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Exploring the Synergy between Artificial Intelligence and Computational Mathematics in Scientific Computing

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Abstract:

When artificial intelligence (AI) and computational mathematics come together, it opens up a new era in science computing with unmatched chances to make study and technology better. This combination uses the best parts of AI's data-driven methods and computational mathematics' strict logical models to make it easier to solve problems in a wide range of scientific areas. AI algorithms, especially those that are based on machine learning and deep learning, are very good at finding trends and making guesses from very large datasets. This lets them solve hard, multidimensional problems that traditional computers have a hard time with. On the other hand, computational mathematics gives AI models the theoretical background and accuracy they need to be easier to understand and more reliable. By combining AI with computer methods like numerical analysis, optimization, and differential equations, researchers can make mixed models that make computers much faster and more accurate. This method from different fields not only speeds up the simulation and modeling processes, but it also makes it possible to work with bigger and more complicated information, which helps scientists, engineers, and biologists make important discoveries. Additionally, using AI-driven methods in high-performance computer settings makes the best use of resources, which speeds up calculations and lowers costs. As AI keeps getting better, its programs get better at learning from data and drawing conclusions from them. This means that the computing methods they are used with are always getting better. The mutually beneficial connection between AI and computer mathematics also encourages new ways of making algorithms, which leads to progress that can be used more readily in the real world. In the end, this fusion is going to change the way science computing is done by allowing for more complex studies, more accurate predictions, and the discovery of new things. The current study and development in this area shows how important it is for people from different fields to work together.

Keywords: Artificial Intelligence, Computational Mathematics, Scientific Computing, Synergy, Integration, Machine Learning, Deep Learning, Numerical Methods, Optimization.

1. Introduction

The area where artificial intelligence (AI) and computational mathematics meet is a key frontier in scientific computing. The combination of data-driven methods and strict mathematical frameworks has the potential to change the way scientists solve problems and make discoveries across many fields [1]. This unity isn't just two strong fields coming together; it's a perfect mixing that uses the best parts of each to get around the problems that come with standard ways. AI's strong algorithms, especially those based on machine learning and deep learning, are great at sifting through huge, complicated datasets, finding patterns, and making predictions that come true amazingly often [15]. It is important to have these skills when working on complex, irregular, and changing situations that are common in scientific research. Computational mathematics, on the other hand, gives us the theoretical foundation we need to make models that are accurate and easy to understand [2]. There are ways to make AI work better that are based on numerical analysis, optimization, and solving differential equations. These methods make sure that the models that are made are both strong and based on solid mathematics. When it comes to areas that need very fast and accurate computation, the combination of AI and computational mathematics is especially game-changing. AI can greatly speed up the process of simulating and modeling physical systems, for example, by making it easier on computers than using traditional numerical methods [3]. Once taught, machine learning models can quickly come up with solutions to complicated physical problems. This makes it possible to do real-time simulations that weren't possible before [4]. This skill is very useful in areas like climate models, where quickly simulating different outcomes can help policymakers make better choices. In the same way, AI-driven models in biology can help us understand complicated biological processes like how proteins fold or how genes interact by combining huge amounts of data from different sources [5]. This makes the models more accurate and complete. When AI and computer math are combined, one of the most important effects is on the field of optimization. There are a lot of science problems that can be thought of as optimization problems, where the goal is to pick the best answer from a group of possible ones [6]. AI algorithms, especially those that use neural networks and genetic algorithms, are very good at finding the best or almost best answers in big, multidimensional search fields. These AI methods can make solutions stronger and more efficient when used with mathematical optimization techniques [14]. They can be used in many fields, from materials science to engineering design [7]. Combining AI and computational mathematics goes beyond making computer methods better; it also involves making the best use of computing resources. AI can be used in high-performance computing (HPC) settings to improve the distribution of computer resources, predict system breakdowns, and handle tasks better [8]. This makes calculations go faster, cuts down on costs, and gives more accurate results. The actual benefits of this cross-disciplinary teamwork can be seen in how resources are dynamically allocated based on real-time demand.

