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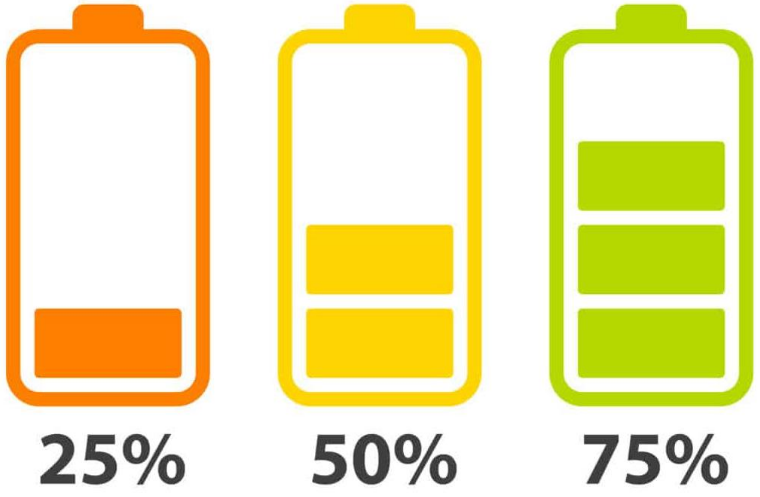
Session 8: Case Study II
SoC Degradation

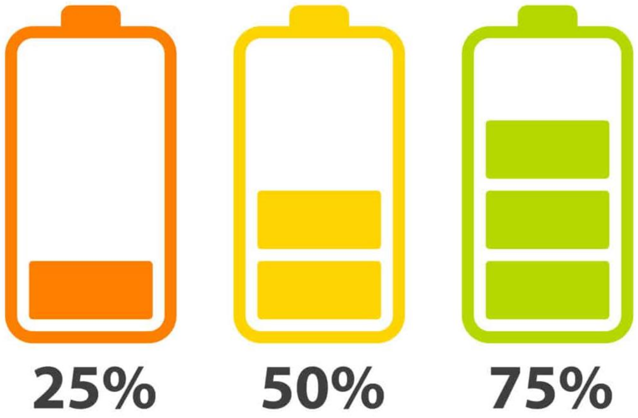


Prof. Carlos Cano Domingo
carlos.cano.domingo@upc.edu
Session 8

Session 8: SoC Degradation

Objective: Study the State of Charge estimation considering aging effects.

Content:
- Review CRISP-DM
- Problem Understanding 1A: Understanding the Problem Itself
- Problem Understanding 1B: Searching for Possible Approaches and Research Opportunities
- Data understandings
- Data preparation
- Modelling
- Evaluation
- Implementation/ Deployment



EU contribution 4.966.935€

NEXTBAT is a European Union-funded project aimed at revolutionizing battery technology for the electrification of various transport sectors.

Objectives:

- **Battery Performance Improvement**: Increase energy and power density by 30-50%, and reduce battery weight by 25% using lightweight materials.
- **Standardized Safety**: Establish safety assessment methodologies with physical and virtual testing.
- **Sustainability**: Achieve up to 100% recyclability for hardware and 50-80% for battery cells, reducing the carbon footprint.
- **Demonstration Across Sectors**: Showcase battery prototypes for on-road, waterborne, airborne, rail, and off-road applications.

https://nextbat.eu/

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Main Research Areas – my part:

1. **Bioinformatics:** We develop computational tools and algorithms to analyse and interpret biological data, facilitating advancements in genomics, proteomics, and systems biology.
2. **Psychology:** Our research delves into cognitive processes and human behaviour, aiming to improve mental health and optimize human-computer interactions.
3. **Green Energy Systems (Focus on Batteries):** We explore sustainable energy solutions by enhancing battery technology, contributing to efficient energy storage and reduced environmental impact.

Main Research Interest:

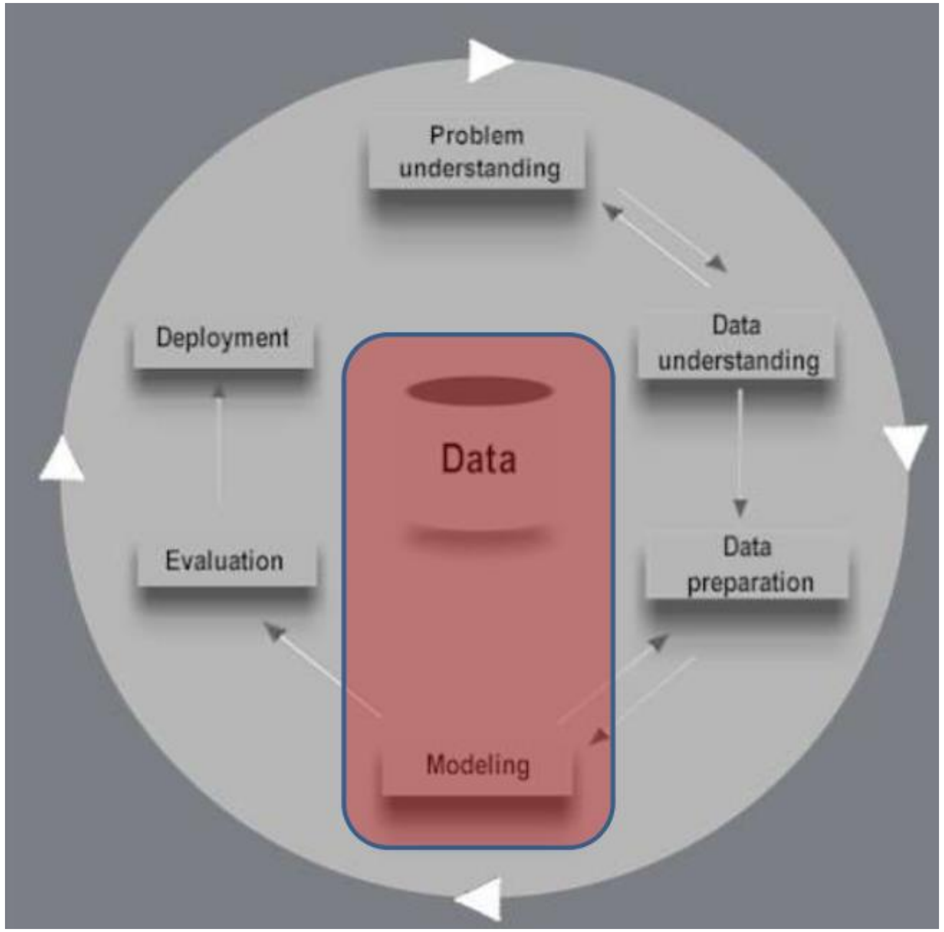
1. Computational Finance
2. Data and Knowledge Visualization
3. Explainability
4. Trustworthiness
5. Responsibility
6. Feature Selection and Extraction
7. Fuzzy Systems and Fuzzy Hybridizations
8. Genetic Algorithms and Evolutionary Strategies
9. Pattern Recognition and Computer Vision
10. Sentiment Analysis
11. Supervised and Unsupervised Neural Networks
12. Support Vector Machines
13. Deep Learning
14. Reinforcement Learning
15. Optimization Techniques
16. Time Series Analysis

1 Review CRISP-DM methodology

CRISP: Description of phases

1. Problem Understanding: Study of targets and requirements form the business/problem viewpoint. Defining it as a DM problem.
   - 1A: Understanding the Problem Itself
   - 1B: Searching for Possible Approaches and Research Opportunities
2. Data Understanding: Data recollection; getting to know the data, trying to detect both quality problems and interesting features.
3. Data Preparation: Preparing the data set to be modelled, starting from raw data. This is an iterative and exploratory process. Selection of files, tables, variables, record samples… plus data cleaning.
4. Modelling: Data analysis using modelling techniques of a sort that are suitable for the problem at hand. Includes fiddling with the models, tuning their parameters, etc.
5. Evaluation: All previous steps must be evaluated as whole (as a unitary process), and we must decide whether deliverables so far meet the DM challenge.
6. Implementation / Deployment: All the knowledge acquired to this point must be organized and presented to the "client" in a usable form. We must define, together with this client, a protocol to reliably deploy the DM findings.

CRISP: Description of phases



2 Problem Understanding 1A: Understanding the Problem Itself

CRISP: Description of phases

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1A Problem Understanding: Batteries

From the most basic to the most complex

Definition and Purpose of Batteries:

- **Energy storage devices** converting **chemical energy** into **electrical energy**.
- Role in portable electronics, electric vehicles, renewable energy storage, etc.

Importance in Modern Technology:

- Enabling **mobility** and **sustainability**.
- Critical component in the **shift towards renewable energy sources**.

Uses

- Electric Vehicles.
- Laptop.
- Smartphone.

1A Probl... ...basic to the most complex


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ELSEVIER
Sustainable Materials and Technologies
Volume 29, September 2021, e00297

An advance review of solid-state battery: Challenges, progress and prospects

Cong Li [a b c], Zhen-yu Wang [a b c], Zhen-jiang He [a b c], Yun-jiao Li [a b c], Jing Mao [d], Ke-hua Dai [e], Cheng Yan [f], Jun-chao Zheng [a b c]

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Journal of Materiomics, Volume 5, Issue 2, 2019, pp. 21..
Yu Huan, ..., Tao Wei

A durable and safe solid-state lithium battery with a hybrid electrolyte membrane
Nano Energy, Volume 45, 2018, pp. 413-419
Wenqiang Zhang, ..., Chunwen Sun

Polymer electrolytes and interfaces toward solid-state batteries: Recent advances and...

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...om/future/article/20240319-the-most-
...atives-to-lithium-batteries

...cedirect.com/topics/engineering/flow-battery

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- No memory effect.

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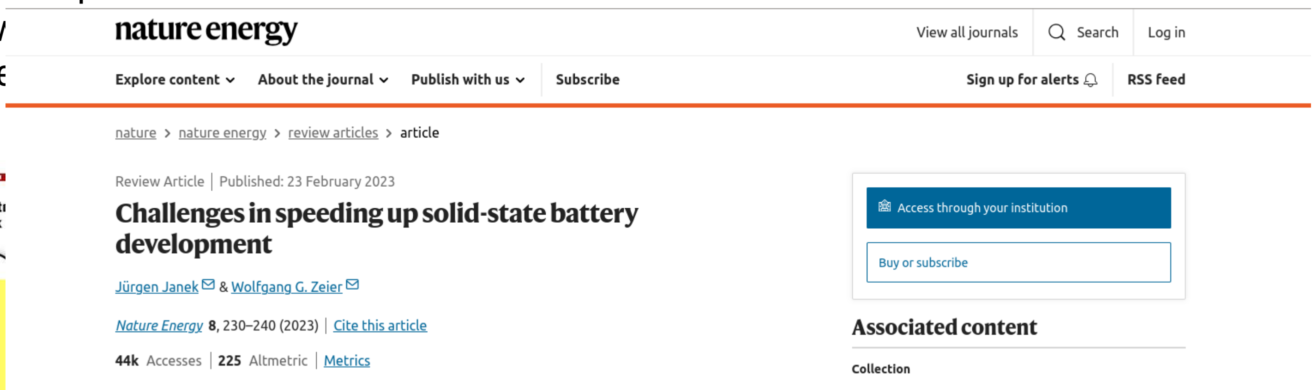
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Review Article | Published: 23 February 2023

Challenges in speeding up solid-state battery development

Jürgen Janek & Wolfgang G. Zeier
Nature Energy 8, 230–240 (2023) | Cite this article
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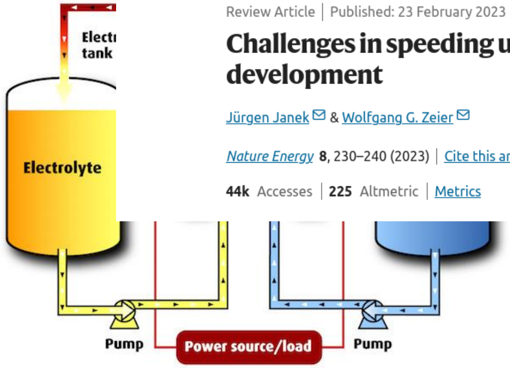

1A Problem Understanding:

From the most basic to the most complex

Main tech

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- Anode: T
- Cathode:
- Electroly
- Separatc

