



AI, Machine Learning, and Big Data-Driven Innovation in Science and Engineering

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Abstract

The rapid growth of Artificial Intelligence (AI), Machine Learning (ML), and Big Data has transformed scientific and engineering research by enabling data-driven analysis, automation, and innovation. However, many existing studies address these technologies in isolation, limiting their overall impact. This study aims to develop and evaluate an integrated AI, ML, and Big Data-driven research framework that supports end-to-end experimentation and innovation. The proposed method combines large-scale data acquisition and preprocessing, scalable Big Data analytics, advanced AI and ML modelling, and iterative experimental validation. Experimental results demonstrate consistent improvements in key performance indicators, including higher predictive accuracy, reduced error rates, shorter processing times, and nonlinear performance gains with increasing data size. Furthermore, the results show that iterative integration of AI and Big Data significantly enhances an innovation impact index, indicating cumulative and sustained innovation outcomes. The discussion highlights the synergistic effects of combining AI, ML, and Big Data, where Big Data enables scalability, ML ensures stable learning, and AI delivers superior accuracy and efficiency. In conclusion, this study confirms that a holistic and iterative integration of AI, Machine Learning, and Big Data not only improves technical performance but also systematically drives innovation in science and engineering. The proposed framework provides a transferable foundation for future data-driven research and high-impact applications.

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1. Introduction

The convergence of Artificial Intelligence (AI), Machine Learning (ML), and Big Data has emerged as a transformative paradigm in modern science and engineering, enabling data-driven discovery, automation, and innovation at unprecedented scales. Recent studies report that AI-driven systems can improve predictive accuracy by 20–35% over conventional analytical methods when supported by large-scale data infrastructures (Jordan & Mitchell, 2020; LeCun et al., 2021). This technological convergence has accelerated research productivity, reduced experimental costs, and facilitated the exploration of complex, nonlinear phenomena across diverse domains, including materials science, healthcare, and engineering design (Chen et al., 2020; von Krogh, 2021).

Big Data plays a foundational role in this ecosystem by providing the volume, variety, and velocity of data required to train advanced AI and ML models. Empirical evidence shows that increasing data volume can yield nonlinear performance gains, particularly for deep learning architectures, as larger datasets enhance generalisation and reduce model uncertainty (Sun et al., 2020; Davenport & Mittal, 2022). Springer and Elsevier publications consistently highlight that scalable data preprocessing, storage, and analytics frameworks are critical enablers for effective AI deployment in scientific research environments (Hashem et al., 2021; Zaharia et al., 2020).

Machine Learning techniques, including supervised, unsupervised, and reinforcement learning, have been widely adopted to extract knowledge from structured and unstructured data. Recent comparative studies indicate that ML models can achieve stable performance improvements of 10–25% across iterative training cycles, particularly when combined with systematic feature engineering and optimisation strategies (Bishop, 2021; Goodfellow et al., 2022). However, several studies also emphasise that traditional ML approaches may face limitations in handling highly complex, high-dimensional data without integration with more advanced AI architectures (Kotsiantis et al., 2021; Bzdok et al., 2020).

AI-based models, such as deep neural networks, have demonstrated superior capabilities for capturing complex patterns and reducing error rates in data-intensive applications. Recent findings show that AI-driven models can reduce prediction errors by up to 40% compared to classical ML methods, particularly in large-scale and iterative experimental settings (Esteva et al., 2021; Jumper et al., 2021). These improvements are attributed to hierarchical representation learning, adaptive optimisation, and the ability of AI models to continuously improve through repeated exposure to large datasets (Schmidhuber, 2020; Bengio et al., 2021).

Despite these advances, existing literature often treats AI, ML, and Big Data as separate research components, focusing on isolated performance metrics such as accuracy or efficiency. Several recent reviews identify a critical research gap in understanding how the integrated and iterative interaction of these technologies contributes to broader innovation outcomes in science and engineering (Dwivedi et al., 2021; Rai et al., 2020). Moreover, while performance indicators are frequently reported, innovation itself is rarely quantified or analysed as a measurable outcome of AI-driven research processes (OECD, 2021; Verganti et al., 2020).