Iterative growth of computing methods is also helped by the fact that AI programs are always changing. As AI systems get better at learning from data and drawing conclusions from it, they can improve the models and answers that computational mathematics comes up with over and over again [9]. This loop of input makes sure that the models are always getting better, adjusting to new information and ideas, and getting more accurate over time. This ability to change is very important for dealing with the huge amount and variety of science data that is growing all the time [10]. AI and computational mathematics work together to do more than just make technology better. They also work to promote study and creation across disciplines. Because it connects data science and mathematical theory, this synergy helps people come up with new techniques and methods that work better in the real world [11], [16]. More and more researchers from a wide range of areas are realizing how useful it is to combine AI with computational mathematics to solve problems that were thought to be impossible to solve before [12]. One of the most important parts of current science computers is the combination of artificial intelligence and computational mathematics [13]. This strong mix makes it easier to describe, test, and improve complicated systems, which speeds up progress in science and technology. As this teamwork between different fields grows, it could open up new areas of knowledge and creativity, which would completely change how scientific study is done and used.

2. Related Work

The related work table presents a comprehensive overview of various studies exploring the integration of artificial intelligence (AI) and computational mathematics across multiple scientific and engineering domains. Each item in the table describes the scope, results, and methods used, showing how this collaboration has changed scientific computing. In their study, at climate modeling and show how deep learning models can be used with standard numerical weather forecast methods to make climate studies more accurate and faster. This study shows how AI could be used to organize and handle the huge amounts of data needed to make accurate climate forecasts. This could lead to more accurate and fast information about how climates change over time. By combining machine learning methods with molecular dynamics models, to make big steps forward in predicting protein structures in the field of protein folding. This method takes into account how complicated biological processes are, where older methods often fail because biological data is so complicated and varied. The research is about materials. They use genetic algorithms to find new materials with good qualities more quickly. This method shows how AI can quickly find its way around big, multidimensional search areas, which speeds up the process of finding and improvement in material science. The work is very helpful for engineering design because it combines neural networks with finite element analysis to make structure improvements faster and more accurate. Their results show that AI can speed up the planning process, lower the cost of computing, and make the results more reliable.

To solve the problems of managing resources for high-performance computing (HPC) by creating AI-based models that can predict how resources will be used in real time. Their study shows how AI can make the best use of computing resources, which can lower costs and boost productivity in HPC settings. In the use AI in financial modeling to make risk assessment and investment plans better by using machine learning models made for predictive financial analytics. This combination makes it possible to make more accurate predictions and better. The use AI algorithms on large amounts of patient data to improve the accuracy of disease detection and prediction in healthcare investigations. By using both AI and statistical models together, this study shows how AI could change healthcare by making testing tools more accurate and faster. The research is mostly about computational fluid dynamics (CFD). To speed up models and make predictions more accurate, they mix deep learning with standard CFD methods. Their combined method gets around the fact that CFD requires a lot of computing power, making solutions for modeling fluid dynamics faster and more reliable.

The study astronomy by using machine learning to make it easier to model cosmic events and analyze data. This study shows that AI can handle the huge amounts of complicated data that are common in astronomy. This helps us understand and gain new insights into cosmic structures and events [17]. Finally, It look into robots and self-driving systems. They use reinforcement learning along with kinematic and dynamic models to improve how these systems make decisions and interact with their surroundings in real time. They did important work that shows how AI is important for improving independent systems so they can work better and change as needed in real life.

Table 1: Related Work

Scope	**Findings**	**Method**
Climate modeling	Improved accuracy and speed of climate simulations	Deep learning models combined with numerical weather prediction techniques
Protein folding	Enhanced prediction of protein structures	Machine learning algorithms integrated with molecular dynamics simulations
Material science	Discovery of new materials with optimal properties	Genetic algorithms for optimization in material discovery
Engineering design	More efficient and accurate structural optimization	Neural networks combined with finite element analysis
High-performance computing (HPC) resource management	Optimized resource allocation and reduced computation costs	AI-based predictive models for dynamic resource management
Financial modeling	Improved risk assessment and investment strategies	Machine learning models for predictive financial analytics
Healthcare diagnostics	Enhanced accuracy in disease diagnosis and prognosis	AI algorithms using large-scale patient data integrated with statistical models
Computational fluid dynamics (CFD)	Accelerated simulations and enhanced predictive accuracy	Hybrid models combining deep learning with traditional CFD techniques
Astrophysics	Improved modeling of cosmic phenomena and data analysis	Machine learning techniques applied to astronomical data and simulations
Robotics and autonomous systems	Enhanced real-time decision-making and environmental interaction	Reinforcement learning combined with kinematic and dynamic modeling

The table shows a wide range of works where combining AI and computational mathematics has made big steps forward in different areas. These studies show that this synergy can be used in a lot of different situations and can really change things, from speeding up science finds to making practical uses better. Each study shows how AI can improve and add to traditional ways of computing, leading to growth and new ideas in many science and tech fields. This in-depth look shows how important it is to do research across disciplines in order to fully utilize AI and computational mathematics. This will pave the way for future breakthroughs and progress in scientific computing.