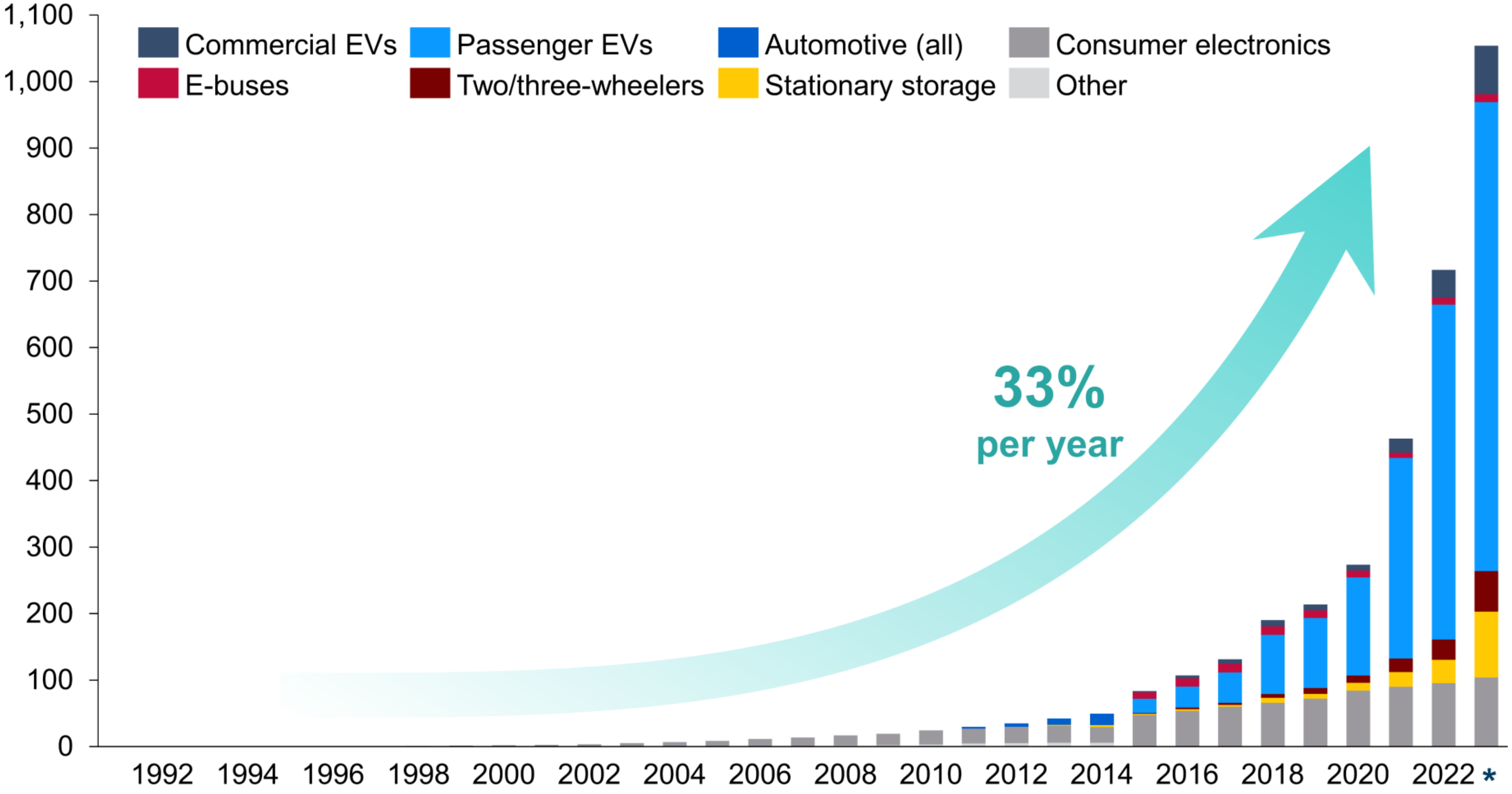


Exhibit 1: Global battery sales by sector, GWh/y

1A Proble… …st complex

Main tech…

Composit…
- Anode: …
- Cathode…
- Electrol…
- Separat…

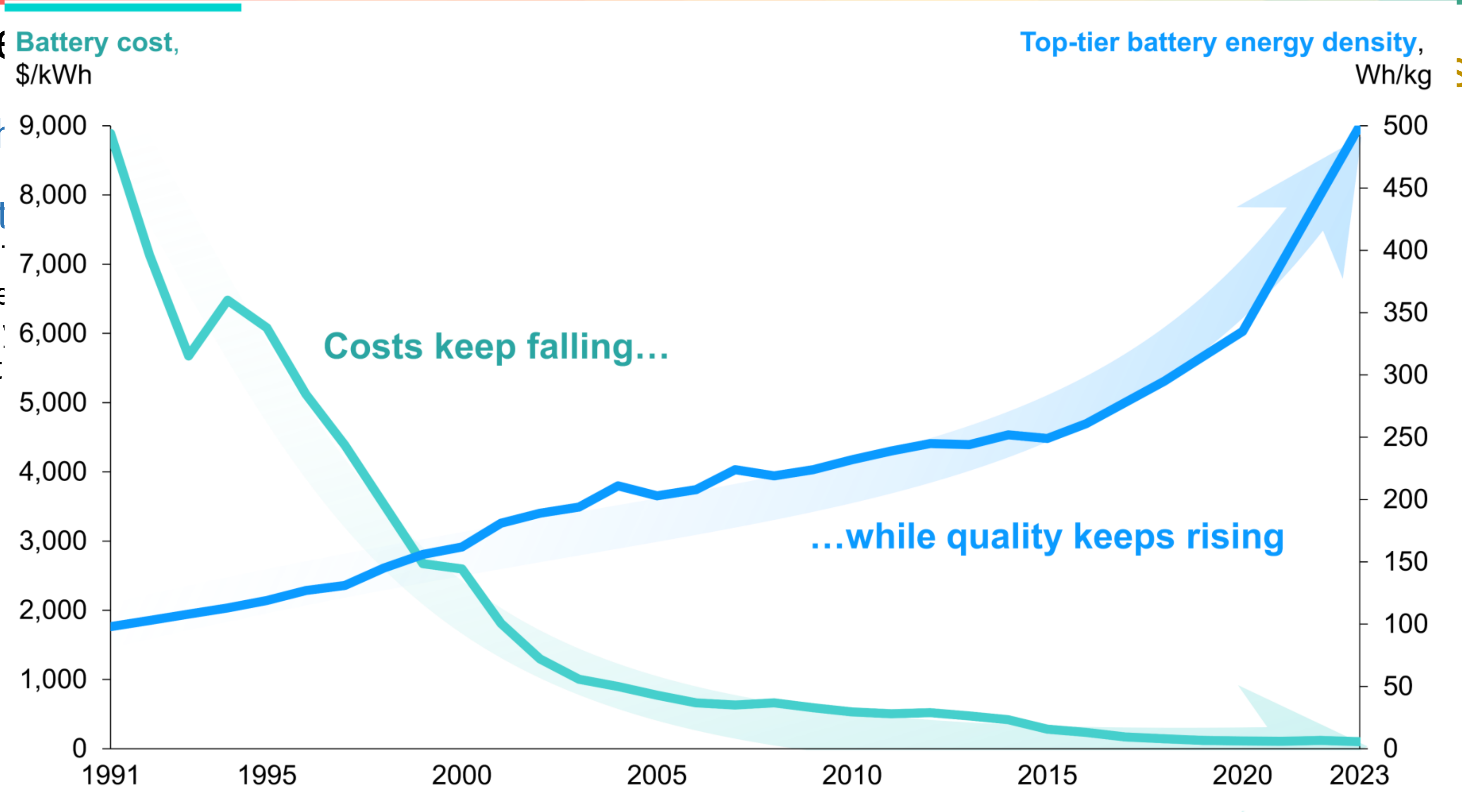


Exhibit 2: Battery cost and energy density since 1990

1A Problem Understanding:

…ost complex

Main tec

Compos

- Anode
- Cathod
- Electr
- Separa

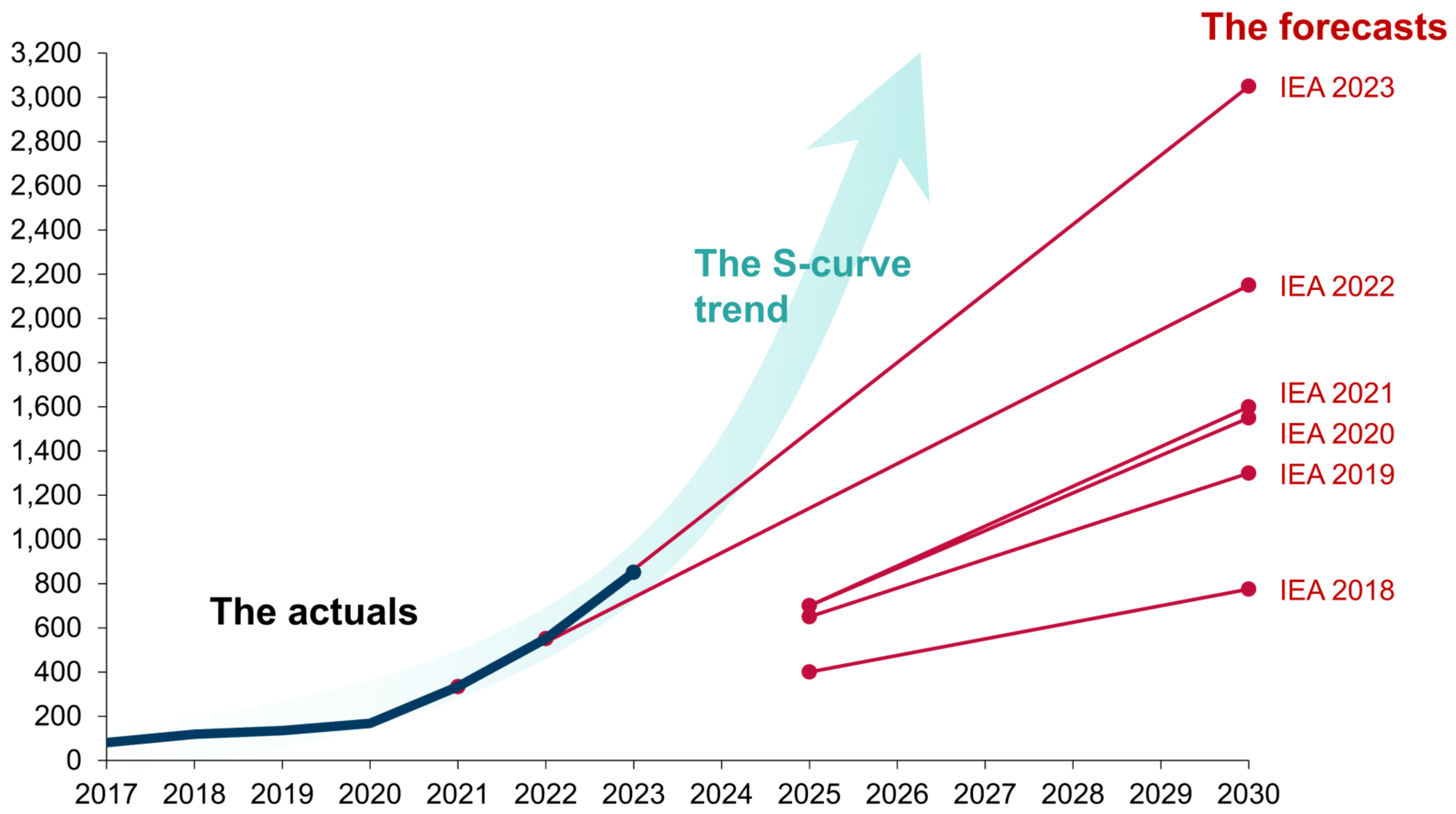


Exhibit 3: Automotive lithium-ion battery demand, IEA forecast vs. actuals, GWh/y

1A Problem Understanding: SoC

From the most basic to the most complex

Definition of State of Charge (SoC)

A measure of the energy available in a battery relative to its full capacity.

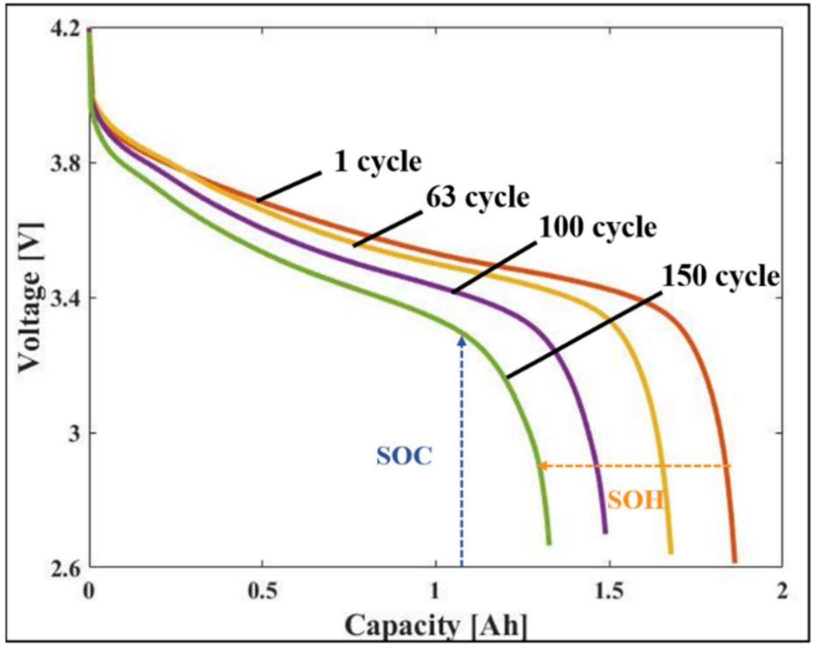
$$SOC(\%) = \left(\frac{Q}{Q_{total}}\right) \times 100\%$$

Key Role of SoC in Battery Systems

- Ensures the battery operates within safe and efficient limits.
- Helps manage charging, discharging, and energy allocation.