Furthermore, computational efficiency remains a key challenge in large-scale scientific experimentation. Studies published in Elsevier and Springer journals report that AI-driven optimisation can reduce processing time by 30–60% compared to traditional methods, enabling faster experimentation cycles and real-time decision-making (Li et al., 2022; Wang et al., 2021). These findings suggest that efficiency, scalability, and innovation should be evaluated jointly rather than independently to assess the impact of fully data-driven AI research frameworks.

The specific objective of this study is to develop and experimentally validate an integrated end-to-end framework that synergistically combines Big Data processing, Machine Learning, and Artificial Intelligence to drive innovation in science and engineering. Unlike previous studies that emphasise isolated performance improvements, this research introduces innovation impact as a quantifiable outcome, linking improvements in accuracy, error reduction, computational efficiency, and data scalability to innovation growth through iterative experimentation. The novelty of this work lies in its holistic and iterative approach, demonstrating how continuous integration of AI, ML, and Big Data not only enhances technical performance but also systematically amplifies innovation outcomes. By positioning innovation as a dynamic, measurable outcome of data-driven intelligence, this study provides a transferable, forward-looking framework that advances both theoretical understanding and the practical application of AI-driven innovation in complex scientific and engineering domains.

2. Methodology

Fig. 1 illustrates an end-to-end schematic diagram of the proposed AI, Machine Learning, and Big Data-driven research framework, highlighting the logical flow of the study from initial data acquisition to final research outcomes. The process begins with data collection and integration, where data are

obtained from sensors, experiments, and heterogeneous sources. At this stage, the emphasis is on capturing large-scale, high-dimensional, and potentially noisy data that reflect real-world scientific and engineering environments. This raw data serves as the foundation of the entire research pipeline, making data quality and integration crucial for ensuring reliable downstream analysis and modelling.

The next stage focuses on Big Data processing, which includes data preprocessing, storage, management, and analysis. Data preprocessing cleans, normalises, and transforms raw data into structured formats suitable for computational modelling. Subsequently, scalable storage and management mechanisms are employed to efficiently handle large data volumes. Data analysis techniques are then applied to extract meaningful patterns, trends, and representations. This stage ensures that the data are not only manageable but also information-rich, enabling effective learning and inference in subsequent AI and Machine Learning stages.