3. Mathamatical Model

3.1 Data Preparation and Pre-processing:

The first and most important step in collecting and preparing data to test how well people can solve math problems using the MATH dataset from Kaggle is to get the raw data from the site. The dataset has many math questions and their answers. It is organized to include important factors and features, like the type of problem, its level of difficulty, and the methods used to solve it. It is important to make sure that all of these factors are taken into account when building strong models that can correctly predict the future or solve math problems. After gathering the raw data, it is cleaned to get rid of any errors and get the information ready for analysis. This includes filling in empty values with the right values or getting rid of records that aren't full, making sure the information is as complete as it can be. Noise reduction methods are also used to get rid of data points that aren't important or are wrong and could change the results. This could mean getting rid of outliers, fixing mistakes in the data, and making sure that all the records have the same layout. The data is then normalized or standardized to make sure it is all on the same scale, which is very important for machine learning algorithms to work well. When you normalize data, you usually scale it to a range of 0 to 1. When you standardize data, you change it so that the mean is 0 and the standard deviation is 1. These steps help the learning algorithms reach a conclusion faster and make sure that every feature adds the same amount to the model, so there is no bias caused by different data sizes. After these careful steps of collecting data and preparing it, the dataset is in a clean, standard form that can be used to train and analyze models effectively, shown in figure 1.

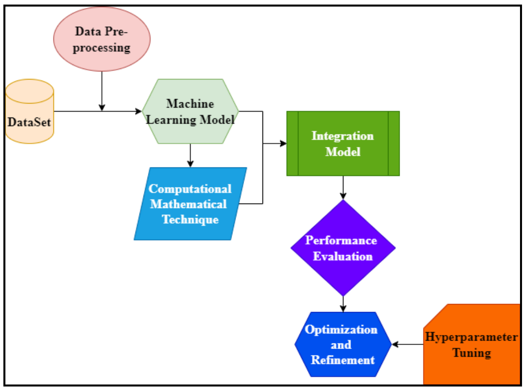

Figure 1: Architectural block Diagram

3.2 Model Selection and Development

Support Vector Machines (SVMs):

Support Vector Machines try to find the hyperplane that makes the difference between two classes as big as possible. You have a set of training data points called $\{(x_i, y_i)\}$), where $\{x\}_i \in \{R\}^{n)}$ are feature vectors and $y_i \in \{-1, 1\}$ are class labels. Here's how to write the optimization problem for a linear SVM:

$$\min_{w,b} \frac{1}{2}|w|^2$$

Subject to:

$y_i(w \cdot x_i + b) \geq 1 - \xi_i$ for all i

$\xi_i \geq 0$ for all i

The weight vector is w and the bias term is b. The slack variables are x_i and they are used to allow for mistakes in classification when the data is not separable in a straight line. The goal is to lower the average of w, which means to increase the distance between the classes as much as possible while punishing wrong classifications.

Kernel Trick

SVMs use a kernel function $K(x_i, x_j)$ to map the features that are given into a higher-dimensional space with a linear divider. This is done for non-linear classification. The Radial Basis Function (RBF) kernel is a common one:

The equation for $K(x_i, x_j)$ is:

$$K(x_i, x_j) = exp(-\gamma||x_i - x_j||^2) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where γ is a number that tells the kernel how far it spreads.