SoC Estimation Challenges

1. Dynamic Nature of SoC: Affected by battery usage, temperature, and aging.
2. Non-Linear Relationships: Voltage vs. SoC curves are non-linear
3. Hysteresis Effects: Difference in voltage during charging and discharging at the same SoC level.
4. Data Limitations: Sensor inaccuracies & Noise and missing data in real-world applications



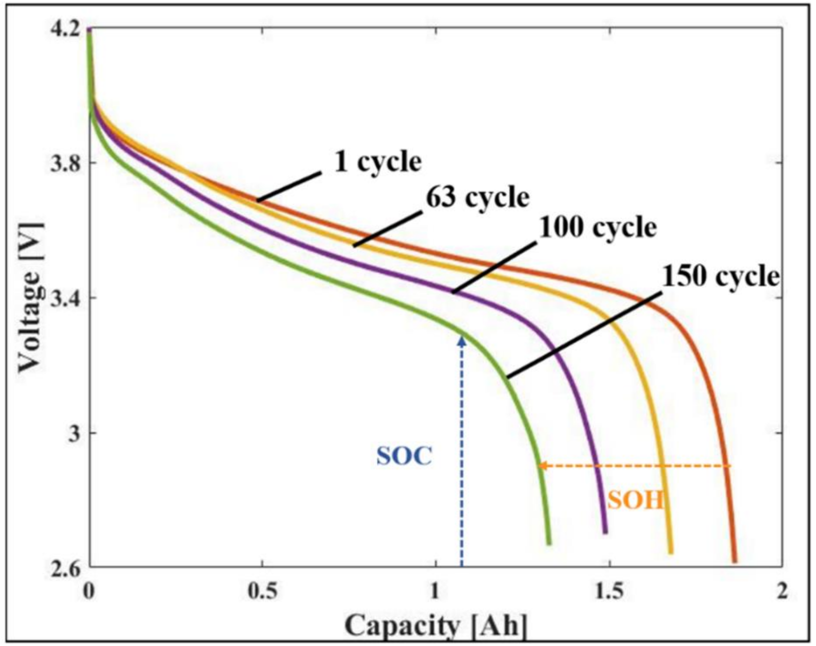
1A Problem Understanding: SoC

From the most basic to the most complex

SoC Estimation Methods

- Direct Measurement: Not Possible
- Coulomb Counting: Very unstable
- Model-Based Methods: Not adaptable to complex situation (Degradation)
- Data-Driven Approaches: Needs huge amount of data in very different situations

$$SOC(\%) = \left(\frac{Q}{Q_{total}}\right) \times 100\%$$



Importance of Accurate SoC Estimation

- **Safety**: Prevents overcharging and over-discharging, which can lead to thermal runaway.
- **Efficiency:** Optimizes battery usage and energy management.
- **Longevity:** Avoids deep discharge cycles, preserving battery health.
- **Real-Time Applications:** Crucial for electric vehicles and energy storage systems where real-time SoC feedback is necessary.

1A Problem Understanding: Battery Degradation

From the most basic to the most complex

What is Battery Degradation?

The gradual loss of a battery's capacity and ability to deliver power over time.

- Cap
- Pov

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1. Solid
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4. Elect

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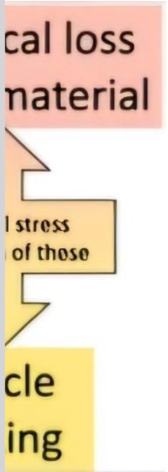
Cite this: *Phys. Chem. Chem. Phys.*, 2022, 24, 7909

Lithium-ion battery degradation: how to model it†

Simon E. J. O'Kane, *[ab] Weilong Ai, ‡[bc] Ganesh Madabattula,§[ab] Diego Alonso-Alvarez,[bd] Robert Timms,[be] Valentin Sulzer,[bf] Jacqueline Sophie Edge,[ab] Billy Wu,[bc] Gregory J. Offer[ab] and Monica Marinescu[ab]

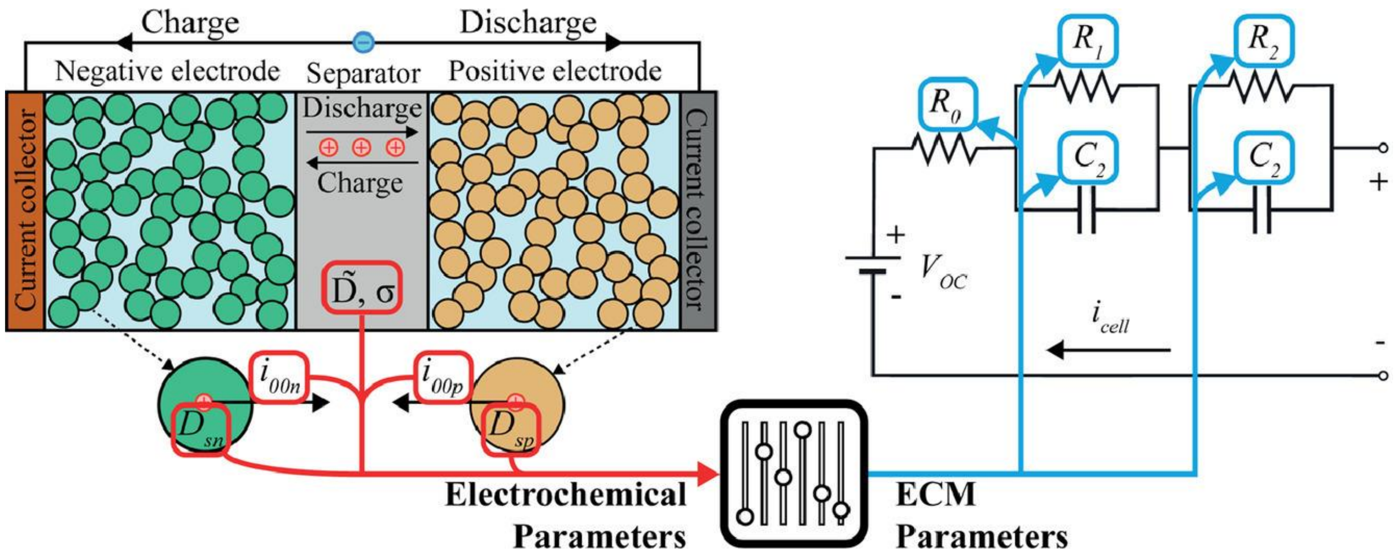
Predicting lithium-ion battery degradation is worth billions to the global automotive, aviation and energy storage industries, to improve performance and safety and reduce warranty liabilities. However, very few



From the most basic to the most complex

Impact of Degradation on SoC Estimation

- Changes in Voltage-SoC Curves: Aging shifts the curves, reducing their accuracy for SoC estimation.
- Increased Variability: Aging introduces noise and inconsistencies in sensor readings.
- Dynamic Parameters: Internal resistance and other parameters vary with degradation, complicating modeling.
- Reduced Predictive Accuracy: Models trained on new batteries may not generalize to degraded ones.



TASK 1: Understand the concept of State of Charge and battery degradation.

Guidelines:

1. Collect: Find and list 7 documents (e.g., scholarly articles, review papers, book chapters, reputable websites) that can help in different aspect of the phenomena.
2. Classify: Categorize the documents (e.g., introductory material, advanced research, theoretical background, applications).
3. Justify: Write a brief note on why each document is useful for understanding the phenomena.

Tools: Encourage the use of academic databases (e.g., Google Scholar, IEEE Xplore), library resources, and reputable websites.

3 Problem Understanding 1B: Searching for Possible Approaches and Research Opportunities

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TASK 2: Identify and understand distinct research approaches in the SoC estimation and battery degradation to help shape potential research directions.

Objective: Identify and understand distinct research approaches in the SoC estimation and battery degradation to help shape potential research directions.

Guidelines:

1. Identify Approaches: Choose three unique research approaches used in the study of SoC estimation
2. Collect: For each approach, find and list 3 papers that showcase how this approach is applied in the field of SoC.
3. Justify: Briefly describe how each approach (and the resources found) could help form a research line or open up new questions for investigation.

Tools: Encourage the use of academic databases (e.g., Google Scholar, IEEE Xplore), library resources, and reputable websites.

Recommended Tools for Exploring Research Approaches

1. Research Rabbit: Discover new research approaches by visualizing connections between papers and finding related studies.
2. Consensus: Pose questions about Schumann Resonance to get summarized responses with linked research articles.
3. Semantic Scholar: Use AI-driven features to find influential papers and specific research methods in SR.
4. Connected Papers: Generate a map of connected papers to explore variations in research approaches.
5. Scite: See how studies are cited (supporting, contrasting, mentioning) to understand the impact of different approaches.
6. Scopus: Comprehensive database for peer-reviewed literature across disciplines, especially useful for identifying trends and widely cited methods in SR research.
7. Google Scholar & IEEE Xplore: Standard platforms for a wide search, especially helpful for finding diverse applications of SR research.

My approach (In order):

1. **Ask Consensus.**
2. **Google Scholar for consolidated lines.**
3. **Scopus for recent papers.**
4. **Create research rabbit for each research line**

Recommended Tools for Exploring Research Approaches

1. Ask Consensus: Start by posing questions related to Schumann Resonance in Consensus to gain initial insights and identify keywords or common themes in SR research.
2. Google Scholar for Consolidated Lines: Use Google Scholar to search for established, consolidated research lines. Look for review articles or highly cited papers to identify main approaches in the field.
3. Scopus for Recent Papers: Search Scopus for recent publications in each identified research line to find the latest advancements and active areas of investigation.
4. Create Research Rabbit Maps: For each research line identified, use Research Rabbit to visualize connections, explore related papers, and deepen understanding of each approach.
5. Classify & Justify: Organize the collected papers by approach and provide a brief justification for how each contributes to understanding Schumann Resonance and supports potential research directions.

My approach (In order):

1. **Ask Consensus.**
2. **Google Scholar for consolidated lines.**
3. **Scopus for recent papers.**
4. **Create research rabbit for each research line**

1B Approaches

From the most basic to the most complex

Can you give three different research line

Pro Filter

1. Model-Based Estimation Techniques
Model-based techniques leverage mathematic
considering the aging effects on battery perfor
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Energy
Volume 220, 1 April 2021, 119767

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State-of-charge estimation tolerant of battery aging based on a physics-based model and an ...man filter

, Yong Tian [a]

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Energy
Volume 174, 1 May 2019, Pages 33-44

Co-estimation of capacity and state-of-charge for lithium-ion batteries in electric vehicles

Xiaoyu Li [a b], Zhenpo Wang [a b], Lei Zhang [a b]

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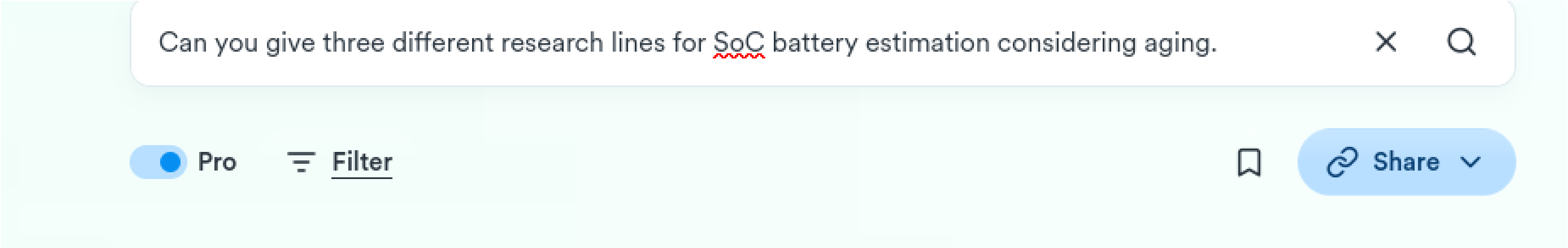
1B Approaches

From the most basic to the most complex

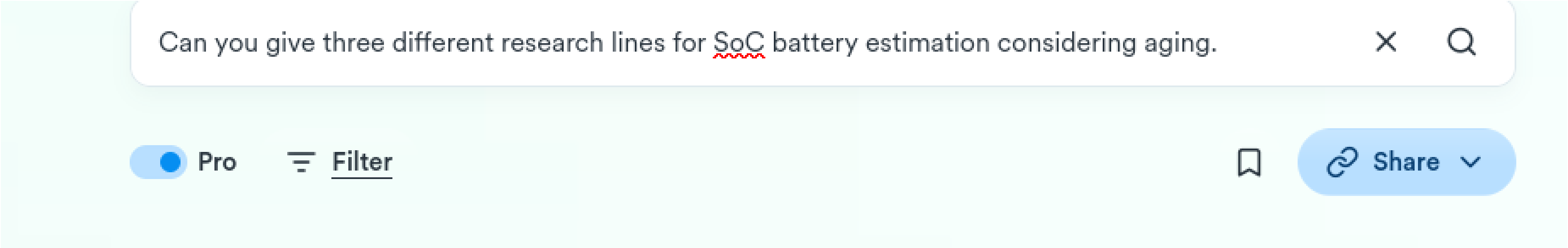


2. Data-Driven and Machine Learning Approaches
Data-driven methods and machine learning algorithms are increasingly being used to enhance SoC estimation by incorporating the effects of battery aging. These methods can adapt to the nonlinear behavior of batteries and improve estimation accuracy.

