

Atomic Orbital Search and Physics-Inspired Algorithms for Feature Selection: A Systematic Review

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Abstract

Data analysis involves feature selection to achieve better performance, increase the speed of the learning algorithm, and get more precise and comprehensible results. Physics models have been widely used to accelerate the search process over the solution space. Moreover, the flexibility of the search process enables flexibility in adapting to the specific problem at hand, for example, by tuning parameters to optimize feature selection for various kinds of problems, or datasets, or learning tasks. The paper investigates the Atomic Orbital Search (AOS) algorithm, which is based on the quantum mechanical formation of electron orbitals, for feature selection. According to the PRISMA 2020 guidelines, literature published from 2019 to 25 October was collected from the Scopus and Web of Science databases. After duplicate removal and multi-stage screening, only 34 studies that strictly focused on AOS algorithms and met the inclusion criteria were included in the qualitative and quantitative synthesis. This paper is a summary of the present developments and applications of the Atomic Orbital Search (AOS) algorithm. The literature review indicates that the publications for the AOS algorithm have grown from 1 in 2019 to 11 in 2024, with the highest number of citations in 2021, 336. Empirical studies reveal that the accuracy of the AOS-based models is always higher than that of any other models, and feature reduction is always greater than 50% with the classification accuracy always higher than reported by several studies. The AOS-based models also have certain drawbacks, such as parameter sensitivity, simulation-verification, and the lack of comparison with other models, including performance indicators and applicability to various datasets, which can make them less effective in practical use and reduce their applicability to a variety of situations. This review focuses on the feature selection using AOS and other physics-inspired optimization methods.

Keywords: Atomic Orbital Search, Feature Selection, Physics-Inspired Optimization, Metaheuristic Algorithms, Hybrid Optimization, Multi-Objective Optimization, Systematic Review.

1 Introduction

In the past, data analysis has been a ubiquitous topic in various domains of research and applications such as machine learning, pattern recognition, and decision-making. In many applications, including medical diagnosis, text mining, bioinformatics, IoT (Internet of Things) analysis, and security analysis, a large volume of data is available, the vast majority of which is irrelevant. Such characteristics may cause misclassification, regression, and clustering models to be less accurate, more complex, and less interpretable. One issue in pre-processing is feature selection, which plays an important role in selecting the most relevant features and can contribute to better performance. Feature selection can be used to reduce the complexity by removing unnecessary features (Faramarzi et al., 2020). Feature Selection can be thought as the task of finding the optimum subset of features. The problem produces a feature space that has many combinations of features. The objectives are not clearly stated. The traditional approach has difficulty finding an optimal set of features, due to the large number of features that can be searched and the lack of guiding goals. However, when there is feature dependency or a large feature space, the traditional approaches are severely hampered by identifying the relevant features and making suboptimal selections. Feature selection is done using search-based techniques. New search strategies are powerful, flexible, and can avoid falling in the local optima, allowing them to explore complex feature spaces and to make the selection of the features accurately. The strategies are successful in traversing the search space. The methods have been proven to be effective in complex feature selection tasks, both supervised and semi-supervised (Abd Elaziz et al., 2022).

Salawudeen et al., (2021) state that metaheuristics could be categorized based on their inspirations. The trigger could be a process, a concept in nature, a physical concept, and/or Physics-Based Optimization Algorithms (PIOA). Some physical phenomena are modelled using physics-inspired algorithms and approaches, such as energy transfer, force interactions, physics of equilibrium, and probabilistic transition. The algorithms essentially follow a paradigm, which translates certain physical principles into solution-exploration procedures. Some examples of these metaheuristics include the Arithmetic Optimization Algorithm (Abualigah et al., 2023), the Equilibrium Optimizer (Faramarzi et al., 2020), the Big Bang-Big Crunch (BB-BC) algorithm, and Atom Search Optimization (Zhao et al., 2019).

This survey categorizes atomic orbital search as a physics-inspired optimization algorithm and, hence, as the focus of this review. Figure 1 shows the taxonomy of representatives of the Physics-Inspired Optimization Algorithms (PIOAs) category, which clearly highlights the multitude of physics-inspired paradigms at various levels of abstraction. It can be seen from figure 1 that PIOAs can be categorized into representatives inspired by the concept of thermodynamics (for instance, simulated annealing), representatives inspired by the concept of gravity and forces (for instance, GSA), representatives inspired by the concept of fluid (for instance, FDA), representatives inspired by the concept of equilibrium chemistry (for instance, EO), representatives inspired by the concept of nuclear physics (for instance, nuclear reaction optimization), and representatives inspired by the concepts of atomic and quantum levels (for instance, ASO and atomic orbital search) (Faramarzi et al., 2020).