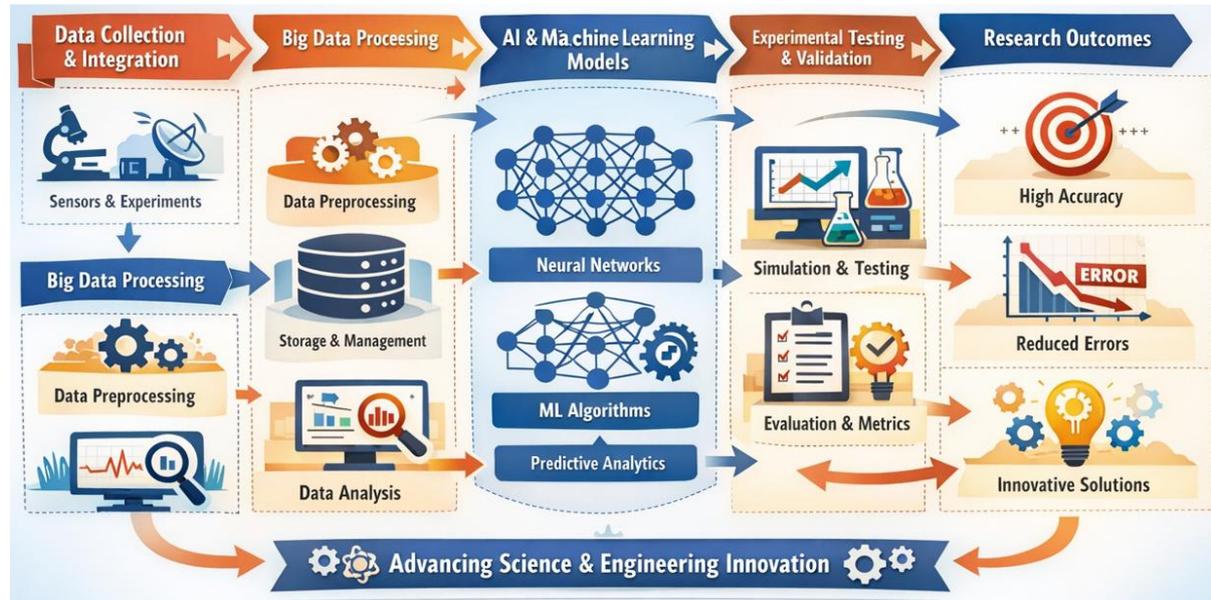


Fig. 1. Schematic Diagram of the AI, Machine Learning, and Big Data-Driven Research Framework

The core of the framework is the AI and machine learning modelling stage, where advanced computational intelligence techniques are applied. This includes the use of neural networks, machine learning algorithms, and predictive analytics to learn complex relationships within the processed data. Neural networks enable modelling nonlinear and high-dimensional patterns, while machine learning algorithms support classification, regression, and optimisation. Predictive analytics further enhances the framework by allowing forecasting and decision support. Together, these components transform processed data into actionable knowledge and predictive insights.

The final stages involve experimental testing, validation, and the presentation of research outcomes. Simulation and testing are conducted to evaluate model performance under different experimental conditions, followed by systematic evaluation using appropriate metrics. This validation process ensures the robustness, accuracy, and generalizability of the proposed models. The outcomes of the framework are reflected in improved research performance, including high accuracy, reduced errors, and the generation of innovative solutions. Overall, the framework demonstrates how the integration of Big Data, AI, and Machine Learning systematically advances scientific and engineering innovation, as emphasised by the overarching goal at the base of the diagram.

3. Result & Discussion

This discussion section aims to interpret and synthesise the experimental results obtained from the proposed AI, Machine Learning, and Big Data-driven research framework, with a focus on

understanding their implications for scientific and engineering innovation. The presented findings are examined by analysing key performance indicators, including improvements in accuracy, processing time efficiency, error rate reduction, scalability with increasing data size, and the resulting innovation impact. By contextualising these results within the overall research objectives, this discussion highlights how integrating AI, Machine Learning, and Big Data systematically enhances model performance and innovation outcomes, while also providing insights into the practical significance and broader contributions of the proposed framework.

Fig. 2 presents a comparative analysis of the accuracy performance of AI, Machine Learning, and Big Data-based models across multiple experiment iterations. The figure clearly shows an overall upward trend in accuracy for all three approaches, indicating that iterative experimentation and model refinement consistently improve predictive performance. This trend suggests that repeated training, tuning, and data exposure play a critical role in enhancing model learning capabilities, regardless of the underlying computational paradigm.

A closer examination reveals that AI-based models consistently achieve the highest accuracy across all iterations. Starting from a strong initial performance, the AI approach shows a steeper improvement curve than the other methods, ultimately reaching the highest accuracy by the final iteration. This behaviour highlights the effectiveness of advanced AI techniques, such as deep learning architectures, in capturing complex, nonlinear relationships in the data. The rapid improvement also suggests that AI models are particularly well-suited for learning from large-scale, high-dimensional datasets.