- **Artificial Neural Networks (ANNs)**: ANNs are used to model actual SoC trajectories and predict SoC by updating the initial SoC value using the updated State of Health (SoH). This method has shown a reduction in errors by up to 45% in mean absolute percentage error, particularly for **aged batteries**.
- **Convolutional Neural Networks (CNNs)**: The use of three-dimensional CNNs (3DCNN) to describe the aging degree and SoC has been proposed. The fused convolutional neural network (FCNN) algorithm, which considers the aging degree of the battery, has shown improved SoC estimation accuracy.

1B Approaches

From the most basic to the most complex



3. Hybrid Estimation Approaches

Hybrid methods combine model-based and data-driven techniques to leverage the strengths of both approaches for more robust SoC estimation.

- **Joint Estimation Using Simplified Pseudo-Two-Dimensional (P2D) Models**: This method simplifies the P2D model into a nonlinear state-space form and uses particle filters to estimate SoC and SoH. It calibrates SoH based on lithium concentration predictions, improving SoC estimation accuracy for aged batteries[6].
- **Enhanced Electrochemical Models with Dual Nonlinear Filters**: This approach uses a reduced-order electrochemical model and dual nonlinear filters to co-estimate SoC and SoH. It identifies key aging factors like lithium ion loss and resistance increment, ensuring precise SoC estimation over the battery's lifespan[7].

1B Approaches

From the most basic to the most complex

1. Adapt Equivalent circuit model using classical parameter extraction.
2. Use Deep Learning to encode Battery data, and use this encode data to predict aging effect.
3. Use a Reinforce Learning approach to learn how to adapt the ECM parameters with the aging effect.
4. Use Deep Learning approach base on physical informed Neural Network to estimate the values of the ECM parameters considering degradation.

4 Data understanding

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TASK 3 Data Collection and Understanding

Objective: Find open-source datasets that contain battery data, with one dataset representing batteries without degradation and another representing batteries with degradation effects

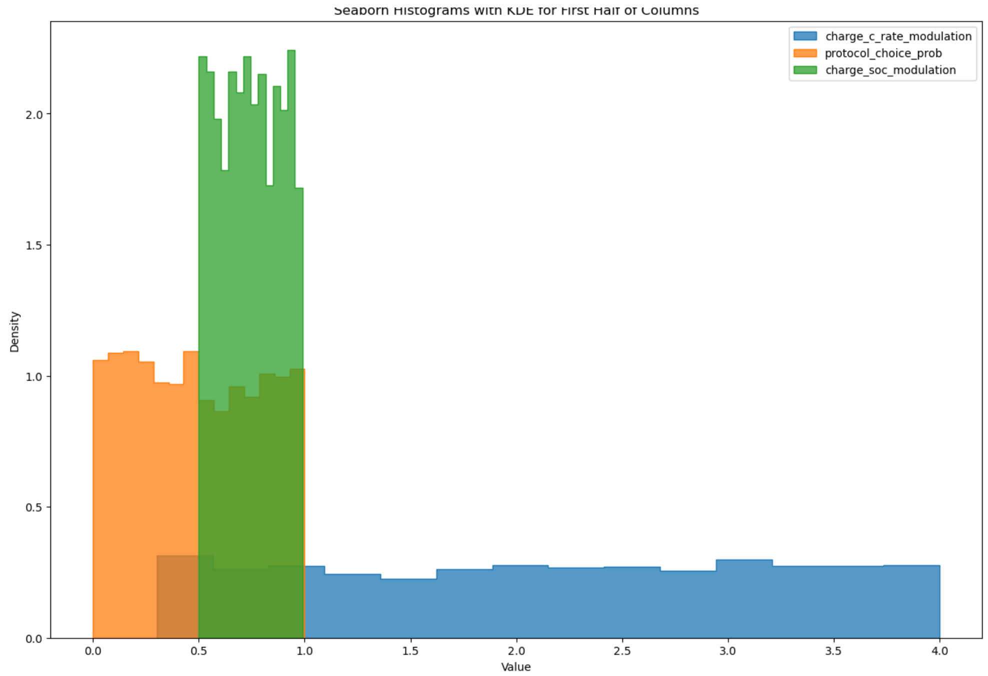
Guidelines:

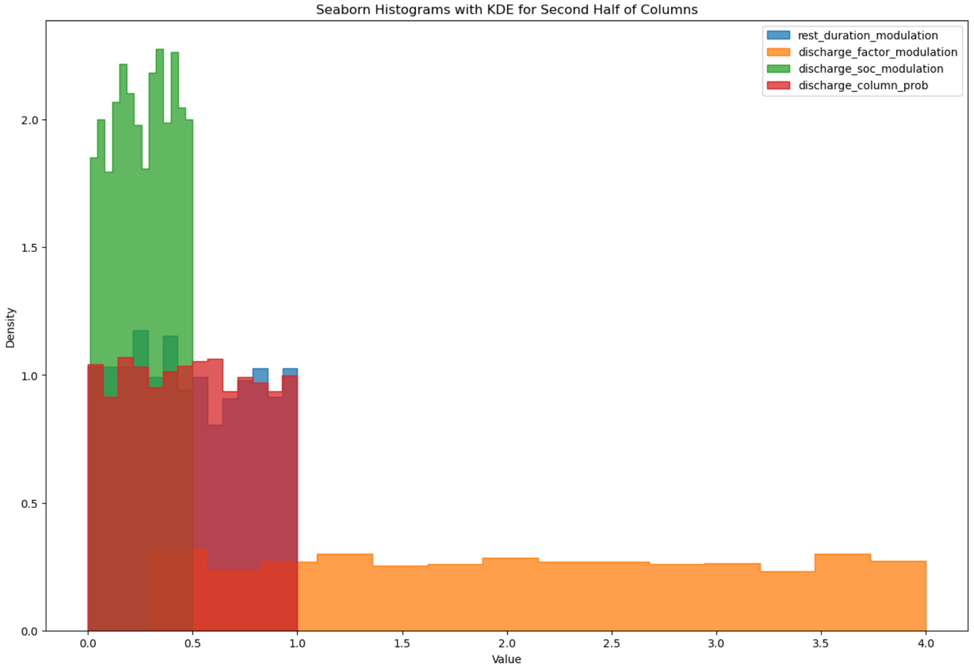
1. Search for two open datasets on battery data: a) Dataset 1: Contains data from batteries that have not experienced significant ii) Dataset 2: Contains data from batteries with evident degradation over time.

2. Analyze and summarize each dataset: a) Data Structure: Indicate the main features or columns present in the datasets (e.g., voltage, current, temperature, cycles). b) Data Purpose: Explain the purpose of each dataset.

	Profile_Path	charge_c_rate_modulation	protocol_choice_prob	charge_soc_modulation	rest_duration_modulation	discharge_factor_modulation	discharge_soc_modulation	discharge_column_prob
0	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	2.779997	0.768552	0.620459	0.966347	3.982351	0.236802	0.068032
1	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	3.068918	0.782052	0.761592	0.657273	0.714661	0.215364	0.466603
2	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	3.663077	0.039440	0.917059	0.081393	0.705596	0.015935	0.941802
3	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	2.224310	0.363964	0.625491	0.054064	2.876392	0.289590	0.464908
4	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	3.468210	0.375017	0.532496	0.416802	3.619987	0.434651	0.485967
...	...	...	...	...	...	...	...	...
2495	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	0.596583	0.164877	0.754615	0.966899	1.914233	0.264069	0.767076
2496	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	1.908112	0.573913	0.692133	0.657531	3.038046	0.017554	0.364355
2497	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	2.740446	0.021113	0.832778	0.891682	2.591752	0.169878	0.033819
2498	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	2.454280	0.807684	0.687955	0.912067	3.239267	0.288956	0.398018
2499	/gpfs/projects/bsc21/bsc021148/nextbat/phase_2...	1.515808	0.003143	0.742159	0.697300	2.715643	0.182991	0.764864

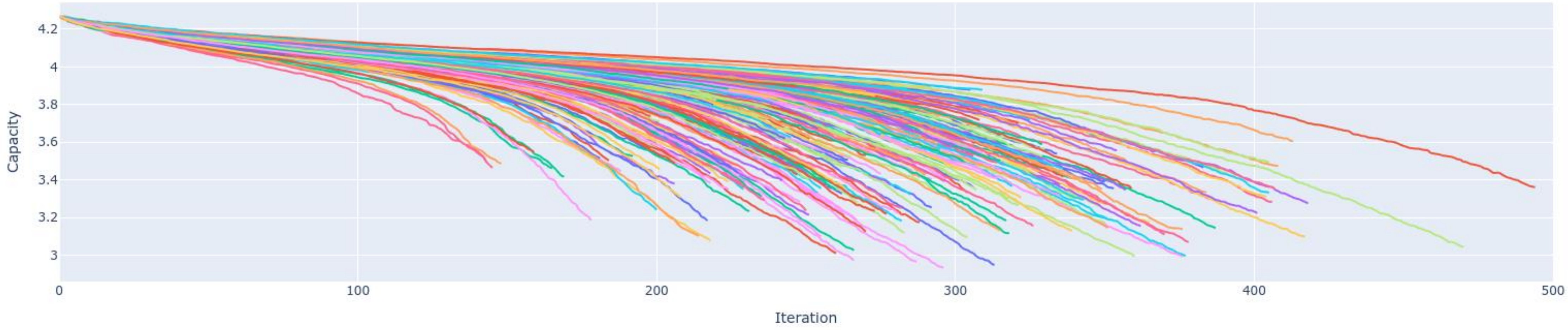
2500 rows × 1008 columns



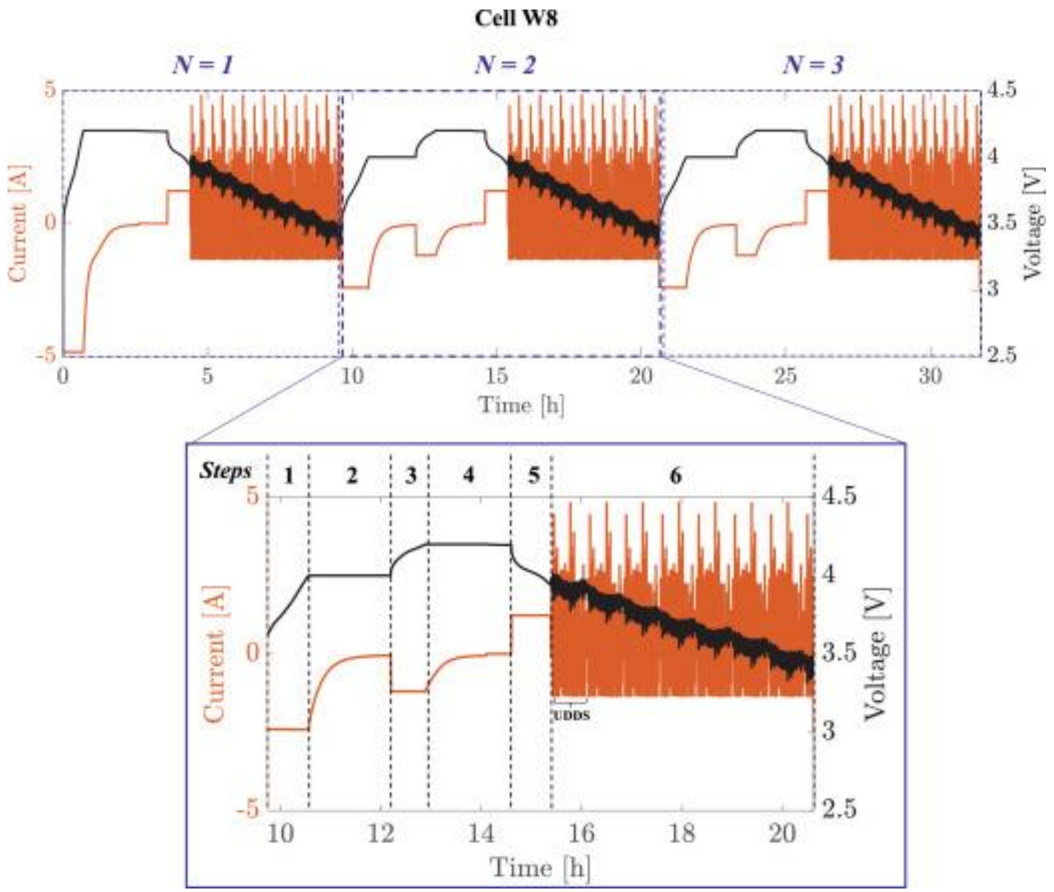


	Iteration_1	Iteration_2	Iteration_3	Iteration_4	Iteration_5	Iteration_6	Iteration_7	Iteration_8	Iteration_9	Iteration_10
0	4.264555	4.259677	4.255673	4.256197	4.251833	4.251424	4.245381	4.242299	4.241299199551259	4.239260
1	4.259917	4.255397	4.251379	4.245856	4.245119	4.23828	4.23532	4.232272	4.230676918424422	4.226894
2	4.259696	4.256866	4.248712	4.242428	4.235675	4.233793	4.22832	4.222586	4.217597901160326	4.211204
3	4.265699	4.259917	4.257934	4.254015	4.251833	4.248057	4.248147	4.246076	4.242471502067588	4.240315
4	4.265322	4.258361	4.257624	4.254703	4.253957	4.253738	4.247608	4.245106	4.243749999999876	4.240619
...	...	...	...	...	...	...	...	...	...	...
2495	4.268000	4.256654	4.253876	4.248321	4.243750	4.240322	4.237568	4.234528	4.232666	4.230307
2496	4.267092	4.262598	4.259025	4.250572	4.247912	4.241801	4.239172	4.234419	4.231494	4.229100
2497	4.258547	4.256802	4.251833	4.248368	4.244671	4.240924	4.23522	4.229786	4.227193	4.225566
2498	4.268000	4.265207	4.259614	4.253890	4.251006	4.246535	4.241823	4.239892	4.23476	4.231890
2499	4.262372	4.255356	4.248702	4.244510	4.240692	4.235731	4.232468	4.231434	4.228894	4.226986