Among these approaches, Atomic Orbital Search (AOS) has emerged as a physics-inspired metaheuristic. In AOS, a potential solution is treated as a state of an electron orbiting a nucleus in an atomic orbit. Based on energy states and random quantum leaps, the electron's path is determined, guiding the search process in the solution space (Elaziz et al., 2021). AOS has attracted considerable attention from researchers and practitioners and has been applied to solve different real-life problems. Feature selection and optimization problems are interesting settings in which candidate solutions can be

sorted by feature values (i.e., quantized energy levels), and the AOS algorithm can be run in a reduced dimensionality without loss of performance. In addition to basic AOS, several improved versions have been proposed in the literature, including evolutionary, opposite-based, chaotic, Lévy-flight search, and hybrid approaches (Karakas & Latifoğlu, 2022; Chao et al., 2026). This special issue also invites high-quality scientific contributions that address AOS applications in real-world problems such as healthcare analytics, engineering applications, optimization of IoT systems, clustering, security problems, and other relevant domains.

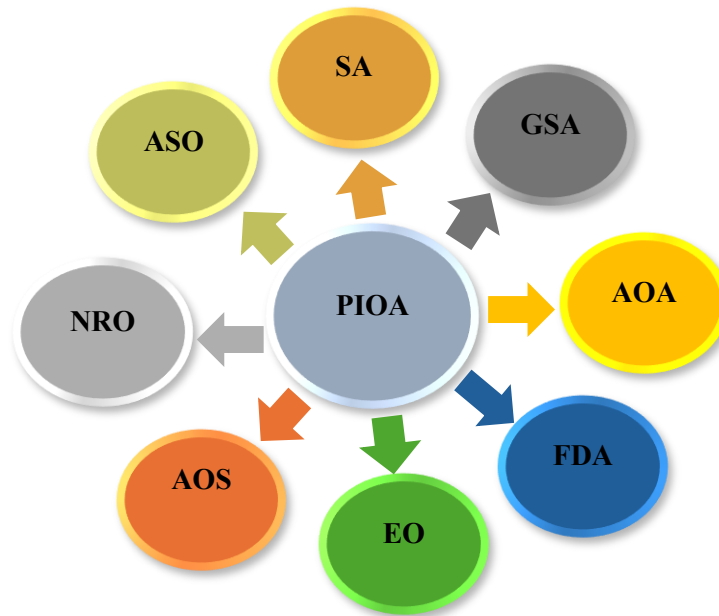


Figure 1: Classification of PIOA algorithms

The Survey of Atomic Orbital Search (AOS) literature reveals that the AOS papers are scattered across many sources. Most existing papers introduce new variants of the AOS algorithm; therefore, the literature lacks comprehensive information on the evolution of AOS, the relationships among the various versions, and comparisons with physics-inspired feature selection methods. In addition, while most reviews treat AOS as a metaheuristic alongside other algorithms, it does not provide a systematic, categorical survey of AOS and other physics-based feature selection methods. Thus, there is a need for a study regarding AOS and physics-based algorithms for feature selection. This study offers a review, a taxonomy, and a critical evaluation of atomic orbital search and physics-inspired algorithms for feature selection. The contribution of this work includes:

1. Presenting a systematic review of current literature, using AOS approaches for feature selection, and discussing the results in the light of the PRISMA statements to guarantee transparency and reproducibility.
2. Organizing current AOS algorithms into standard, modified, and hybrid enhancements as well as multi-objective-based strategies.
3. Providing an empirical survey of trends in bibliometrics for research on Auditory and vestibular Otolaryngology and related areas, with a presentation of publication and citation data and a table with the information on the most highly cited and most frequently publishing journals, authors, institutions, and countries.

4. Synthesizing the application domains of AOS based on feature selection, with emphasis on the characteristics of the dataset and trends in empirical performance.
5. Propose research avenues in the future, emphasizing the potential applications in multi-objective optimization problems, large-scale feature selection, open-source reproducibility, and connection with modern learning paradigms.

The rest of this paper is as follows: Section 2 describes the review method, including the PRISMA-based analysis framework, rules for including and excluding studies, and the strategy for searching the literature. In Section 3, some statistics on publishing trends, citations, and the distribution of published papers across publishers, journals, institutions, and countries are provided as part of a bibliometric study on atomic orbital search research. In Section 4, atomic orbital search optimization is overviewed, and some algorithms are illustrated with their search procedures, time complexity, physical inspiration, and advantages and disadvantages. The AOS and its variants, namely Standard AOS, Hybrid AOS, and Multi-Objective AOS, are covered in Section 5. The application areas for AOS-based feature selection are presented in Section 6. Finally, Section 7 presents the challenges of AOS-based studies, and the study conclusions are demonstrated in Section 8.

2 Review Methodology

This review used an auditable protocol for planning, implementing, and presenting systematic literature reviews in computer science research. This protocol for planning and conducting systematic literature reviews was followed carefully and meticulously in this review to ensure a clear, auditable process. This review aims to analyse, appraise, and synthesize studies associated with the Atomic Orbital Search (AOS)-based feature selection. The process consists of 5 key phases:

- Formulation of research questions,
- Definition of the search strategy and study selection criteria,
- Evaluation of selected studies, and
- Data extraction, and
- Data synthesis.

The complete review process, from identifying the studies for review to including them, is shown in figure 2.