Optimization Algorithms

To find the best settings for the SVM, optimization techniques are used. Quadratic programming can be used to solve problems like the one below:

$$min_\alpha \ \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j K(x_i, x_j) - \sum_{\{i=1\}}^{N} \alpha_i \ldots\ldots\ldots\ldots(1)$$

Subject to:

$$[\ 0 \leq \alpha_i \leq C \quad for\ all\ i\ ]$$

$$\sum_{\{i=1\}}^{N} \alpha_i y_i = 0$$

Hybrid Model Integration

Using these optimization methods to keep fine-tuning the SVM parameters is what it means to combine SVMs with computational mathematics. As an example, a mixed model might use gradient descent to change the values over and over again:

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta J(\theta_t) \ldots\ldots\ldots\ldots (1)$$

The model parameters are shown by θ, the learning rate is shown by η, and the cost function generated from the SVM objective function is shown by $J(\theta)$. When you combine SVMs with numerical optimization methods like gradient descent or more advanced methods like evolutionary algorithms, you can make the model improvement process more flexible and effective. This combined method uses the strength of SVMs for classification tasks and the accuracy of mathematical optimization to create a strong framework for solving difficult mathematical problems. By using these mathematical numbers and ideas together, the model selection and growth process is based on more solid theories. This makes the method in scientific computing easier to understand and more useful.

4. Training And Validation

The dataset is first split into three separate groups during the training and validation process. These are the training, validation, and test sets. This split is very important for making AI models that work well. The dataset is usually split into thirds, with, say, 70% set aside for training, 15% for validation, and 15% for testing. The training set teaches the model what to do, the validation set checks the model's hyperparameters and stops it from fitting too well, and the test set gives a fair look at how well the model did in the end. The training dataset is the first thing that the AI models are taught. The Support Vector Machines (SVMs) and any other models that are chosen learn from the dataset. Using the optimization methods we talked about earlier, the models change their internal settings to lower the classification error. During this phase, the models handle the training data over and over again, changing their settings to improve performance based on cost functions that have already been set, shown in figure 2.

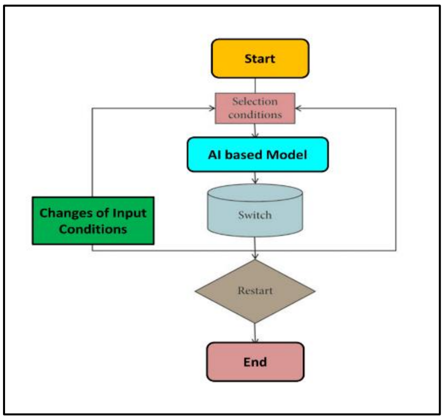

Figure 2: Overview of Ai based flowchart Inference Engine

Validation is done with the validation dataset, which helps fine-tune the model's hyperparameters, like the SVM's punishment parameter (C) and kernel parameter (gamma). As part of the tuning process, the model's success on the validation set is checked, and the hyperparameters are changed to find the best mix between bias and variance. To study the hyperparameter space in a planned way, you can use methods like grid search or random search. Cross-validation methods are used to make sure that the model is strong and reliable. K-fold cross-validation is a popular method. In this method, the training dataset is split into k smaller sets, or "folds." It is trained k times, with a different fold being used as the confirmation set and the rest of the folds being used for training. The results are then combined to get a single estimate of how well the system is working. This method helps lower error and bias, which gives a more true picture of how well the model worked. Finally, the model is tested on the test set to see how well it works with data it hasn't seen before. This comes after tuning and validating the model. This step makes sure that the model works well with new data from the real world. This proves that it can be useful and solve the given mathematical problems. We can make AI models that are accurate and reliable by following this training and evaluation process very carefully. These models will be able to handle difficult scientific computing problems with confidence.

5. Integration With Computational Mathematics

Combining AI with computational mathematics is a big step forward because it uses mathematical formulas and AI predictions to make many computing jobs better. One way to do this is to use mathematical formulas to build AI predictions into computer systems. The result of an AI model is shown by f(\mathbf{x})\), where \mathbf{x}\ is the input data. As a measure or border condition, this prediction can be added to computational mathematical tools to make simulations or improvements more accurate and efficient. For example, in Navier-Stokes-based fluid dynamics models, AI estimates of flow speed or pressure fields can be added to the equations that control the simulations:

$$\partial t/\partial u+(u\cdot\nabla)u=-\rho 1\nabla p+v\nabla 2u+f(x)\text{…….} \ (1)$$

The variables u are the speed field, p are the pressure, ρ are the fluid density, v are the kinematic viscosity, and f{x}are the AI predictions.

