mater.* **2022**, *51*, 223–238.
[26] M. Faraji-Niri, K. Liu, G. Apachitei, L. R. Ramirez, M. Lain, D. Widanage, J. Marco, *J. Cleaner Prod.* **2021**, *324*, 129272.
[27] S. Thiede, A. Turetskyy, T. Loellhoeffel, A. Kwade, S. Kara, C. Herrmann, *CIRP Ann.* **2020**, *69*, 21–24.
[28] Y. Takagishi, T. Yamanaka, T. Yamaue, *Batteries* **2019**, *5*, 54.
[29] M. Duquesnoy, T. Lombardo, M. Chouchane, E. N. Primo, A. A. Franco, *J. Power Sources* **2020**, *480*, 229103.
[30] T. Lombardo, J.-B. Hoock, E. N. Primo, A. C. Ngandjong, M. Duquesnoy, A. A. Franco, *Batteries & Supercaps* **2020**, *3*, 721–730.
[31] A. Shodiev, M. Duquesnoy, O. Arcelus, M. Chouchane, J. Li, A. A. Franco, *J. Power Sources* **2021**, *511*, 230384.
[32] E. Rohkohl, M. Kraken, M. Schönemann, A. Breuer, C. Herrmann, *Int. J. Adv. Manuf. Technol.* **2022**, *119*, 4829–4843.
[33] M. Duquesnoy, I. Boyano, L. Ganborena, P. Cereijo, E. Ayerbe, A. A. Franco, *Energy and AI* **2021**, *5*, 100090.
[34] E. N. Primo, M. Touzin, A. A. Franco, *Batteries & Supercaps* **2021**, *4*, 834–844.
[35] M. Faraji-Niri, G. Apachitei, M. Lain, M. Copley, J. Marco, *J. Power Sources* **2022**, *549*, 232124.
[36] M. Faraji-Niri, G. Apachitei, M. Lain, M. Copley, J. Marco, *Energy Technol.* **2022**, *10*, 2200893.

[37] T. Kornas, R. Daub, M. Z. Karamat, S. Thiede, C. Herrmann, in *2019 IEEE 15th International Conference on Automation Science and Engineering (CASE)*, **2019**, pp. 380–385.
[38] K. Liu, M. F. Niri, G. Apachitei, M. Lain, D. Greenwood, J. Marco, *Control Engineering Practice* **2022**, *124*, 105202.
[39] J. Schnell, C. Nentwich, F. Endres, A. Kollenda, F. Distel, T. Knoche, G. Reinhart, *J. Power Sources* **2019**, *413*, 360–366.
[40] S. Stock, S. Pohlmann, F. J. Günter, L. Hille, J. Hagemeister, G. Reinhart, *J. Energy Storage* **2022**, *50*, 104144.
[41] S. Thiede, A. Turetskyy, A. Kwade, S. Kara, C. Herrmann, *CIRP Ann.* **2019**, *68*, 463–466.
[42] A. Turetskyy, S. Thiede, M. Thomitzek, N. von Drachenfels, T. Pape, C. Herrmann, *Energy Technol.* **2020**, *8*, 1900136.
[43] A. Turetskyy, J. Wessel, C. Herrmann, S. Thiede, *Procedia CIRP* **2020**, *93*, 168–173.
[44] A. Turetskyy, J. Wessel, C. Herrmann, S. Thiede, *Energy Storage Mater.* **2021**, *38*, 93–112.
[45] Y. Wang, W. Li, R. Fang, H. Zhu, Q. Peng, *Control Engineering Practice* **2022**, *125*, 105224.
[46] R. P. Cunha, T. Lombardo, E. N. Primo, A. A. Franco, *Batteries & Supercaps* **2020**, *3*, 60–67.
[47] R. Leithoff, N. Dilger, F. Duckhorn, S. Blume, D. Lembcke, C. Tschöpe, C. Herrmann, K. Dröder, *Batteries* **2021**, *7*, 19.
[48] K. Liu, X. Hu, H. Zhou, L. Tong, W. D. Widanage, J. Marco, *IEEE/ASME Transactions on Mechatronics* **2021**, *26*, 2944–2955.
[49] K. Liu, K. Li, T. Chen in 2021 IEEE Sustainable Power and Energy Conference (iSPEC), **2021**, pp. 3653–3658.
[50] K. Liu, Z. Wei, Z. Yang, K. Li, *J. Cleaner Prod.* **2021**, *289*, 125159.