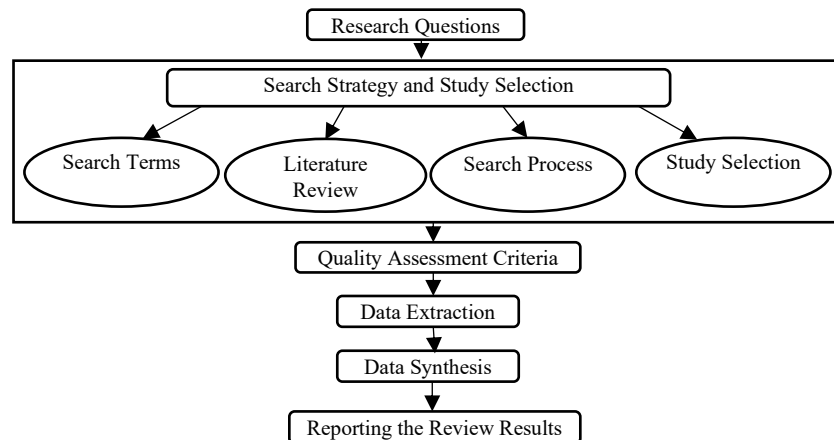


Figure 2: Steps of the review methodology

Research Questions

The objective of this literature review is to analyse and summarize all the literature available related to feature selection methods based on AOS. These research questions are designed in such a way that they would cover the progressions and applications of the discussed methodologies:

- RQ1: What are the bibliometric characteristics and research trends of Atomic Orbital Search (AOS) in the literature between 2019 and 2025?
- RQ2: What are the underlying physical inspirations, algorithmic mechanisms, computational properties, and inherent strengths and weaknesses of the Atomic Orbital Search algorithm?
- RQ3: Which variants of Atomic Orbital Search have been proposed? Additionally, how to classify various atomic orbital search algorithms into standard, modified, hybrid, and multi-objective search algorithms?
- RQ4: What application domains and problem scenarios have been tackled, and what is the achieved performance, for AOS-based feature selection methods?
- RQ4: In which application areas and problem situations has AOS-based feature selection been used? What performance results have been reported for AOS-based feature selection?
- RQ5: What trends and open research problems emerge when comparing AOS variants across different application areas?

Search Strategy and Study Selection

This review used a methodical approach to derive search terms in five stages, following recommendations for developing search terms in systematic reviews (Malhotra, 2020). The five stages are:

1. Extracting key terms from the defined research questions.
2. Determining synonyms and alternative spellings of the identified key terms
3. Researching and listing relevant keywords and themes from relevant studies.
4. Using “OR” with synonyms and spelling variation.
5. Combine Search Terms using "AND" to combine all search phrases.

These terms pertain to "Atomic Orbital Search and feature selection" evaluation. This study also employs feature selection, attribute selection, Atomic Orbital Search, Atom Search Optimization, and metaheuristic optimization. The last search query is as follows:

((“feature selection” OR “attribute selection”) AND (“Atomic Orbital Search” OR “AOS” OR “Atom Search Optimization”) AND (“metaheuristic” OR “meta-heuristic”))

The use of the search strategy was consistent across all available databases for bibliographic data. The literature search involved using Scopus and Web of Science to search literature between 2019 and 2025 relating to AOS and variations of feature selection. The initial set had $N = 410$, which was reduced to $N = 282$ after eliminating duplicates. Screening based on criteria removed literature in which only AOS served as a baseline, literature lacking feature selection, and literature consisting of surveys, short communications, or non-English literature. After screening, 38 articles were selected for detailed scrutiny; however, 4 were excluded because it was not based on AOS, leaving 34 that met all criteria

and were included in the qualitative synthesis. The search strategy used to select literature is shown in the flow diagram in figure 3, and details of the inclusion and exclusion criteria are provided in table 1.