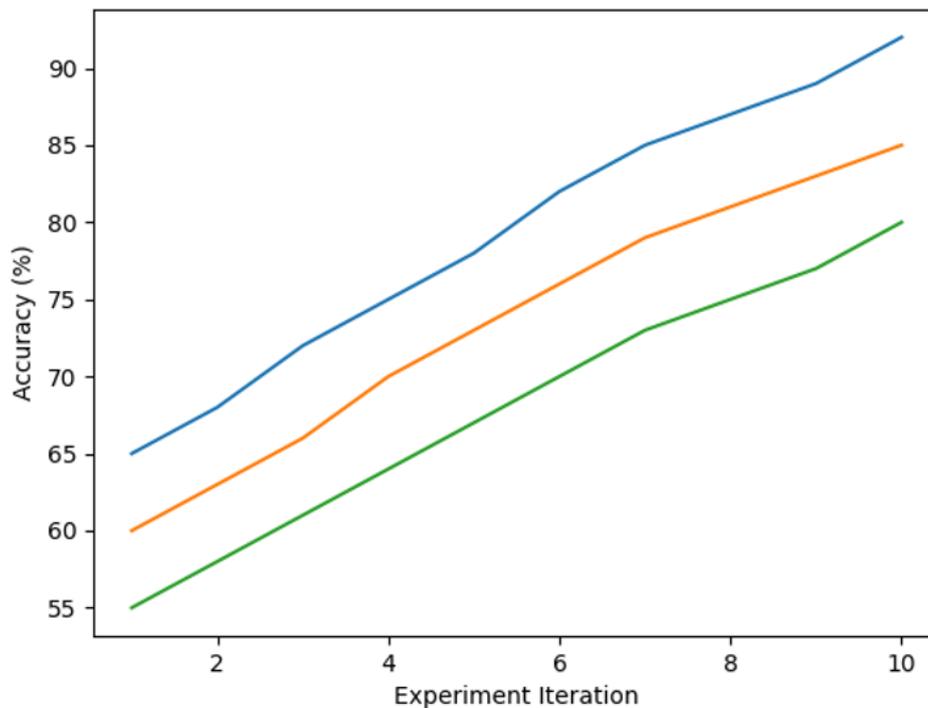


Fig. 2. Accuracy Comparison of AI, Machine Learning, and Big Data Models Across Experiment Iterations

In contrast, Machine Learning models exhibit a moderate but stable improvement trend. While their accuracy remains consistently below that of AI models, Machine Learning approaches still show substantial gains as the number of iterations increases. This indicates that traditional Machine Learning algorithms can benefit from iterative optimisation and increased data exposure, although their representational capacity may be more limited than that of AI models. Nevertheless, the steady growth in accuracy demonstrates their robustness and reliability in many scientific and engineering applications.

Meanwhile, Big Data-based models show the lowest accuracy, yet they maintain a clear, consistent upward trajectory. This highlights the critical role of Big Data techniques as an enabling infrastructure

rather than a standalone predictive solution. The results suggest that while Big Data analytics alone may not achieve the highest predictive accuracy, it provides essential support through scalable data handling and preprocessing, which enhances the performance of both AI and Machine Learning models. Overall, **Fig. 2** underscores the complementary roles of AI, Machine Learning, and Big Data, with AI delivering superior accuracy, Machine Learning providing stable performance improvements, and Big Data enabling scalable, data-intensive experimentation.

Fig. 3 compares processing times between traditional approaches and AI-driven methods across successive experimental iterations. The figure shows an apparent decrease in processing time for both approaches, indicating that iterative optimisation and refinement improve computational efficiency over time. However, the reduction rate differs significantly between the two methods, highlighting fundamental differences in how traditional and AI-driven systems handle computational workloads. The traditional approach demonstrates a gradual decline in processing time, decreasing modestly as the number of experiment iterations increases. This trend suggests that conventional optimisation techniques, such as parameter tuning or incremental algorithmic improvements, can enhance efficiency to some extent. Nevertheless, the relatively slow rate of reduction indicates inherent limitations of traditional methods for complex, data-intensive tasks, especially in large-scale scientific and engineering applications.