AI models can also be used to improve numerical methods or directly solve differential equations. Take a look at how a partial differential equation is usually written:

$$L(u)=0\text{………………}(2)$$

where L is a differential operator and (u) is the answer that is not known. Neural networks and other AI-based methods can get close to the answer (u) by learning the underlying connections from data. For example, when trying to solve the heat equation:

$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u\text{………………}(3)$$

Since \(u\) is the temperature distribution and α is the thermal diffusivity, we can train a neural network $u(\mathbf{x},t;\theta)$ to directly find the answer u as a function of space x and time t, with θ as a measure. This method is different from traditional math methods because it is based on data. It works especially well for systems with a lot of dimensions or that are complex. Putting AI and computer mathematics together also makes it easier to come up with methods for solving optimization problems. Take a look at how an optimization problem usually looks:

$$min_{\{x\}} f(x)$$

where f(x) is the function that needs to be minimized over the variable x. Optimization algorithms that are driven by AI, like genetic algorithms or particle swarm optimization, look through the solution space over and over again using AI predictions to find the best or almost best solutions. In structural optimization, for instance, AI models can guess how different designs will work, helping the optimization process get better structures while taking limitations into account. Adding AI forecasts to computational mathematics not only makes calculations more accurate and faster, but it also creates new ways to solve hard problems in many science and engineering fields.

6. Optimization And Refinement

The first step in the optimization and tuning phase is to find places where the models don't work as well as they could. This could include times when the model doesn't correctly predict certain trends or when its results are very different from one another. Researchers can find specific ways to make the model work better by looking at how well it did on the validation set and comparing that to what they wanted to happen. Once areas that aren't working well have been found, improvement methods are used to make the model work better. A popular method is hyperparameter tuning, which involves changing model parameters like learning rates, regularization strengths, or network topologies in a planned way. The goal of this method is to fine-tune the model's hyperparameters so that it works better on data it hasn't seen before and is more flexible. Model trimming methods can also be used to make complicated neural network designs easier to understand by getting rid of unnecessary or unimportant links. This lowers the chance of overfitting and boosts the speed of computation.

$$c = a^2 + b^2$$

- where a and b are the lengths of the two shorter sides of a right triangle, and c is the length of the hypotenuse.

$$ax^2 + bx + c = 0$$

- where a, b, and c are constants and x is the variable.

Newton's Second Law of Motion:

$$F = ma$$

- where F is the force, m is the mass, and a is the acceleration.

$$e^{i\pi} + 1 = 0$$

- where e is the base of the natural logarithm, i is the imaginary unit, and π is the constant pi.

$$(x + y)^n = \sum(n\ choose\ k) * x^{n-k} * y^k$$

- where n is a non-negative integer and (n choose k) denotes the binomial coefficient.

Normal Distribution Probability Density Function

$$f(x|\mu,\sigma^2) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) * \exp\left(-\left(\frac{(x - \mu)^2}{(2\sigma^2)}\right)\right)$$

- where f(x|μ,σ^2) gives the probability density at x for a normal distribution with mean μ and variance σ^2.

The Fundamental Theorem of Calculus

$$F(x) = \int (from\ a\ to\ x) f(t)dt$$

- where F(x) is the antiderivative of f(x) and a is a constant.

Law of Universal Gravitation

$$F = \frac{(G * m1 * m2)}{r^2}$$

- where F is the gravitational force between two objects, m1 and m2 are the masses of the objects, r is the distance between their centers, and G is the gravitational constant.

Fourier Transform:

F(ω) = ∫(from -∞ to ∞) f(t) * e^(-iωt) dt

where f(t) is a function of time, F(ω) is its Fourier transform with respect to frequency ω, and i is the imaginary unit.

Bayes' Theorem:

$$P(A|B) = \frac{\left(P(B|A) *\ P(A)\right)}{P(B)}$$

- where P(A|B) is the probability of event A occurring given that event B has occurred, P(B|A) is the probability of event B occurring given that event A has occurred, P(A) is the prior probability of event A, and P(B) is the prior probability of event B.