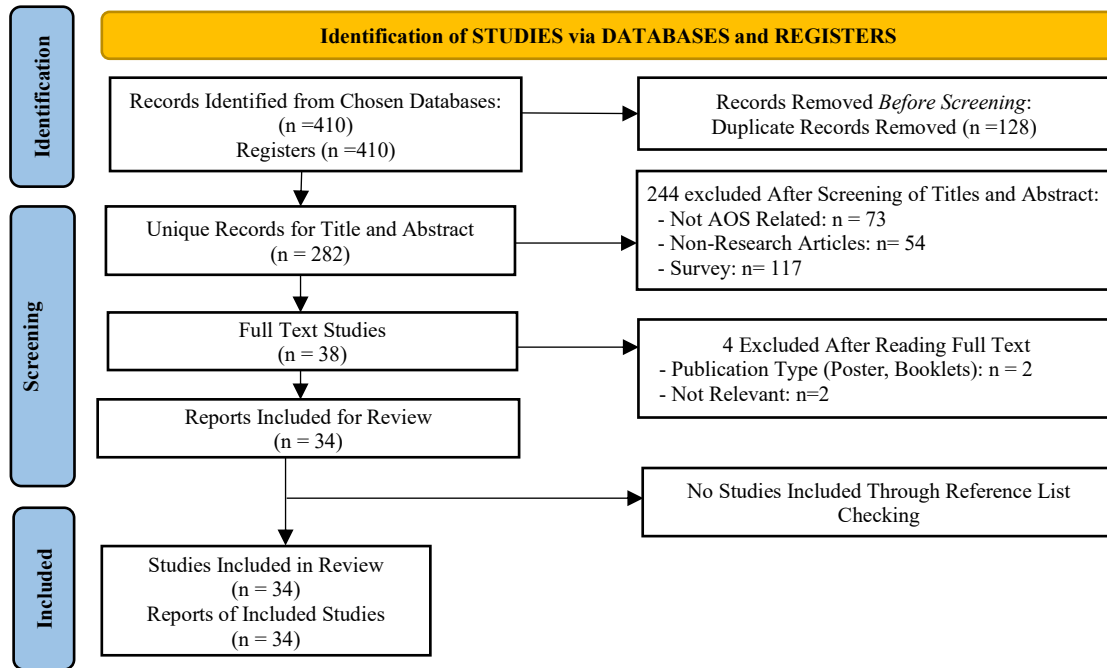


Figure 3: Study selection process

Table 1: Inclusion and exclusion criteria

| Inclusion Criteria | Exclusion Criteria |
|---|--|
| English-language papers | Non-English publications |
| Studies explicitly addressing the Atomic Orbital Search (AOS) for feature selection | Studies with no direct relevance to AOS-based feature selection |
| Papers that answer at least one research question of this review | Papers that do not address any of the defined research questions |
| Full-length papers (≥ 3 pages) | Short papers (< 3 pages) |
| Peer-reviewed journal articles | Conference papers, books, book chapters, editorials, and letters |

Quality Assessment

To ensure the credibility and relevance of the synthesized evidence, a quality assessment was conducted on the included studies. The quality assessment process examined aspects such as the relevance of the AOS-based approach proposed in the study, the quality of the study design, the use of either a benchmark dataset or real-world data, and the comprehensive presentation of data on study assessment metrics. Only peer-reviewed journal articles that met the minimum level of quality assessment criteria were selected. This quality assessment has been included to ensure the credibility of the final list of included studies.

Data Extraction

Relevant information has been extracted using a standardized data extraction form from among the included studies (n=34). The details extracted included publication information, the type of AOS used,

and the feature selection method. The application domain, datasets, learning models, evaluation methods, and performance measures were also recorded. A summary of the extracted details on AOS-based feature selection studies is presented in table 2.

Table 2: Categories and variables extracted from the included AOS-based feature selection studies

| Category | Extracted Variables | Purpose |
|-----------------------------|---|---|
| Bibliographic Information | Title, authors, year of publication, journal/publisher | Enables analysis of publication trends, temporal evolution, and distribution of AOS-based feature selection research. |
| Algorithmic Characteristics | AOS variant type (standard, binary, chaotic, hybrid, multi-objective), enhancement strategy | Identifies how Atomic Orbital Search has evolved for feature selection and supports taxonomy development (RQ1). |
| Feature Selection Type | Wrapper, hybrid filter, wrapper, embedded, unsupervised | Distinguishes the role of AOS within different feature selection paradigms and methodological frameworks (RQ1). |
| Application Domain | Healthcare, engineering, IoT, clustering, data mining, security, benchmarking | Captures the problem domains in which AOS-based feature selection has been applied (RQ2). |
| Evaluation Metrics | Accuracy, precision, recall, F-score, AUC, feature count, fitness value, silhouette score | Supports comparison of evaluation practices and performance reporting across studies (RQ3). |
| Key Findings | Empirical improvements, comparative rankings, validated advantages | Synthesizes major empirical contributions and insights derived from each study (RQ4). |
| Limitations | Premature convergence, parameter sensitivity, scalability constraints | Identifies reported weaknesses and challenges associated with AOS-based feature selection (RQ4). |
| Future Research Directions | Hybridization, multi-objective FS, large-scale datasets, reproducibility | Highlights open research gaps and opportunities for advancing AOS-based feature selection methods (RQ4). |

Data Synthesis

Data synthesis is where the collected data are summarized to answer the research questions raised. This process was examined from two perspectives. First, categorization of the papers using the AOS family taxonomy revealed that the papers were categorized into binary AOS, chaotic AOS, hybrid AOS, learning-based AOS, multi-objective AOS, and unsupervised AOS. Second, the studies were evaluated by application domain, enabling the synthesis process to reveal trends and performance across domains. The outcome of the data synthesis is expressed in a tabular form. The discussion section interprets the results across the sections. Each research question is dealt with within its corresponding section: RQ1 is dealt with in Section 3, followed by RQ2 in Section 4, then RQ3 in Section 5, followed by RQ4 in Section 6, and concluding with RQ5 in Section 7.