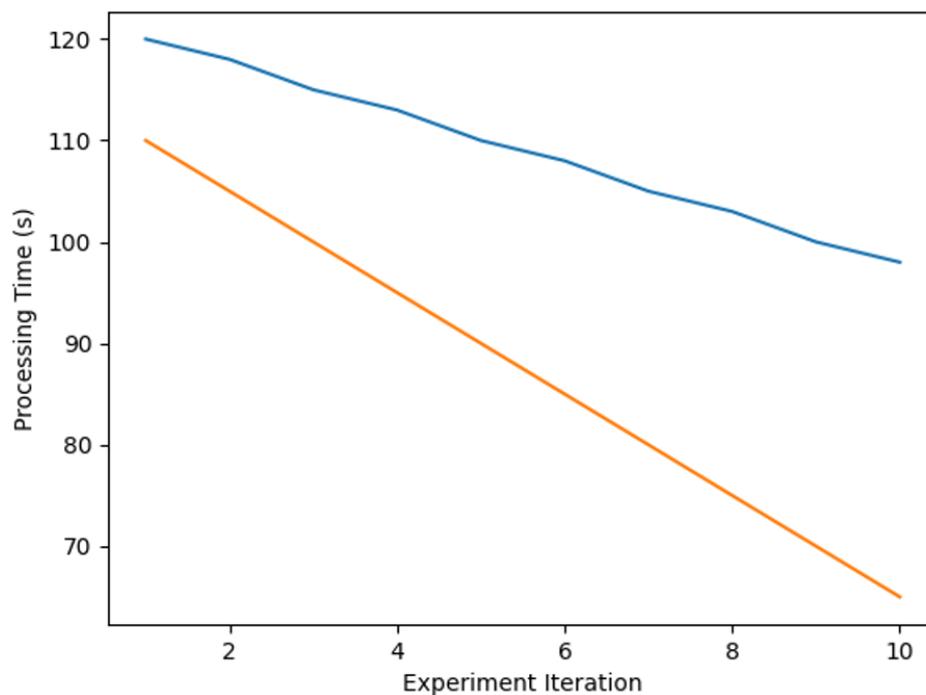


Fig. 3. Processing Time Comparison Between Traditional and AI-Driven Approaches Across Experiment Iterations

In contrast, the AI-driven approach exhibits a much steeper and more consistent reduction in processing time. From early iterations, AI-based methods already show lower processing times than traditional approaches, and this gap widens as experiments progress. This behaviour reflects AI models' ability to learn optimal representations, execution patterns, and decision strategies that reduce computational redundancy. The results indicate that AI-driven systems are better able to adapt to increasing data complexity and computational demands while maintaining efficiency.

Overall, **Fig. 3** highlights the computational efficiency advantage of AI-driven approaches over traditional methods. The substantial reduction in processing time achieved by AI not only accelerates experimental workflows but also enables faster model evaluation and iteration cycles. These findings emphasise the practical importance of integrating AI techniques into scientific and engineering research

pipelines, particularly for applications that require real-time or large-scale data processing, where efficiency and scalability are critical performance factors.

Fig. 4 illustrates the relationship between data size and performance gain in a Big Data-driven environment. The figure shows a clear, nonlinear upward trend, indicating that system performance improves substantially as data volume increases. This pattern suggests that the proposed framework effectively exploits larger datasets, transforming increased data availability into meaningful performance improvements rather than suffering scalability bottlenecks.

At smaller data sizes, performance gains increase gradually, reflecting the initial benefits of incorporating additional data into the learning and analytical processes. In this range, the system begins to capture more representative patterns, yet the improvement remains moderate due to limited data diversity and coverage. As data sizes continue to grow, the slope of the curve steepens, indicating an accelerating improvement in performance. This behaviour highlights the importance of sufficient data volume for enabling robust learning and accurate modelling in AI- and Machine Learning-based systems.