2500 rows × 999 columns



2 Data Understanding



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Data in Brief

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ELSEVIER

Data Article

Lithium-ion battery aging dataset based on electric vehicle real-driving profiles

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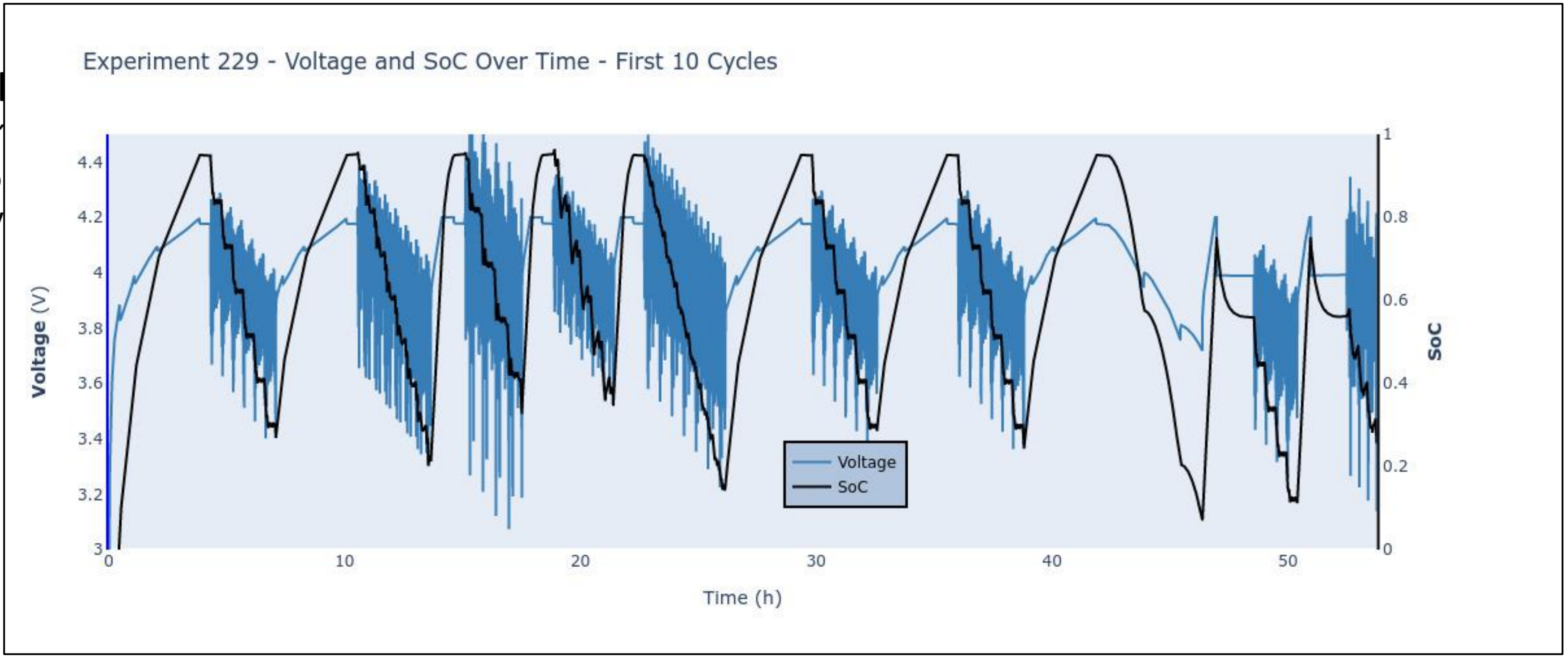
Battery aging
Reference performance tests
Aging campaign
NMC 2170

ABSTRACT

This paper describes the experimental dataset of lithium-ion battery cells subjected to a typical electric vehicle discharge profile and periodically characterized through diagnostic tests. Data were collected at the Stanford Energy Control Laboratory, at Stanford University. The INR21700-M50T battery cells with graphite/silicon anode and Nickel-Manganese-Cobalt cathode were tested over a period of 23 months according to the Urban Dynamometer Driving Schedule (UDDS) discharge driving profile and the Constant Current (CC)-Constant Voltage (CV) charging protocol designed at different charging rates – ranging from C/4 to 3C. Ten (10) cells are tested in a temperature-controlled environment (23°C). A periodic assessment of battery degradation during life testing is accomplished via Reference Performance Tests (RPTs) comprising of capacity, Hybrid Pulse Power Characterization (HPPC), and Electrochemical Impedance Spectroscopy (EIS) tests. The dataset allows for the characterization of battery aging under real-driving scenarios, enabling the development of models and management strategies in electric vehicle applications.

2 Data Understanding

EO High-Order
Carlos Cano[a], Albert Jim
[a] Barcelo
[b] Univ



5 Data preparation

CRISP: Description of phases

1. Problem Understanding: Study of targets and requirements form the business/problem viewpoint. Defining it as a DM problem.
   - 1A: Understanding the Problem Itself
   - 1B: Searching for Possible Approaches and Research Opportunities
2. Data Understanding: Data recollection; getting to know the data, trying to detect both quality problems and interesting features.
3. Data Preparation: Preparing the data set to be modelled, starting from raw data. This is an iterative and exploratory process. Selection of files, tables, variables, record samples… plus data cleaning.
4. Modelling: Data analysis using modelling techniques of a sort that are suitable for the problem at hand. Includes fiddling with the models, tuning their parameters, etc.
5. Evaluation: All previous steps must be evaluated as whole (as a unitary process), and we must decide whether deliverables so far meet the DM challenge.
6. Implementation / Deployment: All the knowledge acquired to this point must be organized and presented to the "client" in a usable form. We must define, together with this client, a protocol to reliably deploy the DM findings.

TASK 3: Students have 10 minutes to search online for preprocessing techniques applied to SR

Objective: Identify and understand preprocessing techniques relevant to Schumann Resonance data.
Guidelines:

1. Identify Techniques: Choose three unique preprocessing techniques commonly used in signal processing or time-series analysis that could be applied to Schumann Resonance data (e.g., noise reduction, feature extraction, normalization).
2. Collect: For each technique, find at least 1 paper or resource that discuss how the technique is applied in the field of Schumann Resonance or similar domains.
3. Justify: Briefly describe how each preprocessing technique (and the resources found) could help refine data for analysis or support further research.

Let’s Review Task 3 Results

Objective: Discuss preprocessing techniques each student found for Schumann Resonance data.
Discussion Points:

- Overview of the preprocessing techniques identified.
- Justifications for how each technique improves data quality or prepares it for analysis.
- Potential applications of these preprocessing methods in SR research.

6 Modelling

CRISP: Description of phases

1. Problem Understanding: Study of targets and requirements form the business/problem viewpoint. Defining it as a DM problem.
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Overview of the Modeling Phase in CRISP-DM

Objective of the Modelling Phase:

- Select and apply appropriate modelling techniques.
- Calibrate model settings to optimal values.

Key Steps:

1. Select Modelling Techniques:
   Choose algorithms suitable for the problem.
2. Generate Test Design:
   Plan for model evaluation (e.g., cross-validation).
3. Build Models:
   Train models using prepared data.
4. Assess Models:
   Evaluate models against success criteria.

Building and Evaluating SoC

Model Training:

- Hyperparameter Tuning.

  Using tools like Ray Tune for optimization.

- Experiment Tracking:

  Leveraging MLflow to log experiments and results.

Evaluation Metrics:

Mean Absolute Error (MAE), R2.

Accuracy.

Model Validation:

Cross-Validation.

Residual Analysis.

Selection of Best Model:

Performance vs. Business Requirements.

Deployment Readiness.

7 Explainable ML

Why do we need model explainability

- Use Machine Learning to review resumes:
  - Based on your capability or gender?
- Use Machine Learning to detect fraud transactions?
  - Why does the model think this transaction is suspicious?
- The above examples all belong to high-stakes decisions. The decisions have a huge impact on human well-being.

Black-box Model

- If the ML system is deployed in high-stakes decisions environment:
  - Is accuracy important?
  - Can we trust the machine learning model?
- In banking, insurance and other heavily regulated industries, model interpretability is a serious legal mandate
- In lots of critical areas such as healthcare, government, bioinformatics, etcs, rationale for models' decision is necessary for trust

Goals of Interpretability

- Model debugging
  - Why did my model make mistake?
- Feature Engineering
  - How can I improve my model?
- Detecting fairness issues
  - Does my model have biases?
- Human-AI cooperation
  - How can I understand and trust model's decision?
- Regulatory Compliance
  - Does my model satisfy legal requirements?
- High-stake Decisions
  - Healthcare, Finance..

InterpretML - Alpha Release

license MIT | python 3.6 | 3.7 | 3.8 | pypi v0.2.7 | build failing | coverage 88% | code quality: python A | maintained yes

> In the beginning machines learned in darkness, and data scientists struggled in the void to explain them.
>
> Let there be light.

InterpretML is an open-source package that incorporates state-of-the-art machine learning interpretability techniques under one roof. With this package, you can train interpretable glassbox models and explain blackbox systems. InterpretML helps you understand your model's global behavior, or understand the reasons behind individual predictions.

Interpretability is essential for:

- Model debugging - Why did my model make this mistake?
- Feature Engineering - How can I improve my model?
- Detecting fairness issues - Does my model discriminate?
- Human-AI cooperation - How can I understand and trust the model's decisions?
- Regulatory compliance - Does my model satisfy legal requirements?
- High-risk applications - Healthcare, finance, judicial, ...

Cae Study

Training Data

Digimon

Pokemon

Testing Data

Digimon or Pokemon?

Linear models first

- Prediction is the linear combinations of the features values, weighted by the model coefficients

Students A's chance = 0.2 + 0.1* GPA - 0.005 * Hours on Tiktok

One student's feature
GPA: 5
Hours on Tiktok: 60 hours

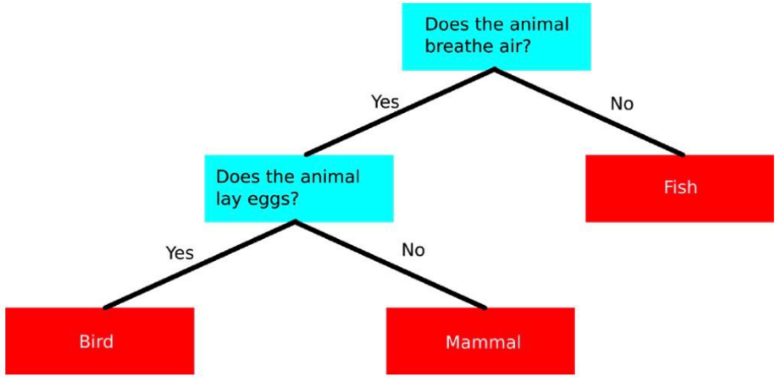
→

Feature Contributions
GPA: 0.5
Hours on Tiktok: -0.3

- Capability of linear models is limited.

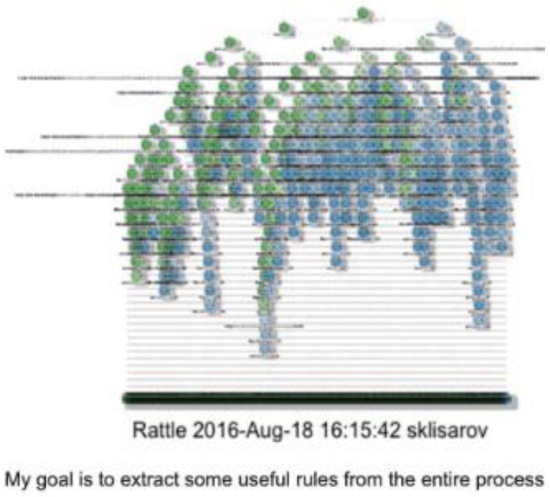
Decision tree

- It is “interpretable”.
- More powerful compared to linear models.