3 Atomic Orbital Search (AOS) Research Trends

Publication and Citation Trends

The publication and citation dynamics of Atomic Orbital Search (AOS) literature from 2019 to 2025 are shown in figure 4. After the inception of AOS, there were only one to three publications per annum until 2022. There has been a considerable increase in publication output from 2023 through 2024, as AOS has been widely adopted across domains ranging from scheduling to energy and power systems to artificial intelligence (Durmus et al., 2024; Noman et al., 2024). The citation dynamics follow a similar trend. There has also been a culmination in the citation for the AOS paper in 2021. There has also been an increase in citations for the AOS paper in 2024; however, it decreased in 2025, mainly because the relevant literature is not very old. Based on citation dynamics, it is concluded that AOS has evolved

from a conceptual metaheuristic into a mature optimization algorithm widely cited and adopted by researchers.

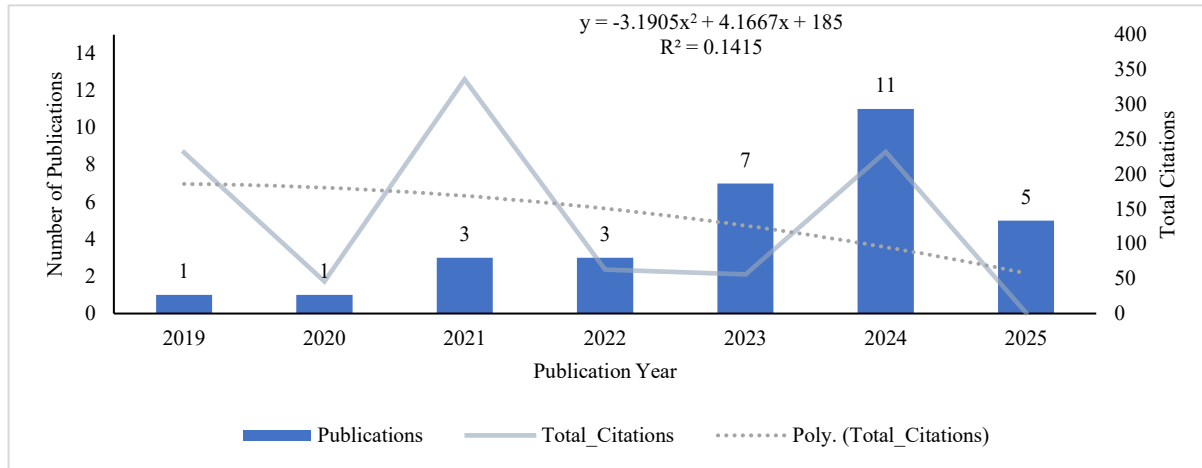


Figure 4: Annual citations of AOS papers

Keyword Co-Occurrence and Burst Detection

The keyword co-occurrence graph in figure 5 illustrates the thematic structure of research on AOS. The graph divides research work into five groups. Orbital, optimization, and search algorithms appear as key terms in the keyword co-occurrence graph. It indicates that AOS, which stands for Algorithmic Optimization Strategies, has applications in the evolution of search techniques and in optimization research. Other groups include applications of AOS in machine learning research and in learning and feature extraction. Other groups include applications in engineering design and the handling of constraints, such as optimizing structural components and improving design efficiency across various engineering projects. The keyword co-occurrence graph indicates that AOS has widespread applications across various fields. Links among various keywords suggest that AOS is a versatile technique with applications in computer science and practical settings.