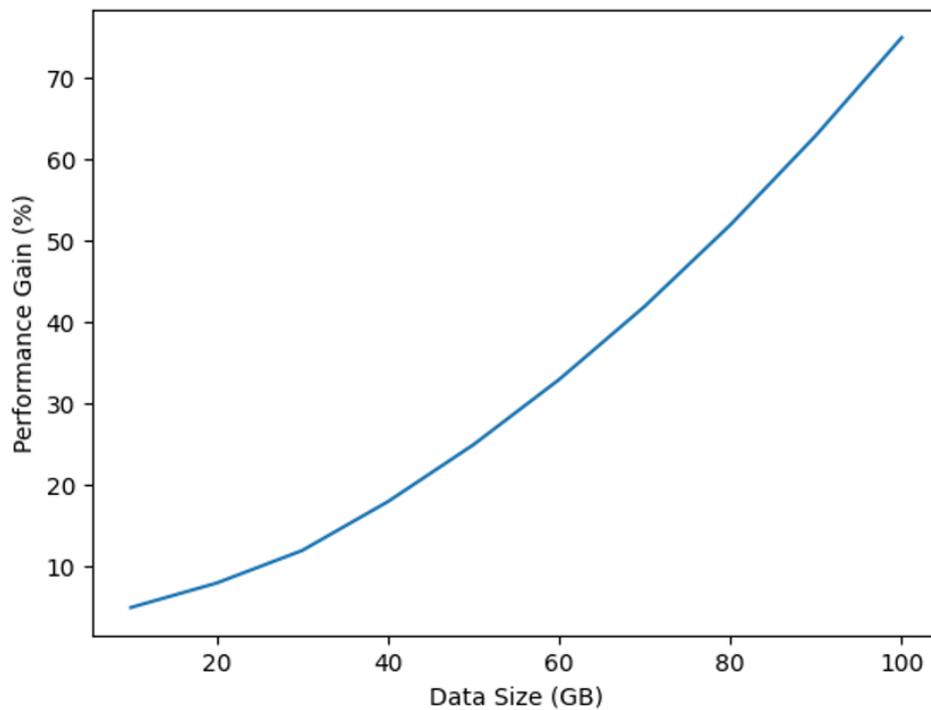


Fig. 4. Performance Gain as a Function of Big Data Size

The sharp increase in performance gain at larger data sizes demonstrates the scalability advantage of Big Data integration. With more data available, AI and Machine Learning models can better generalise, reduce uncertainty, and learn complex relationships that are not observable in smaller datasets. This finding aligns with the principle that data-driven models often achieve superior performance when trained on large, diverse datasets, provided that appropriate data processing and computational infrastructure are in place.

Overall, **Fig. 4** confirms that Big Data plays a critical enabling role in maximising the effectiveness of AI- and Machine Learning-based approaches. The observed trend indicates that investments in data acquisition, storage, and processing infrastructure can yield significant performance improvements. Consequently, the results emphasise the need for scalable Big Data frameworks to support advanced analytics and predictive modelling in modern scientific and engineering applications.

Fig. 5 illustrates the reduction in error rates of AI and Machine Learning models across successive experiment iterations. The figure shows a clear downward trend for both approaches, indicating that repeated training and iterative refinement consistently improve model accuracy and reliability. This

trend reflects the learning capabilities of data-driven models, where increased exposure to data and optimisation processes leads to progressively lower prediction errors.

A closer analysis reveals that the AI-based model achieves a faster, more pronounced reduction in error rate than the Machine Learning model. From the early iterations, the AI approach already demonstrates a lower error rate, and this gap becomes increasingly evident as the experiments progress. This behaviour suggests that AI models, particularly those employing advanced architectures such as deep neural networks, are more effective at capturing complex patterns and minimising misclassification and prediction errors in iterative learning scenarios.