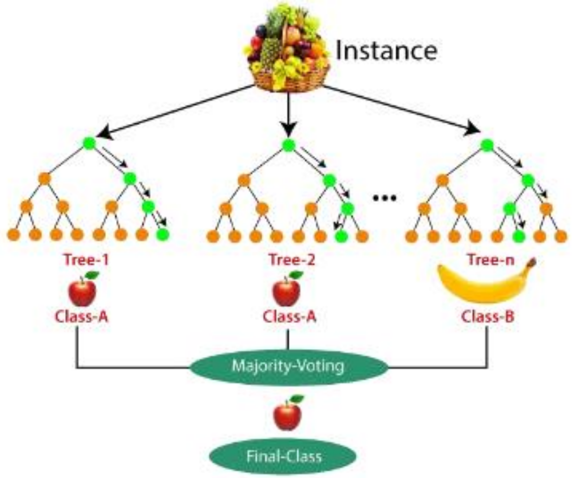


Decision tree can be complex

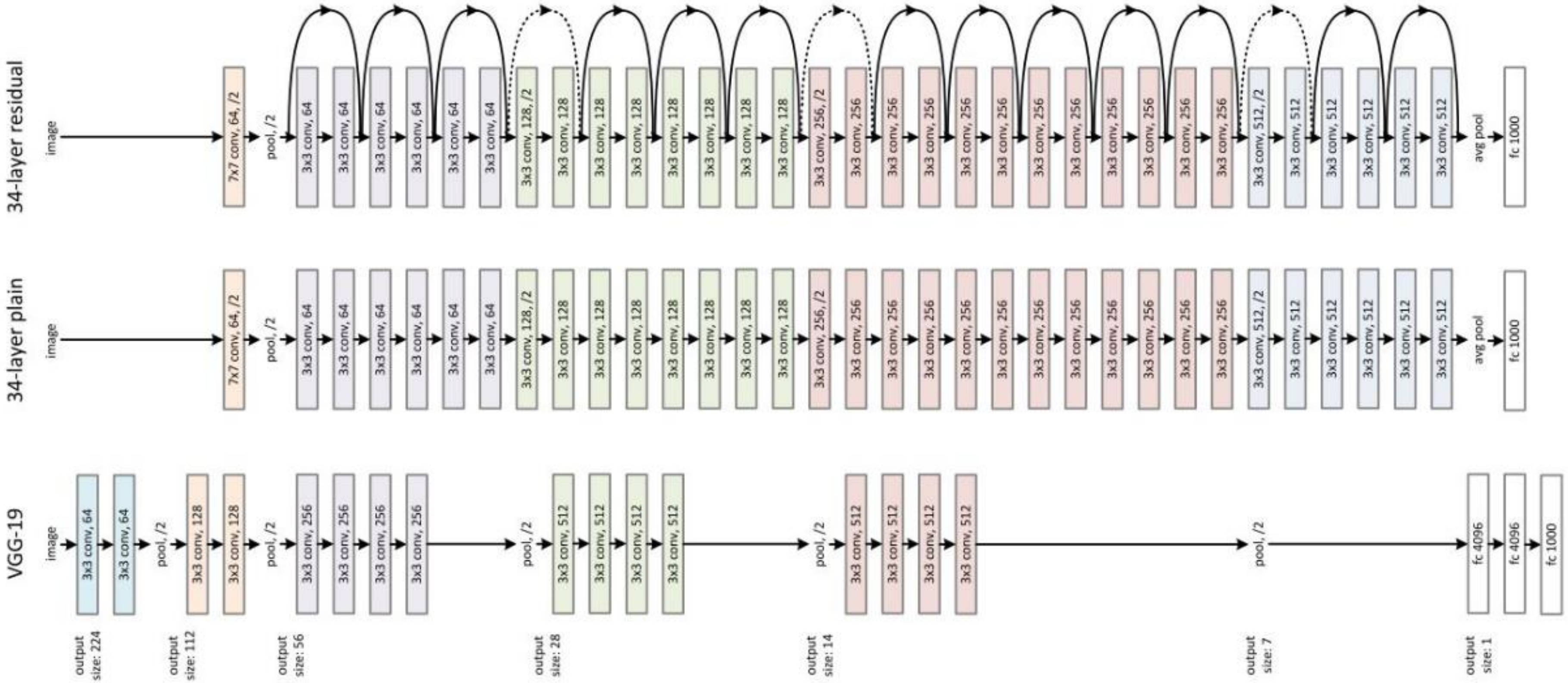
- It can be a huge and complex tree.



- It can be a forest.

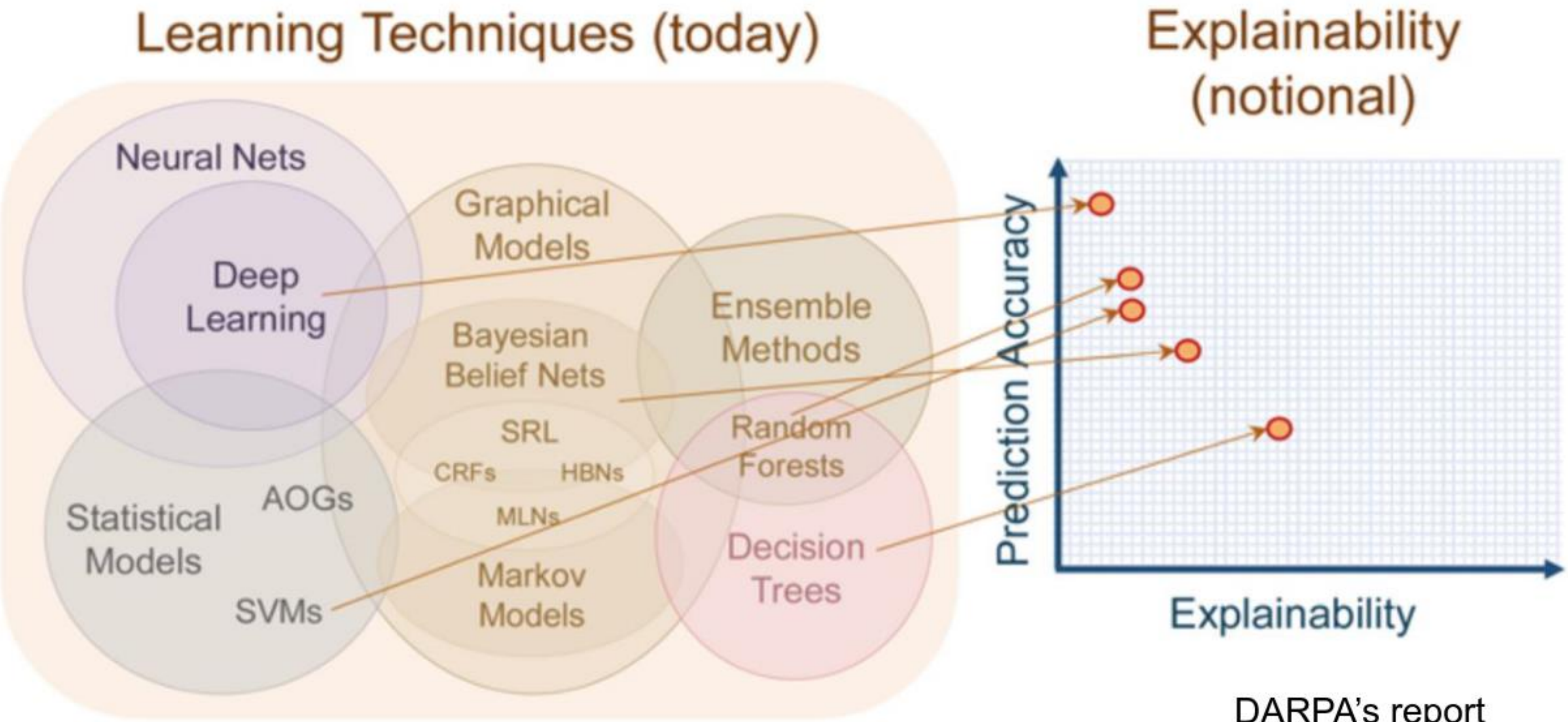


Complex models



For imagenet, they use 152 layers, which firstly achieved lower error rate compared to Humans in image recognition tasks.

Trade-off



DARPA's report

Decision tree

- Self-Explaining
  - Directly interpretable.
  - Generates the explanations at the same time as the prediction
  - Rule-based System, Decision Trees, Logistic Regression, Hidden Markov Model, etc.
- Post hoc:
  - Additional operation is performed after the predictions are made
  - Open-source packages: tf-keras-vis (gradient-based methods for deep learning), LIME, SHAP, etc

Categorization of interpretability

- Global
  - Explanation or justification by revealing how the model's predictive process works
  - What do you think pokemon looks like?
- Local:
  - Provide information or justification for the model's prediction on a specific input
  - Why do you think this image is pokemon?

Post-Hoc

Perform additional operations to explain the entire model's predictive reasoning

Explain a single prediction by performing additional operations (after the model has made the prediction)

Global

Local

Use the predictive model itself to explain the entire model's predictive reasoning (directly interpretable model)

Explain a single prediction using the model itself (calculated from information made available from the model as part of making the prediction)

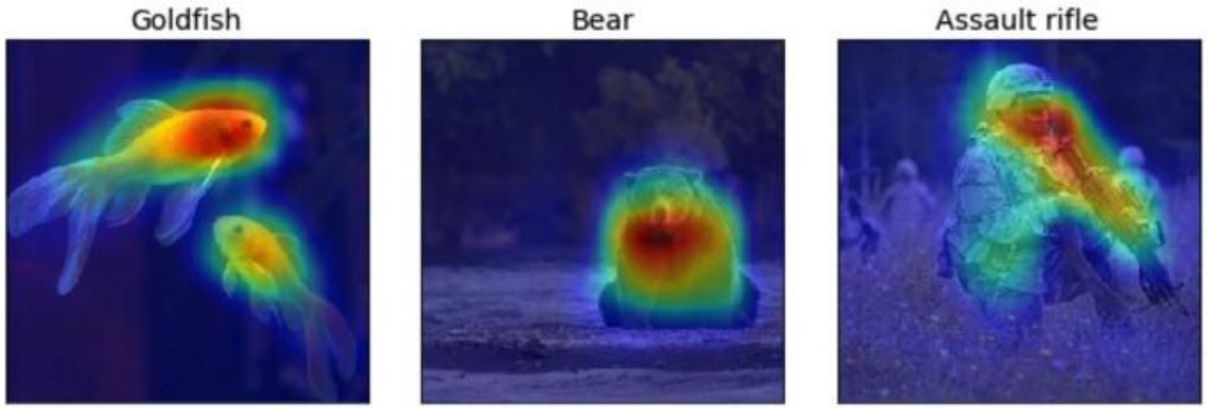
Self-Explaining

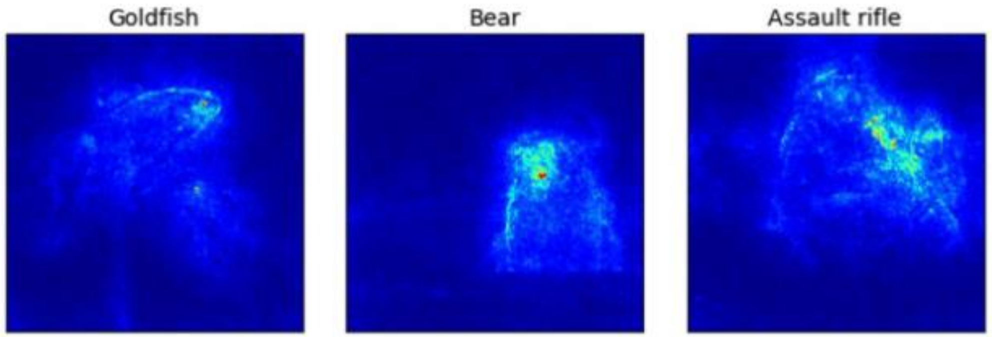
Example-driven

- Reasoning with examples
  - Explain the prediction of an input instance by identifying and presenting other instances
  - Eg. patient A has a tumor because he is similar to these k other data points with tumors
- Similar to nearest neighbor-based approaches

Feature importance

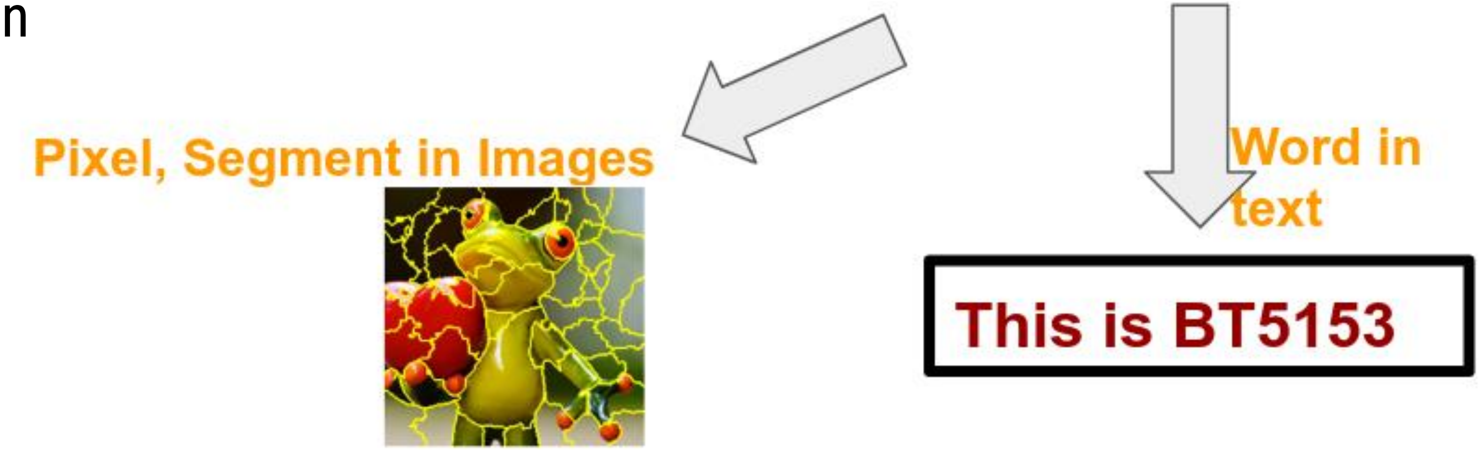
- Derive explanation by investigating the importance scores of different features used to output the final prediction
- It can be computed from
  - Attention Layer Approach
  - Gradient-based Saliency Approach





Gradient-based method

- Explain the decision made by the model
    - Eg, Why do you think this image is pokemon not digimon?
- Motivation: we want to know the contribution of each component/feature in the input data for prediction



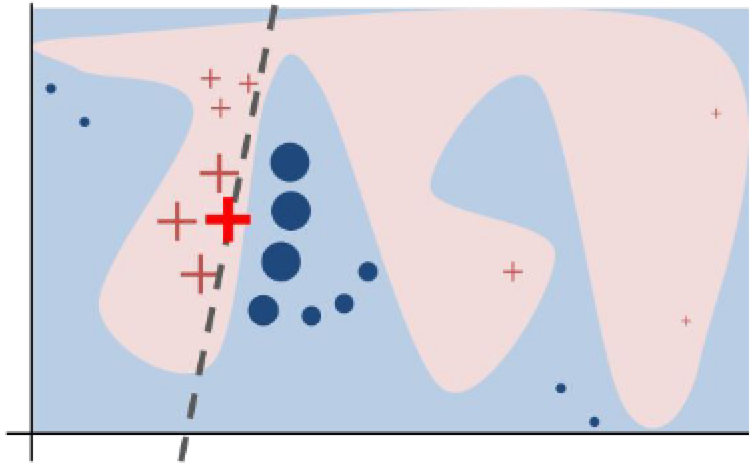
- Solution: Removing or modifying the partial parts of the components, observing the change of decision.