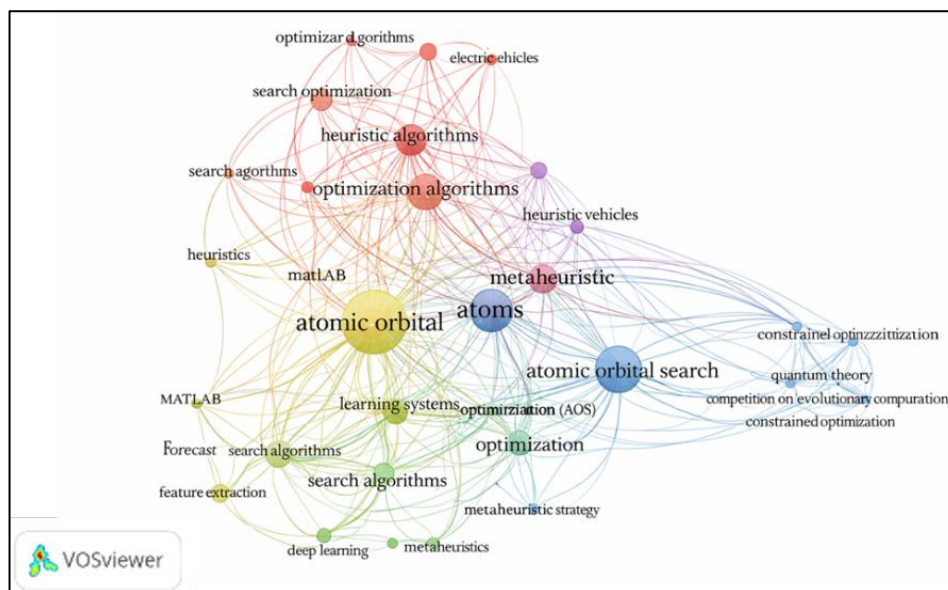


Figure 5: The network of keywords

Top Contributing Authors

In table 3 lists the five most successful and influential authors in atomic orbital search studies. The five most successful and influential researchers in atomic orbital search studies have a cumulative citation of 362, or an average of 90.5 per paper, addressing the validation of the research originally developed in AOS (Hussain et al., 2023; Iqbal et al., 2024). Siamak Talatahari from Iran has two studies with a cumulative citation count of 87 (an average of 43.5 per paper) and engages with the reference (Hussain et al., 2023; Azizi et al., 2022) in an early-influence manner. Adil Sarwar from India has two studies with a cumulative citation count of 85 (an average of 42.5 per paper), indicating early visibility and influence in their research. Iran remains at the forefront, with Turkey and India showing increased participation in this nascent technology. Iran appears as the leader in making initial contributions to atomic orbital search studies, with increased participation from India and Turkey. The citation indices of nearly all contributors here appear to be sufficiently high, indicating initial influence in atomic orbital search studies by a limited number of contributors.

Geographical Distribution of Publications

The publications on Atomic Orbital Search (AOS) included authors representing around 20 international countries, highlighting the international reach of the scientific efforts. Using VOSviewer for country co-authorship analysis with a minimum of 2 publications per country, the network showed clusters that were connected (Figure 6).

Table 3: Top 5 contributing authors

| Rank | Author | Documents | Citations | Avg. Citations | H-Index | Country |
|------|--------------------|-----------|-----------|----------------|---------|---------|
| 1 | Azizi, Mahdi | 4 | 362 | 90.5 | 4 | Iran |
| 2 | Talatahari, Siamak | 2 | 87 | 43.5 | 2 | Iran |
| 3 | Sarwar, Adil | 2 | 85 | 42.5 | 2 | India |
| 4 | Durmuş, Ali | 2 | 8 | 4.0 | 2 | Turkey |
| 5 | Karakose, Ercan A. | 2 | 8 | 4.0 | 2 | Turkey |

Among the collaborating countries for each publication involving multiple countries, Iran had the highest number of publications, with 13 (50.0%), followed by China with 9 (34.6%), the United Kingdom, and Russia, each with 7 (26.9%). Other prominent publishers included Saudi Arabia with 6 (23.1%), Mexico with 7 (26.9%), Egypt with 4 (15.4%), Italy with 3 (11.5%), and other countries, including Pakistan, the United Arab Emirates, and Japan, with 2 (7.7%) publications. Further, several other countries, including Germany, Malaysia, South Korea, Tunisia, and Turkey, each had only one publication (3.8% of publications). Analysis highlights that while the scientific investigation into atomic orbital search is dominated by a few highly productive international nations, such as Saudi Arabia and Mexico, there has been immense international collaboration that has enabled the field to grow so quickly, as evidenced by the diverse contributions from countries like Pakistan, the United Arab Emirates, and Japan.

Top Journals and Publication Venues

In table 4 shows the distribution of AOS-related papers published in some major journals. IEEE Access is the most-published journal, with a cumulative total of 4 papers, constituting the majority of the output. But given that this publication is categorized as a Q2 publication, has a quite wide scope, and, in 2022, had an impact factor of 3.9, its status indicates that it plays a particularly important role in publishing early AOS applications in engineering and computational circles. Other journals contain AOS-related papers and are categorized as having a high overall impact factor and as Q1. Some journals worth noting

include “Applied Mathematical Modeling” (impact factor 5.0), “Applied Soft Computing” (impact factor 8.7), and “Energy Conversion and Management” (impact factor 11.2). This figure is even higher than in other journals. PLOS ONE (impact factor 3.7 and a Q2 ranking) further indicates this work’s applicability in AOS across a whole range of disciplines. Taken as a whole, this analysis indicates that AOS is not merely getting mainstream notice in terms of output.

Table 4: Top 5 journal ranks

| Rank | Journal | Count | Country | IF (2022) | JCR (2022) |
|------|----------------------------------|-------|----------------|-----------|------------|
| 1 | IEEE Access | 4 | USA | 3.9 | Q2 |
| 2 | Applied Mathematical Modelling | 1 | Netherlands | 5.0 | Q1 |
| 3 | Energy Conversion and Management | 1 | United Kingdom | 11.2 | Q1 |
| 4 | Applied Soft Computing | 1 | Netherlands | 8.7 | Q1 |
| 5 | PLOS ONE | 1 | USA | 3.7 | Q2 |

4 Atomic Orbital Search (AOS) Algorithm

Atomic Orbital Search (AOS) by Azizi (Azizi, 2021) is an optimization technique developed using concepts of physics, specifically the atomic theory of quantum mechanics. The conceptual basis of AOS is the layered, quantized energy structure, which permits a natural equilibrium between exploitation and exploration. AOS capability is demonstrated in a population-based stochastic optimization method that treats each possible solution as an electron and a real-valued vector. Each candidate solution is represented as a d-dimensional vector (Equation 1); all solutions form the population matrix (Equation 2), and the fitness (energy) of each solution is evaluated using the objective function in equation 3.