[51] K. Liu, Z. Yang, H. Wang, K. Li, in *Recent Advances in Sustainable Energy and Intelligent Systems: 7th International Conference on Life System Modeling and Simulation, LSMS 2021 and 7th International Conference on Intelligent Computing for Sustainable Energy and Environment*, ICSEE 2021, Han, Springer, Singapore, **2021**, pp. 23–34.
[52] K. Liu, Q. Peng, K. Li, T. Chen, *Automot. Innov.* **2022**, *5*, 121–133.
[53] E. Rohkohl, M. Schönemann, Y. Bodrov, C. Herrmann, *Advances in Industrial and Manufacturing Engineering* **2022**, *4*, 100078.
[54] M. Duquesnoy, T. Lombardo, F. Caro, F. Haudiquez, A. C. Ngandjong, J. Xu, H. Oularbi, A. A. Franco, *NPJ Comput. Mater.* **2022**, *8*, 1–9.
[55] S. Kim, Z. Yi, B.-R. Chen, T. R. Tanim, E. J. Dufek, *Energy Storage Mater.* **2022**, *45*, 1002–1011.
[56] M. Quartulli, A. Gil, A. M. Florez-Tapia, P. Cereijo, E. Ayerbe, I. G. Olaizola, *Energies* **2021**, *14*, 4115.
[57] A. Turetskyy, V. Laue, R. Lamprecht, S. Thiede, U. Krewer, C. Herrmann, in *2019 IEEE 17th International Conference on Industrial Informatics (INDIN)*, **2019**, pp. 53–58.
[58] O. Badmos, A. Kopp, T. Bernthaler, G. Schneider, *J. Intell. Manuf.* **2020**, *31*, 885–897.
[59] M. Faraji-Niri, J. Mafeni Mase, J. Marco, *Energies* **2022**, *15*, 4489.
[60] A. Gayon-Lombardo, L. Mosser, N. P. Brandon, S. J. Cooper, *NPJ Comput. Mater.* **2020**, *6*, 1–11.
[61] Q. Demlehner, D. Schoemer, S. Laumer, *Int. J. Information Management* **2021**, *58*, 102317.
[62] C. Shen, L. Wang, Q. Li, *J. Mater. Process. Techn.* **2007**, *183*, 412–418.
[63] D. F. Cook, C. T. Ragsdale, R. L. Major, *Engineering Applications of Artificial Intelligence* **2000**, *13*, 391–396.
[64] P. S. Grant, D. Greenwood, K. Pardikar, R. Smith, T. Entwistle, L. A. Middlemiss, G. Murray, S. A. Cussen, M. J. Lain, M. J. Capener et al, *J. Phys. E* **2022**, *4*, 42006.
[65] W. van der Aalst, A. Adriansyah, A. K. A. de Medeiros, F. Arcieri, T. Baier, T. Blickle, J. C. Bose, P. van den Brand, R. Brandtjen, J. Buijs, et al., in *Lecture Notes in Business Information Processing*, *Vol. 99* (Eds.: F. Daniel, K. Barkaoui, S. Dustdar), Springer, Berlin, **2012**, pp. 169–194.
[66] C. Ortmeier, N. Henningsen, A. Langer, A. Reiswich, A. Karl, C. Herrmann, *Procedia CIRP* **2021**, *98*, 163–168.
[67] S. Haghi, A. Summer, P. Bauerschmidt, R. Daub, *Energy Technol.* **2022**, *10*, 2200657.
[68] S. Jaiser, A. Friske, M. Baunach, P. Scharfer, W. Schabel, *Drying Technol.* **2017**, *35*, 1266–1275.
[69] M. Schmitt, M. Baunach, L. Wengeler, K. Peters, P. Junges, P. Scharfer, W. Schabel, *Chem. Eng. Process.* **2013**, *68*, 32–37.
[70] E. Wiegmann, A. Kwade, W. Haselrieder, *Energy Technol.* **2022**, *10*, 2200020.
[71] F. Huttner, A. Diener, T. Heckmann, J. C. Eser, T. Abali, J. K. Mayer, P. Scharfer, W. Schabel, A. Kwade, *J. Electrochem. Soc.* **2021**, *168*, 90539.
[72] D. L. Wood, J. Li, C. Daniel, *J. Power Sources* **2015**, *275*, 234–242.
[73] P. Linardatos, V. Papastefanopoulos, S. Kotsiantis, *Entropy* **2020**, *23*, 18.
[74] G. James, D. Witten, T. Hastie, R. Tibshirani, *An introduction to statistical learning. With applications in R*, Springer, New York, **2021**.
[75] F. Doshi-Velez, B. Kim, Towards A Rigorous Science of Interpretable Machine Learning, **2017**.