Surrogate model

- Model predictions are explained by learning a second, usually more explainable model, as a proxy
- Model-agnostic (applicable for any machine learning models)l prediction
- The learned surrogate models and the original models may have completely different mechanisms to make predictions

Surrogate model: local explanations

- Hard to explain a complex model in its entirety
  - How about explaining smaller regions?
  - Explain decisions of any model in a local region around a particular point
  - Learns sparse linear model

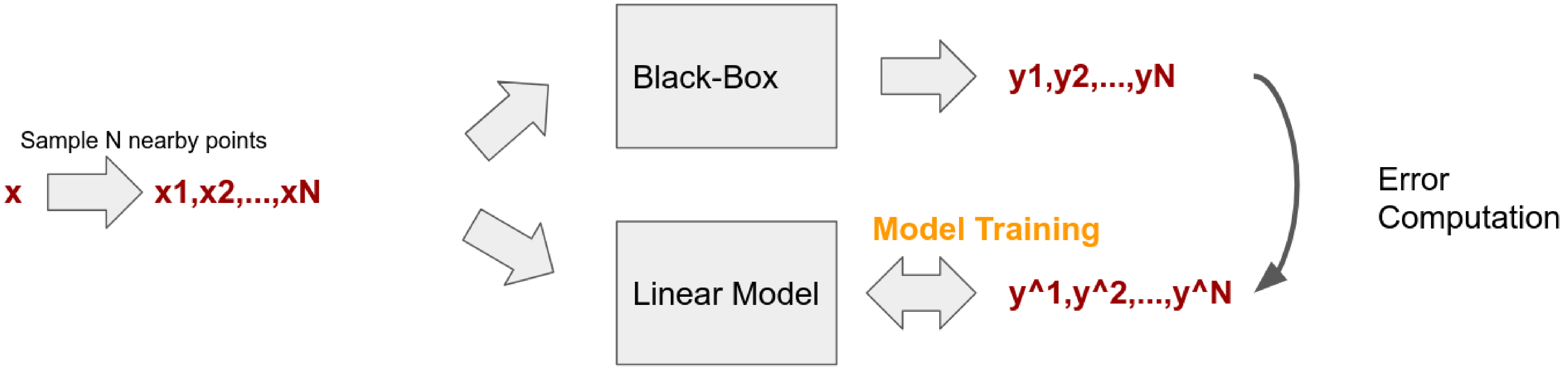


LIME (Ribeiro et. al)

Linear model can not mimic neural networks..but it may mimic a local region

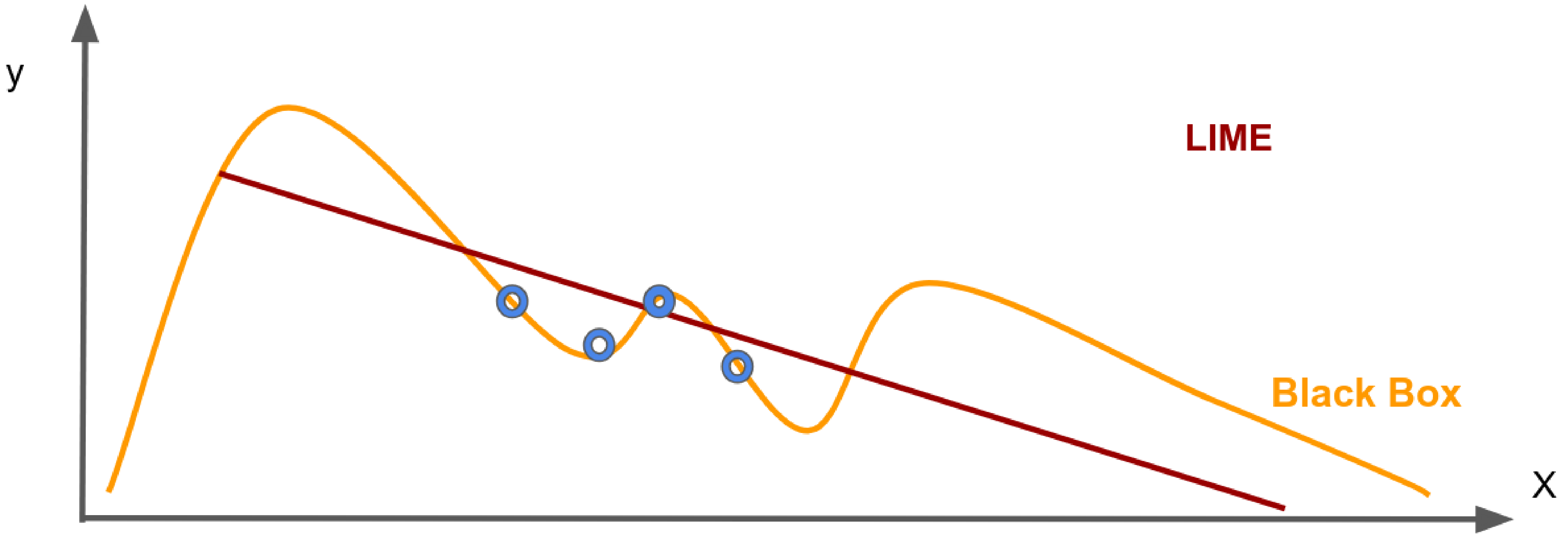
Surrogate model: local explanations

- Interpretable model can be used to mimic the actions of an complex model



Local interpretable model-agnostic explanations

- Given a data point you want to explain
- Sample at the nearby
- Fit with linear model (or other interpretable models)
- Interpret the linear model



XGBoost's feature importance

- XGBoost use boosting to combine weak learners to make accurate predictions.
- Feature importance for XGBoost could be checked in the following methods:
  - Built-in Function
  - Permutation method
  - SHAP method

Miscellaneous Details

- **Origin**
  The origin of the boston housing data is **Natural**.
- **Usage**
  This dataset may be used for **Assessment**.
- **Number of Cases**
  The dataset contains a total of **506** cases.
- **Order**
  The order of the cases is **mysterious**.
- **Variables**
  There are **14** attributes in each case of the dataset. They are:

  1. CRIM - per capita crime rate by town
  2. ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
  3. INDUS - proportion of non-retail business acres per town.
  4. CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
  5. NOX - nitric oxides concentration (parts per 10 million)
  6. RM - average number of rooms per dwelling
  7. AGE - proportion of owner-occupied units built prior to 1940
  8. DIS - weighted distances to five Boston employment centres
  9. RAD - index of accessibility to radial highways
  10. TAX - full-value property-tax rate per $10,000
  11. PTRATIO - pupil-teacher ratio by town
  12. B - 1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
  13. LSTAT - % lower status of the population
  14. MEDV - Median value of owner-occupied homes in $1000's

Housing price prediction

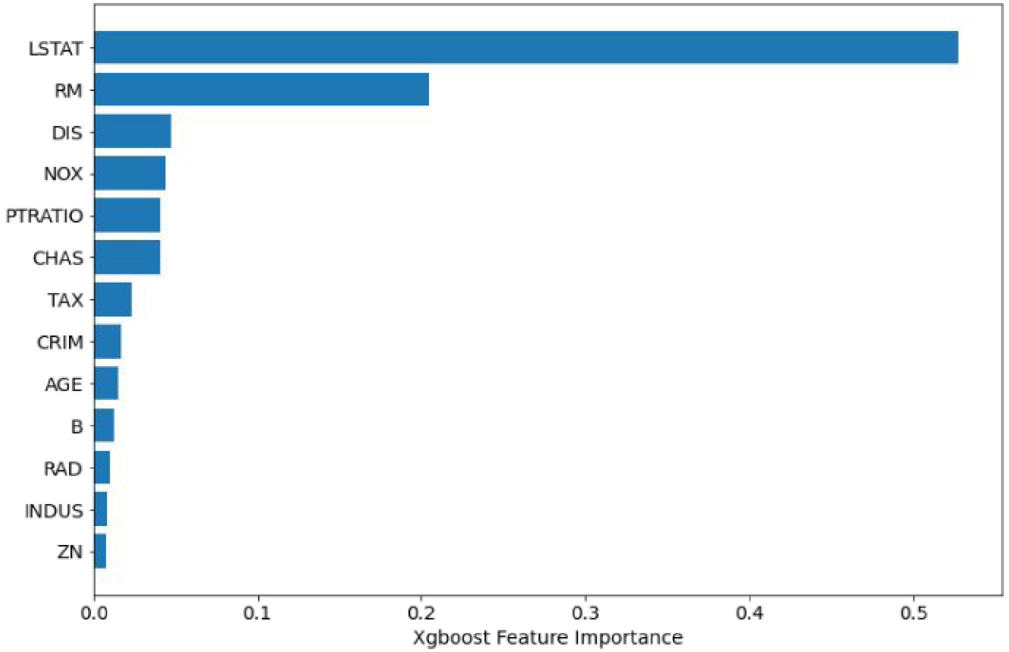
XGBoost built-in function

- XGBoost

get_score(*fmap='', importance_type='weight'*)

Get feature importance of each feature. For tree model Importance type can be defined as:

- 'weight': the number of times a feature is used to split the data across all trees.
- 'gain': the average gain across all splits the feature is used in.
- 'cover': the average coverage across all splits the feature is used in.
- 'total_gain': the total gain across all splits the feature is used in.
- 'total_cover': the total coverage across all splits the feature is used in.



Permutation based feature importance

- Randomly shuffle each feature and compare the model's performance change. The most important feature impact the performance the most.
- Well-supported in sklearn
- A bit slow!

sklearn.inspection.permutation_importance

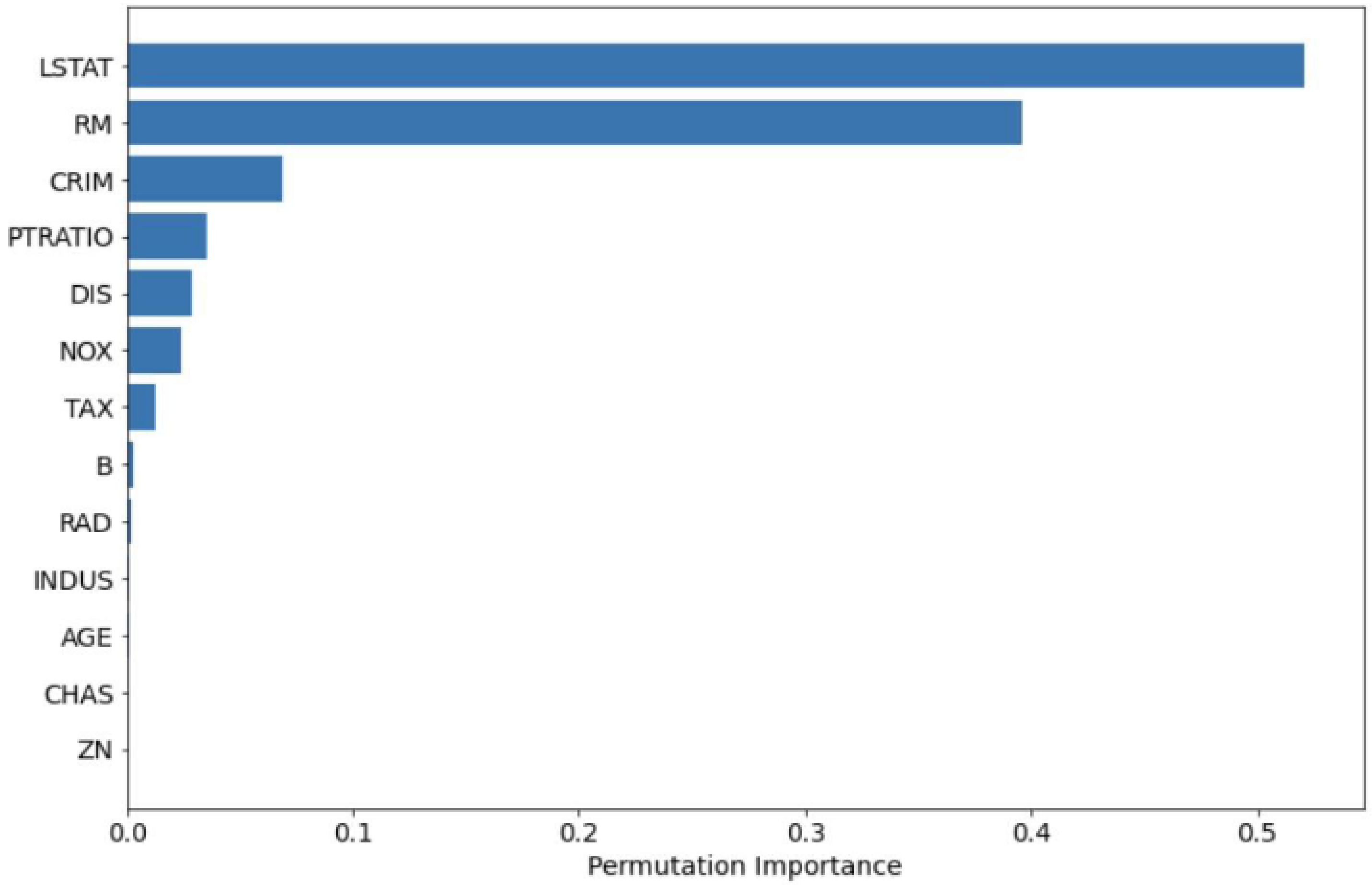
sklearn.inspection.permutation_importance(*estimator, X, y, *, scoring=None, n_repeats=5, n_jobs=None, random_state=None, sample_weight=None, max_samples=1.0*) [source]

Permutation importance for feature evaluation [BRE].