$$X_i = [x_{i,1}, x_{i,2}, \dots, x_{i,d}], i = 1, 2, \dots, m \tag{1}$$

$$X = \begin{bmatrix} X_1 \\ \vdots \\ X_m \end{bmatrix} = \begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,d} \\ \vdots & \ddots & & \vdots \\ x_{m,1} & x_{m,2} & \dots & x_{m,d} \end{bmatrix} \tag{2}$$

$$E_i = f(X_i) \tag{3}$$

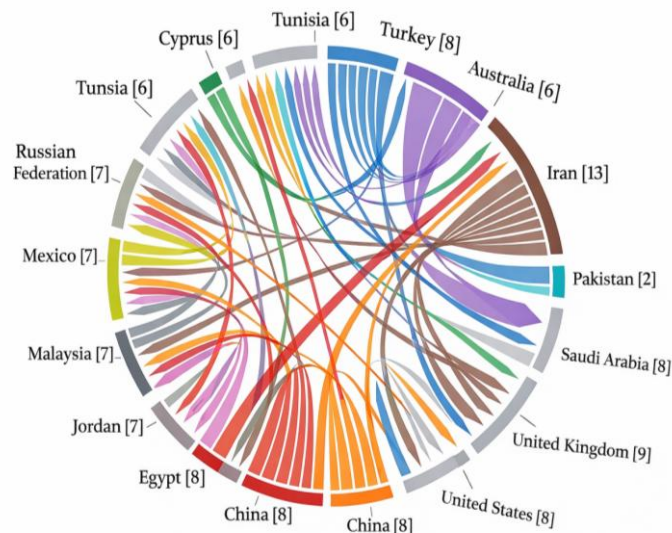


Figure 6: Collaboration network analysis of countries/regions

To imitate the atomic structure, the AOS method uses the probability density function to distribute the solutions into the orbital layers. And then, the solutions are sorted by energy. The better solutions are assigned to the inner orbitals, and the worse solutions are assigned to the outer orbitals. The binding state and binding energy for each layer are defined in equation (4) and equation (5), while the global binding state and energy are defined in equation (6).

$$BS_k = \frac{\sum_{i=1}^p x_i^k}{p}, \quad \begin{cases} i = 1, 2, 3, \dots, p \\ k = 1, 2, 3, \dots, n \end{cases} \quad (4)$$

$$BE_k = \frac{\sum_{i=1}^p E_i^k}{p}, \quad \begin{cases} i = 1, 2, 3, \dots, p \\ k = 1, 2, 3, \dots, n \end{cases} \quad (5)$$

$$BS = \frac{\sum_{i=1}^m X_i}{m}, \quad BE = \frac{\sum_{i=1}^m E_i}{m} \quad (6)$$

The parameter represents the probabilistic transition mechanism governing the AOS algorithm's search behavior. If the energy absorbed exceeds a certain level, a photon-electron collision is initiated, intensifying the search. In particular, equation (7) gives the photon-electron collision that generates photons to explore promising areas of the search space. On the other hand, equation (8) explains the photon absorption process that helps exploration through the update of potential solutions, while the use of equation (9), a random interaction approach, keeps the population diversity.

$$X_{k,i}^{new} = X_{k,i} + \alpha_i(\beta_i LE - \gamma_i BS) \quad (7)$$

$$X_{k,i}^{new} = X_{k,i} + \alpha_i(\beta_i LE_k - \gamma_i BS_k) \quad (8)$$

$$X_{k,i}^{new} = X_{k,i} + r_i \quad (9)$$

The computational and memory complexities are also determined as $O(T(m \log m + md))$, and $O(md)$. AOS demonstrates strong performance in optimization and feature selection problems, although it is sensitive to parameter settings and requires careful tuning.

5 Variants of the Atomic Orbital Search (AOS) Algorithm

In figure 7 gives the taxonomy for all the different Atomic Orbital Search (AOS) algorithms. This taxonomy outlines the development process of the basic algorithm into the modified, hybrid, and multi-objective versions. The taxonomy is then divided, and each type of AOS algorithm is considered. The importance of the different types of AOS algorithms relative to the basic quantum-inspired search algorithm and how it overcomes different limitations and needs is emphasized.

Standard Atomic Orbital Search (AOS) Algorithm

Atomic orbital search (AOS) optimization is a physics-inspired optimization technique discussed in (Iqbal et al. 2024) and based on principles of quantum atomic physics. Candidates for solution are represented as electrons that revolve around a nucleus and are placed in quantum energy levels determined by the value of an objective function, which makes up a self-organizing population that resembles atomic orbitals. The process of searching proceeds through electrons' transition from one energy level to another. Excitation implies searching (exploration), while de-excitation shows that the solution is about to be found. The process depends on the current energy level of the electron and the likelihood of emitting a photon. The basic algorithm of AOS locates a global optimum in simple benchmark problems. Several modifications have been introduced to enhance AOS's performance and versatility.