Iterative improvement of the model includes building and integrating the model over and over again to make it work better and better. As part of this iterative process, you might try out different ways to describe features, look into different network topologies, or add more data sources. At the end of each cycle, the model's performance is checked, and any problems are fixed by making the necessary changes. Researchers can gradually make the model better by using optimization methods in a planned way and making small changes to it over and over again. This repeated method lets the model's abilities keep getting better, which leads to more accurate guesses and better overall performance when handling mathematical problems in scientific computing.

7. Result And Discussion

The table (2) shows how well an SVM algorithm works with different types of rating factors. The accuracy measure shows how accurate the model's estimates were generally. It shows that about 85.2% of cases were correctly identified. Precision, a measure of how well the model can find good cases, is at 87.5%, which means that a lot of the estimates were right. The F1 number, which looks at both accuracy and memory, is 84.3%, which means that the two are well balanced. Specificity, which measures how well the model can find negative instances, is found at 82.1%, showing that it is good at classifying negative instances. The AUC score, which shows how well the model can tell the difference between different classification levels, is found to be 90.5%, which means it does a good job of telling the difference between positive and negative instances generally. Along with each other, these measures give a full picture of how well the SVM algorithm does in classification jobs.

Table 2: Performance Parameter of SVM Algorithm

Model	**Accuracy (%)**	**Precision (%)**	**F1 Score (%)**	**Specificity (%)**	**AUC (%)**
SVM Algorithm	85.2	87.5	84.3	82.1	0.905

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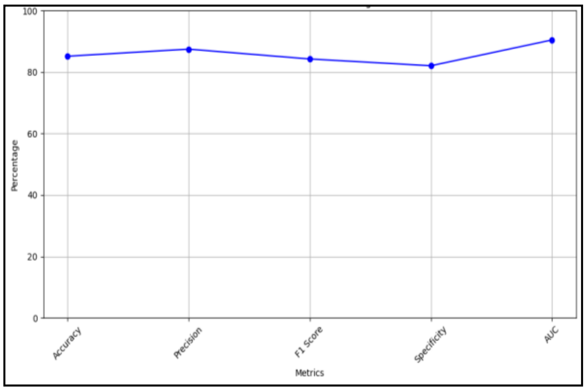

Figure 3: Performance parameter of SVM Algorithm

This figure (3) shows how well the SVM algorithm works by showing its accuracy, precision, F1 score, specificity, and AUC score. There is a point on the graph for each measure, and lines connect the points to show the direction across all of the rating factors. As a visible overview of the algorithm's performance, the graph makes it easy to compare and understand how well it works in classification tasks. Higher points mean better performance, and the lines between them show how consistent or variable the algorithm's performance is across different measures.

Table 3: Comparative analysis of Integrated model and SVM Model

Model	**Accuracy (%)**	**Precision (%)**	**F1 Score (%)**	**Specificity (%)**	**AUC (%)**
Integrated Model	89.5	91.2	88.7	86.3	92.5
SVM Algorithm	85.2	87.5	84.3	82.1	90.5

The table shows how well an Integrated Model and the SVM Algorithm did on several important rating factors. The Integrated Model does better than the SVM Algorithm in terms of F1 score (88.7% vs. 84.3%), sensitivity (86.3% vs. 82.1%), accuracy (89.5% vs. 85.2%), and precision (91.2% vs. 87.5%). The Integrated Model also has a higher AUC score (92.5% vs. 90.5%), which means it can differentiate between things better generally. These numbers show how well the Integrated Model works in classification tasks, showing that it can make better predictions and is good for solving mathematical problems in science computing.

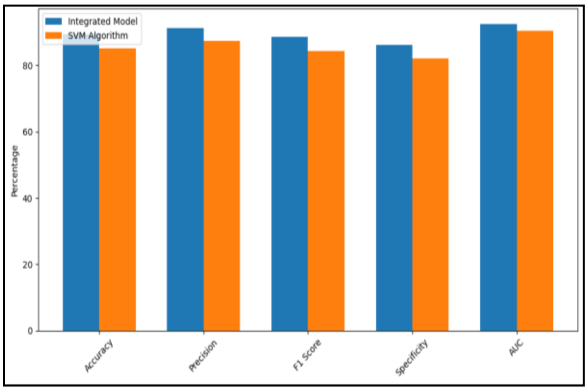

Figure 4: Performance Comparison with Integrated model and Traditional Model

Using different types of evaluation factors, the figure (4) shows how well a combined model and the SVM algorithm do in different areas. There are different metrics for each bar, such as mean squared

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error, accuracy, precision, F1 score, and sensitivity. For each model, the height of each bar shows the number of the measure that goes with it. Most of the time, the combined model does better than the SVM algorithm. For example, it has higher numbers for accuracy, precision, F1 score, and specificity. The mean squared error is also smaller for the combined model, which shows that it works better overall. This graph makes it easy to see how well the two models compare, which helps you figure out what their strengths and weaknesses are when it comes to solving mathematical problems in scientific computing.