The estimator is required to be a fitted estimator. `X` can be the data set used to train the estimator or a hold-out set. The permutation importance of a feature is calculated as follows. First, a baseline metric, defined by scoring, is evaluated on a (potentially different) dataset defined by the `X`. Next, a feature column from the validation set is permuted and the metric is evaluated again. The permutation importance is defined to be the difference between the baseline metric and metric from permutating the feature column.

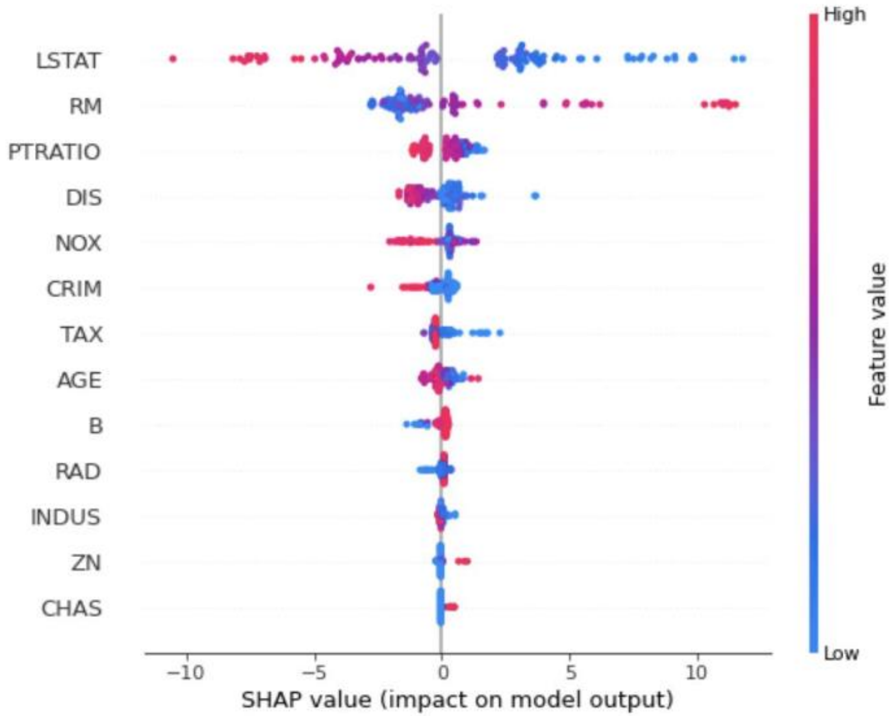
Read more in the User Guide.

Permutation importance



SHAP: SHapley Additive exPlanations

- Similar to LIME, it is also model-agnostic and compute the shapley value based on game theory to measure the contribution from each feature.
- Measuring the feature importance to the entire model



8 Responsible M

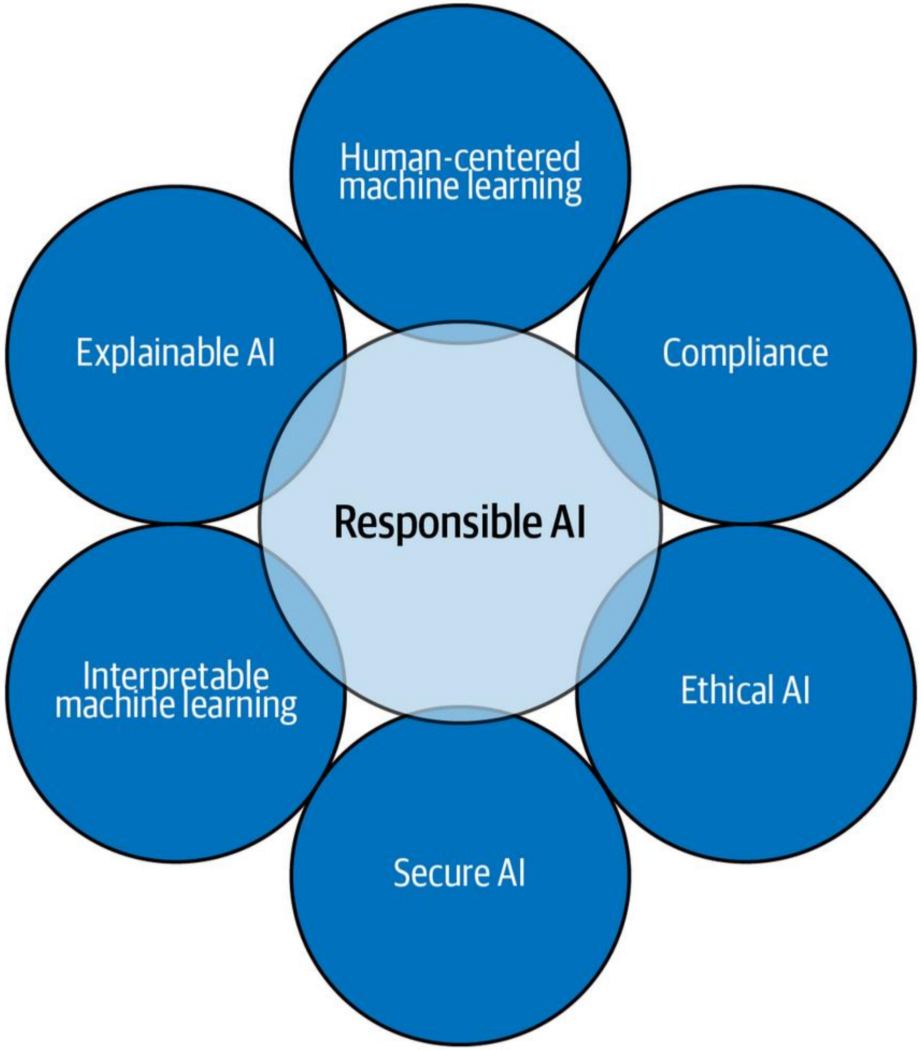
Introduction to Responsible Machine Learning

Responsible Artificial Intelligence is about human responsibility for the development of intelligent systems along fundamental human principles and values, to ensure human-flourishing and well-being in a sustainable world.

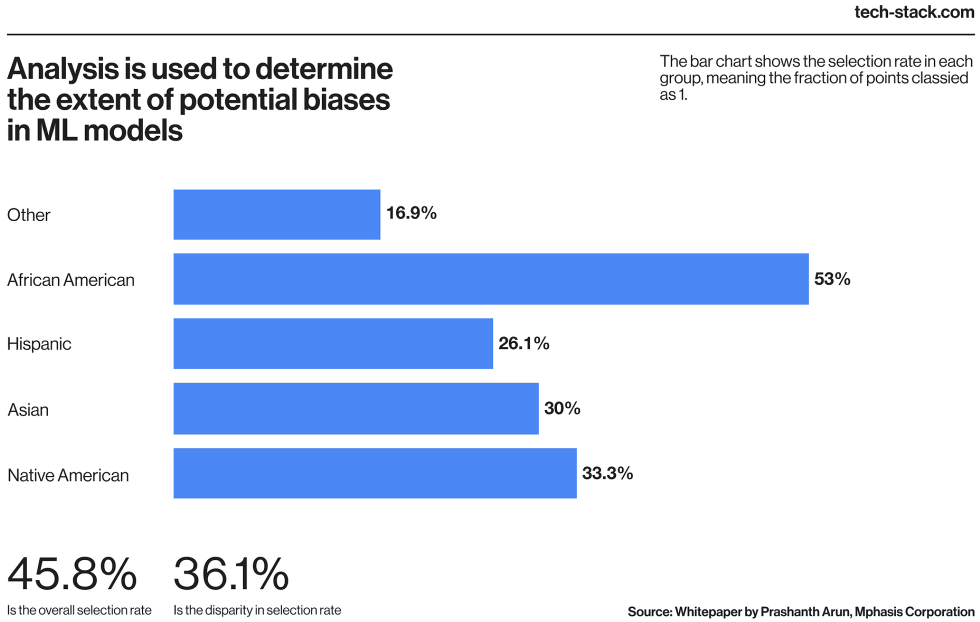
- Definition: The practice of developing and using machine learning (ML) algorithms in a way that empowers humans while minimizing negative impacts.
- Relevance: ML and AI are increasingly integrated into products we use daily, affecting user experience and societal outcomes.
- Objective: Ensure ethical, compliant, secure, and human-centered AI that benefits users and society.

Importance of Responsible ML

- User Impact:
  - Risk of offensive or discriminatory outputs without responsible practices.
  - Potential for privacy breaches and poor user experiences.
- Business Impact:
  - Harm to company reputation and customer trust.
  - Legal and ethical consequences from irresponsible ML use.
- Societal Impact:
  - Perpetuation of biases and discrimination.
  - Influence on social dynamics and equity.



Principles of Responsible Machine Learning



1. Human augmentation. The belief that ML can offer incorrect predictions, which is why it always needs humans to supervise it.
2. Bias evaluation. The commitment to continuously analyze potential biases in ML to correct them.
3. Explainability by justification. Anyone developing ML-based tools should aim to improve their transparency.
4. Reproducible operations. ML should have the proper infrastructure to guarantee reproducibility across the operations of ML systems.

Principles of Responsible Machine Learning

5. Displacement strategies. ML development should mitigate the human impact of ML adoption, especially when automation solutions displace workers.
6. Practical accuracy. ML solutions should be as precise as possible, which can only be achieved through high-quality processes.
7. Trust by privacy. The commitment to build processes that protect the data handled by ML and guarantee its privacy.
8. Data risk awareness. The belief that ML is vulnerable to attacks, which is why engineers have to constantly develop new processes to ensure a high level of security.

Incorporating Responsible ML

Selecting a Dataset Responsibly:

- Use diverse and representative data.
- Verify data sources and obtain necessary permissions.
- Ensure data is anonymized to protect privacy.

Applying Basic ML Methods Responsibly:

- Choose algorithms that are interpretable and explainable.
- Implement bias detection and mitigation techniques.
- Maintain human oversight throughout the ML process.

Extracting Conclusions Ethically:

- Interpret results within the proper context.
- Be transparent about methodologies and limitations.
- Consider the societal impact of your conclusions.

9 Trustworthy ML

Trustworthy Artificial Intelligence (AI) defining it as programs and systems designed to solve problems like humans, providing benefits and convenience without posing threats or risks of harm.

3 Perspectives:

1. Technical Perspective: Trustworthy AI should exhibit accuracy, robustness, and explainability.
2. User Perspective: AI should possess availability, usability, safety, privacy, and autonomy.
3. Social Perspective: Trustworthy AI should be law-abiding, ethical, fair, accountable, and environmentally friendly.

Technical Perspective

- Accuracy: AI systems should produce outputs that are as consistent with the ground truth as possible.
- Robustness: They should be resilient to changes and perturbations in complex and volatile real-world environments.
- Explainability: AI should be transparent and allow human understanding and analysis to minimize potential risks.

User Perspective:

- Availability: AI systems should be accessible whenever users need them.
- Usability: They should be easy to use for people with different backgrounds.
- Safety: AI should avoid causing harm under any conditions, prioritizing user safety.
- Privacy: AI must protect user privacy and handle data responsibly.
- Autonomy: The decision-making power of AI should always be under human control.

Social Perspective

- Law-abiding and Ethical: AI should comply with all relevant laws and ethical principles.
- Fairness: AI should be non-discriminatory and ensure justice among all users.
- Accountability: There should be clear responsibility for each part of the AI system.
- Environmentally Friendly: AI should minimize energy consumption and pollution for sustainable development.