[76] M. H. Kutner, C. J. Nachtsheim, J. Neter, W. Li, *Applied linear statistical models*, McGraw-Hill Irwin, Boston, Mass., **2005**.
[77] D. C. Montgomery, *Design and analysis of experiments*, John Wiley & Sons Inc, Hoboken, NJ, **2013**.
[78] R. A. Johnson, D. W. Wichern, *Applied multivariate statistical analysis*, Pearson/Prentice Hall, Upper Saddle River, NJ, **2007**.
[79] C. M. Bishop, *Pattern recognition and machine learning*, Springer Science + Business Media LLC, New York, NY, **2006**.
[80] G. Rebala, *An Introduction to Machine Learning*, Springer International Publishing AG, Cham, **2019**.
[81] C. C. Aggarwal, *Neural Networks and Deep Learning. A Textbook*, Springer International Publishing AG, Cham, **2018**.
[82] L. Breiman, Machine Learning 2001, Kluwer Academic Publishers, *45*, 5–32.
[83] J.-O. Palacio-Niño, F. Berzal, Evaluation Metrics for Unsupervised Learning Algorithms, **2019**.
[84] P. J. Rousseeuw, *Journal of Computational and Applied Mathematics* **1987**, *20*, 53–65.
[85] M. Halkidi, Y. Batistakis, M. Vazirgiannis, *Journal of Intelligent Information Systems* **2001**, *17*, 107–145.
[86] A. V. Joshi, Machine Learning and Artificial Intelligence, Springer, Cham, **2020**.
[87] M. Sokolova, G. Lapalme, *Inf. Process. Manage.* **2009**, *45*, 427–437.
[88] D. M. W. Powers, International Journal of Machine Learning Technology 2:1, **2011**.
[89] J. Fan, F. Han, H. Liu, *Natl. Sci. Rev.* **2014**, *1*, 293–314.
[90] A. Alwosheel, S. van Cranenburgh, C. G. Chorus, *Journal of Choice Modelling* **2018**, *28*, 167–182.
[91] D. Rajput, W.-J. Wang, C.-C. Chen, *BMC Bioinf.* **2023**, *24*, 48.
[92] I. Balki, A. Amirabadi, J. Levman, A. L. Martel, Z. Emersic, B. Meden, A. Garcia-Pedrero, S. C. Ramirez, D. Kong, A. R. Moody et al, *Canadian Association of Radiologists journal = Journal l'Association canadienne des radiologistes* **2019**, *70*, 344–353.
[93] M. Keppeler, H.-Y. Tran, W. Braunwarth, *Energy Technol.* **2021**, *9*, 2100132.
[94] J. Freiesleben, J. Keim, M. Grutsch, *Qual. Reliab. Engng. Int.* **2020**, *36*, 1837–1848.
[95] V. Banna, A. Chinnakotla, Z. Yan, A. Vegesana, N. Vivek, K. Krishnappa, W. Jiang, Y.-H. Lu, G. K. Thiruvathukal, J. C. Davis, *An Experience Report on Machine Learning Reproducibility: Guidance for Practitioners and TensorFlow Model Garden Contributors*, **2021**.
[96] E. Breck, S. Cai, E. Nielsen, M. Salib, D. Sculley, The ML Test Score: A Rubric for ML Production Readiness and Technical Debt Reduction, **2017**.
[97] S. Amershi, A. Begel, C. Bird, R. DeLine, H. Gall, E. Kamar, N. Nagappan, B. Nushi, T. Zimmermann, in *2019 IEEE/ACM 41st International Conference on Software Engineering: Software Engineering in Practice (ICSE-SEIP)*, **2019**, pp. 291–300.
[98] N. Kühl, R. Hirt, L. Baier, B. Schmitz, G. Satzger, *Communications of the Association for Information Systems* **2021**, *48*, 589–615.
[99] T. Lombardo, F. Caro, A. C. Ngandjong, J.-B. Hoock, M. Duquesnoy, J. C. Delepine, A. Ponchelet, S. Doison, A. A. Franco, *Batteries & Supercaps* **2022**, *5*, e202100324.
[100] X. Liu, L. Zhang, H. Yu, J. Wang, J. Li, K. Yang, Y. Zhao, H. Wang, B. Wu, N. P. Brandon et al, *Adv. Energy Mater.* **2022**, *12*, 2200889.
[101] D. Gunning, M. Stefik, J. Choi, T. Miller, S. Stumpf, G.-Z. Yang, *Science Robotics* **2019**, *4*.

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