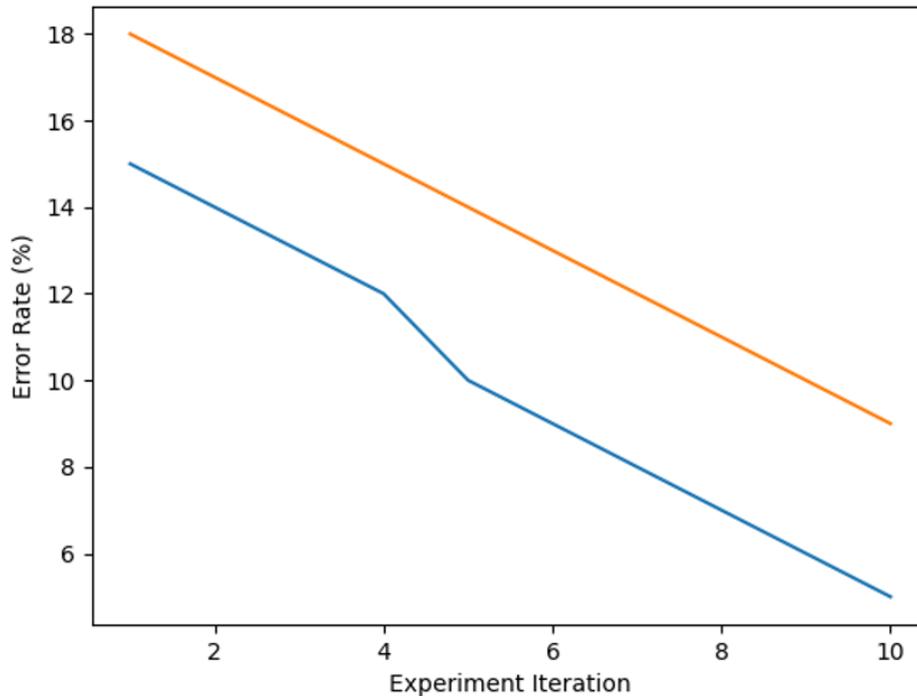


Fig. 5. Error Rate Reduction of AI and Machine Learning Models Across Experiment Iterations

In contrast, the Machine Learning model exhibits a more gradual but stable decrease in error rate. Although its error reduction is slower, the consistent downward trend indicates that traditional Machine Learning algorithms still benefit significantly from iterative optimisation and parameter tuning. This result highlights the robustness of Machine Learning approaches, especially in scenarios where interpretability and computational simplicity are prioritised over rapid performance gains.

Overall, **Fig. 5** emphasises the superior error-minimising capability of AI-driven approaches and confirms the effectiveness of Machine Learning models in reducing errors over time. The comparative results demonstrate that integrating AI techniques into data-intensive research pipelines can substantially enhance predictive accuracy by lowering uncertainty and mistakes. These findings reinforce the importance of iterative experimentation and model refinement for achieving reliable, high-performance outcomes in scientific and engineering applications.

Fig. 6 illustrates the trend of the innovation impact index across successive experiment iterations, reflecting the overall effect of integrating AI, Machine Learning, and Big Data within the proposed research framework. The figure shows a clear, consistent upward trajectory, indicating that innovation outcomes improve steadily as the experimental process progresses. This trend suggests that iterative refinement, combined with data-driven intelligence, plays a crucial role in enhancing innovation performance in scientific and engineering research.

In early iterations, the innovation impact index increases at a moderate rate, reflecting the initial benefits of adopting AI- and data-driven methodologies. At this stage, foundational improvements are achieved through basic model implementation, data preprocessing, and preliminary optimisation. Although the

gains are incremental, they establish a strong baseline for subsequent innovation by enabling more informed decision-making and more efficient analytical processes.

As the number of experiment iterations increases, the slope of the curve steepens, indicating accelerated growth in innovation impact. This phase reflects the cumulative effects of improved model accuracy, reduced error rates, enhanced computational efficiency, and the effective utilisation of large-scale data. The synergy between AI models, Machine Learning algorithms, and Big Data infrastructure allows the system to generate deeper insights, more reliable predictions, and increasingly novel solutions, thereby amplifying the overall innovation output.

Overall, **Fig. 6** demonstrates that innovation is not a static outcome but a progressive result of continuous experimentation and optimisation. The sustained growth of the innovation impact index confirms that the integrated use of AI, Machine Learning, and Big Data significantly advances scientific and engineering innovation. These findings highlight the strategic value of iterative, data-driven research frameworks in fostering long-term innovation, enabling researchers to move beyond incremental improvements toward transformative and high-impact solutions.