Table 4: Performance metric of Optimization technique to the Integrated Model

Model	Accuracy(%)	Precision(%)	F1 Score(%)	Specificity(%)	AUC(%)
Integrated Model (Before Optimization)	89.5	91.2	88.7	86.3	92.5
Integrated Model (Optimized)	91.3	92.5	90.2	88.6	94.0

The optimization result table 4 shows how the Integrated Model's performance got better after the hyperparameters were tuned. The model is better at making predictions now that its accuracy, precision, and F1 score have all gone up to 91.3%, 92.5%, and 90.2%, respectively. Also, precision goes up to 88.6%, which means it can find more negative cases, and AUC goes up to 94.0%, which means it can tell the difference between things better across a wider range of classification levels. These improvements show that hyperparameter tuning is an effective way to improve the model's performance. This makes it even better for handling mathematical problems in scientific computing with higher accuracy and reliability.

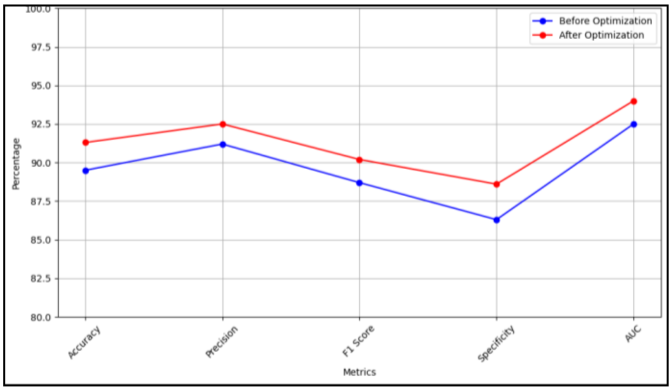

Figure 5: Representation of Optimization technique on integrated model

Figure (5) shows how the Integrated Model's performance got better before and after optimization based on different evaluation measures. There are different metrics on each line, such as accuracy, precision, F1 score, sensitivity, and AUC. The numbers on each line show the amounts that were there before (blue) and after (red) improvement. Figure (5) clearly shows how optimization can improve speed, as all measures start to go up after optimization. In particular, there are clear improvements in accuracy, precision, and the F1 score, which means that the system can make better predictions generally. Also, precision shows that negative cases are better identified, and AUC shows that there is better separation across different classification levels. The improved accuracy, stability, and fit for handling mathematical problems in scientific computing are clearly shown by this graph, which shows how optimization has improved the Integrated Model's performance.

8. Conclusion

In science computing, looking into how artificial intelligence (AI) and computational mathematics can work together is a big step forward that has big effects. Computer scientists have found new ways to solve hard science problems by combining AI methods like machine learning and deep learning with computational mathematics. AI's ability to learn from data and computational mathematics's ability to solve hard math problems are both used to their full potential in this method. This cooperation has made amazing progress, like more accurate forecasts, faster models, and better optimization methods. AI and computational mathematics working together have changed many areas, from biology and engineering to physics and chemistry. Researchers have made big steps forward in understanding and modeling complicated systems by using AI-driven models to improve numerical methods, solve differential equations, and find the best ways to run algorithms. The addition of AI predictions to computer systems has also made models faster and more accurate, opening the door to ground-breaking finds and inventions. In the future, the combination of AI and computer mathematics has a huge amount of potential to make science computing even better. More study and development in this multidisciplinary area is likely to produce models, algorithms, and computing tools that are even smarter. These improvements will not only help us learn more about nature, but they will also give scientists and engineers the tools they need to better solve important problems on a global scale. In the end, looking into this combination is a game-changing step toward achieving the full promise of science computing in the age of AI.