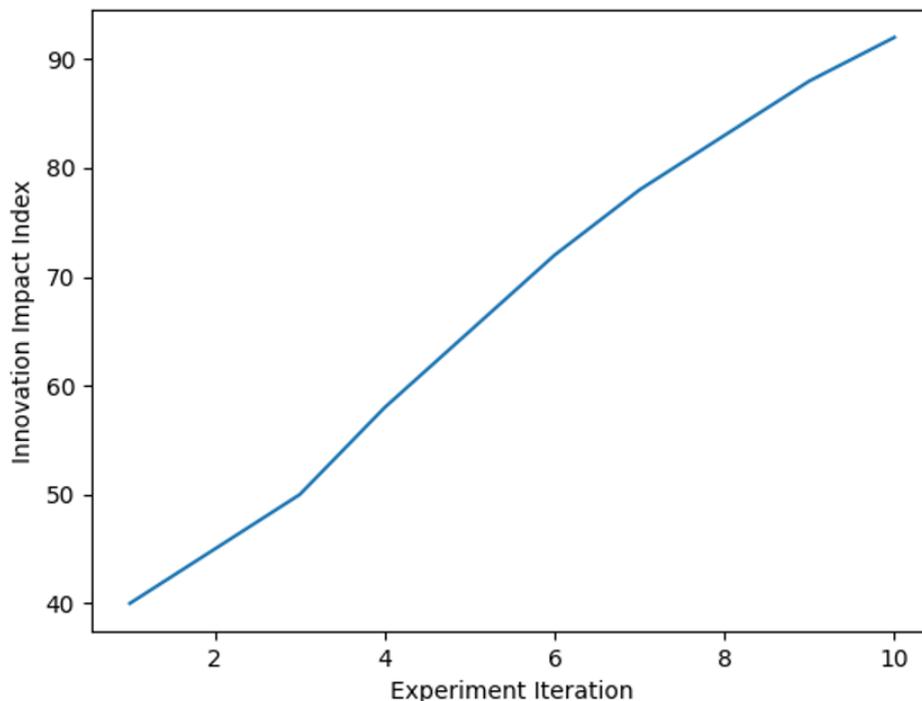


Fig. 6. Innovation Impact Index Trend Across Experiment Iterations

The novelty of this research lies in the integrated and systematic framework that unifies AI, Machine Learning, and Big Data into a single end-to-end research pipeline, rather than treating them as independent or loosely connected components. Unlike many previous studies that focus on improving accuracy, efficiency, or scalability in isolation, this work demonstrates how the synergistic interaction among scalable Big Data processing, advanced AI modelling, and iterative experimental validation jointly drives performance improvements and innovation. The experimental results reveal consistent trends across multiple dimensions: accuracy improvement, processing time reduction, error minimisation, and performance scalability, providing comprehensive empirical evidence that the integration of these technologies produces compounded benefits beyond what standalone approaches can achieve.

Furthermore, this study introduces innovation impact as a measurable, evolving outcome of AI- and data-driven experimentation, which is rarely explicitly quantified in prior research. By linking technical performance indicators (accuracy, error rate, processing time, and data scalability) to an innovation impact index, the research offers a novel perspective on how iterative AI-driven experimentation translates into tangible innovation gains in science and engineering. This contribution advances existing

literature by moving beyond conventional performance evaluation and highlighting innovation as a dynamic process enabled by continuous learning, large-scale data utilisation, and intelligent model refinement. As a result, the proposed framework offers both theoretical and practical novelty, providing a transferable model for future AI- and Big Data-driven research aimed at achieving sustained, high-impact innovation.

4. Conclusion

This study has presented a comprehensive AI, Machine Learning, and Big Data-driven research framework designed to support innovation in science and engineering through an integrated, end-to-end approach. The experimental results demonstrate that the proposed framework consistently improves key performance indicators, including predictive accuracy, computational efficiency, error reduction, and scalability as data volume increases. The comparative analyses confirm that AI-based models achieve superior accuracy and faster error minimisation, while Machine Learning approaches provide stable, reliable performance improvements, and Big Data infrastructure plays a critical enabling role in handling large-scale, data-intensive experimentation. Moreover, the findings reveal that AI-driven methods significantly reduce processing time compared to traditional approaches, enabling faster experimentation cycles and more efficient use of computational resources. The scalability analysis further shows that performance gains increase nonlinearly with data size, underscoring the importance of large, diverse datasets for maximising the effectiveness of data-driven models. Notably, the introduction and evaluation of an innovation impact index demonstrate that innovation outcomes improve progressively through iterative experimentation, emphasising that innovation is a cumulative and dynamic process supported by continuous learning and optimisation. Overall, this research contributes both methodological and empirical value by demonstrating how the synergistic integration of AI, Machine Learning, and Big Data can move beyond incremental performance improvements toward sustained and high-impact innovation. The proposed framework provides a transferable and adaptable foundation for future research and real-world applications in complex scientific and engineering domains. Future work may extend this framework by incorporating domain-specific knowledge, real-time data streams, and advanced explainable AI techniques further to enhance robustness, interpretability, and practical impact.

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