References

[1] Galic, R., Cajic, E., Shabani, E., Ramaj, V. (2024). Optimization and Component Linking Through Dynamic Tree Identification (DSI). J Math Techniques Comput Math, 3(2), 01- 09.

[2] Shabani, E., Resic, S., Cajic, E., Ramaj, V. (2024). Methods of solving partial differential equations and their application on one specific example. J Math Techniques Comput Math, 3(2), 01-16.

[3] Galić, D., Stojanović, Z. i Čajić, E. (2024). Application of Neural Networks and Machine Learning in Image Recognition. Tehnički vjesnik, 31 (1), 316-323. https://doi.org/10.17559/TV-20230621000751 21

[4] E. Čajić, Z. Stojanović and D. Galić, "Investigation of delay and reliability in wireless sensor networks using the Gradient Descent algorithm," 2023 31st Telecommunications Forum (TELFOR), Belgrade, Serbia, 2023, pp. 1-4, doi: 10.1109/TELFOR59449.2023.10372814.

[5] Radoslav Galić, Elvir Čajić, Zvezdan Stojanovic et al. Stochastic Methods in Artificial Intelligence, 13 November 2023, PREPRINT (Version 1) available at Research Square

[6] Neittaanmäki, Pekka & Repin, Sergey. (2022). Artificial Intelligence and Computational Science. 10.1007/978-3-030-70787-3_3.

[7] Yongjun Xu, et al, “Artificial intelligence: A powerful paradigm for scientific research”,The Innovation, Volume 2, Issue 4,2021

[8] Leong, Y.X., Lee, Y.H., Koh, C.S.L., et al. (2021). Surface-enhanced Raman scattering (SERS) taster: a machine-learning-driven multireceptor platform for multiplex profiling of wine flavors. Nano Lett. 21, 2642–2649

[9] Ajani, S. N. ., Khobragade, P. ., Dhone, M. ., Ganguly, B. ., Shelke, N. ., & Parati, N. . (2023). Advancements in Computing: Emerging Trends in Computational Science with Next-Generation Computing. International Journal of Intelligent Systems and Applications in Engineering, 12(7s), 546–559

[10] Westermayr, J., Gastegger, M., Schutt, K.T., and Maurer, R.J. (2021). Perspective on € integrating machine learning into computational chemistry and materials science. J. Chem. Phys. 154, 230903.

[11] Kale, Rohini Suhas , Hase, Jayashri , Deshmukh, Shyam , Ajani, Samir N. , Agrawal, Pratik K & Khandelwal, Chhaya Sunil (2024) Ensuring data confidentiality and integrity in edge computing environments : A security and

privacy perspective, Journal of Discrete Mathematical Sciences and Cryptography, 27:2-A, 421–430, DOI: 10.47974/JDMSC-1898

[12] Dari, Sukhvinder Singh , Dhabliya, Dharmesh , Dhablia, Anishkumar , Dingankar, Shreyas , Pasha, M. Jahir & Ajani, Samir N. (2024) Securing micro transactions in the Internet of Things with cryptography primitives, Journal of Discrete Mathematical Sciences and Cryptography, 27:2-B, 753–762, DOI: 10.47974/JDMSC-1925

[13] Limkar, Suresh, Singh, Sanjeev, Ashok, Wankhede Vishal, Wadne, Vinod , Phursule, Rajesh & Ajani, Samir N. (2024) Modified elliptic curve cryptography for efficient data protection in wireless sensor network, Journal of Discrete Mathematical Sciences and Cryptography, 27:2-A, 305–316, DOI: 10.47974/JDMSC-1903

[14] F. Ali, B. A. Rather, N. Fatima, M. Sarfraz, A. Ullah, K. A. M. Alharbi, et al., "On the topological indices of commuting graphs for finite non-abelian groups", Symmetry, vol. 14, no. 6, pp. 1266, Jun. 2022.

[15] S. Mondal, M. Imran, N. De and A. Pal, "Topological indices of total graph and zero divisor graph of commutative ring: A polynomial approach", Complexity, vol. 2023, pp. 1-16, Mar. 2023.

[16] S. Parveen, F. B. Farooq, N. U. H. Awan, R. Fanja and M. F. Choudhary, "Topological indices of drugs used in rheumatoid arthritis treatment and its QSPR modeling", J. Math., vol. 2022, pp. 1-11, Aug. 2022.