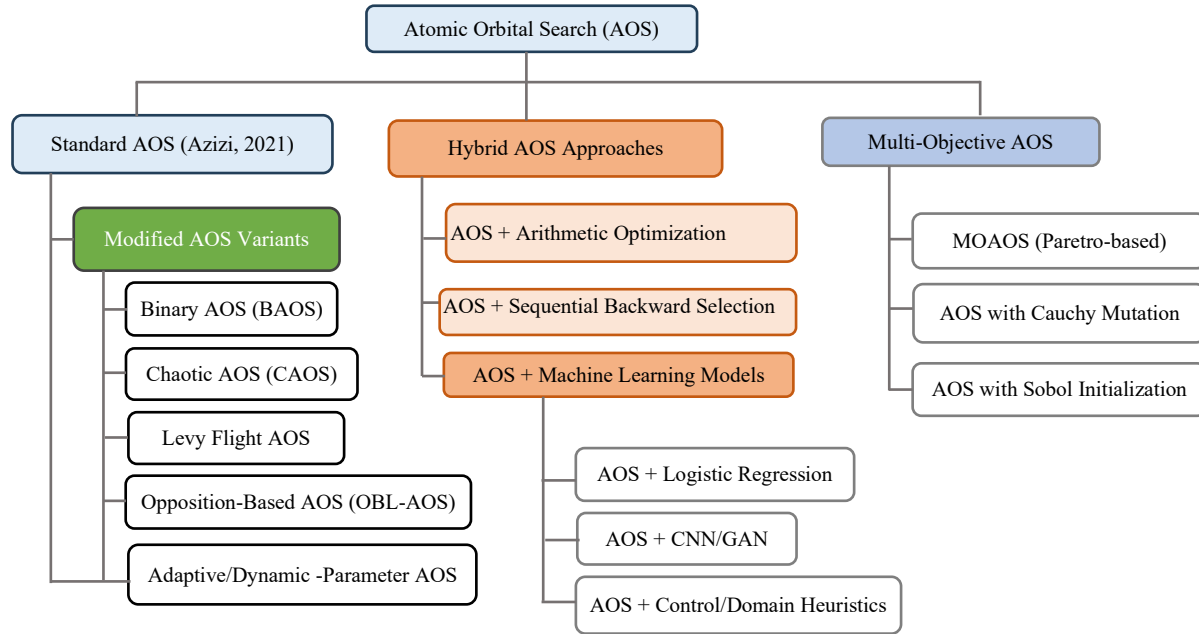


Figure 7: Structured taxonomy of atomic orbital search (AOS) variants

Revised and Improved Editions of AOS

The studies validated the basics of AOS and revealed slow evolutions and sensitivity to parameters. The atomic orbital structure (AOS) calls for enhanced iterations. Opposite-based learning uses search spaces on the opposite sides of the search region for better diversification of the starting point population (Abd Elaziz et al., 2022); hence, the process will benefit from better exploration of possible solutions (Zafar et al., 2021). Energy update: Energy controls the search space. The energy transition algorithm uses energy levels to determine whether to move to another place or raise (Hussain et al., 2023). Additionally, adaptive updating and convergence control enhance the convergence of the optimization processes, whereas chaos and Levy flight improve global search by promoting both exploration and exploitation in the search space (Manita et al., 2023; Revanesh et al., 2023). Thus, fundamental AOS and other optimization methods improve accuracy, convergence, and objective function values.

Hybrid Variants that Combine AOS with Other Methods

AOS is used as the core optimization engine along with other optimization or machine learning techniques to identify the solution. AOS is responsible for global and local search in the solution space. In contrast, other optimization techniques are used to gain domain knowledge of the problem and accelerate the solution-finding process. As a result, hybrid models like Capsule GAN (Zhang et al., 2023) and logistic regression (Elaziz et al., 2021) have shown better classification performance. For hybrid models, AOS is combined with crossover and mutation operators inspired by PSO, genetic algorithms, and the arithmetic optimization algorithm (Abd Elaziz et al., 2022). Integrating an AOS into engineering and scheduling heuristics for solving optimization problems has been studied extensively in recent years to improve solution quality and running time. This paper tackles a complex multi-criteria optimization problem to design a practical and efficient scheduling model for prioritized jobs with due dates across multiple production lines with limited capacity.

AOS Extensions for Multiple Objectives

Recently, multi-objective AOS methods have been developed to address problems involving multiple criteria. As noted in (Asna et al., 2022; Zhang et al., 2023), multi-objective AOS involves multiple energy values, and multi-objective optimization employs methods such as Cauchy mutation and Sobol sequence sampling to identify Pareto-optimal solutions and avoid being trapped in local optima. The multi-objective developments of AOS confirm AOS's ability to address multi-criteria optimization problems. Hence, AOS can be used in cases where a decision must be made based on multiple criteria. As shown in figure 8, the accuracy of all algorithms increases, and the modified AOS version clearly has higher accuracy than the basic AOS version. Also, most hybrid versions of AOS achieved accuracy above 95%. On the other hand, PSO, GA, and GWO yield less accurate results, underscoring the advantages of hybridization and improved methods for the feature selection problem and AOS, particularly in applications such as image recognition, data classification, and predictive modeling.

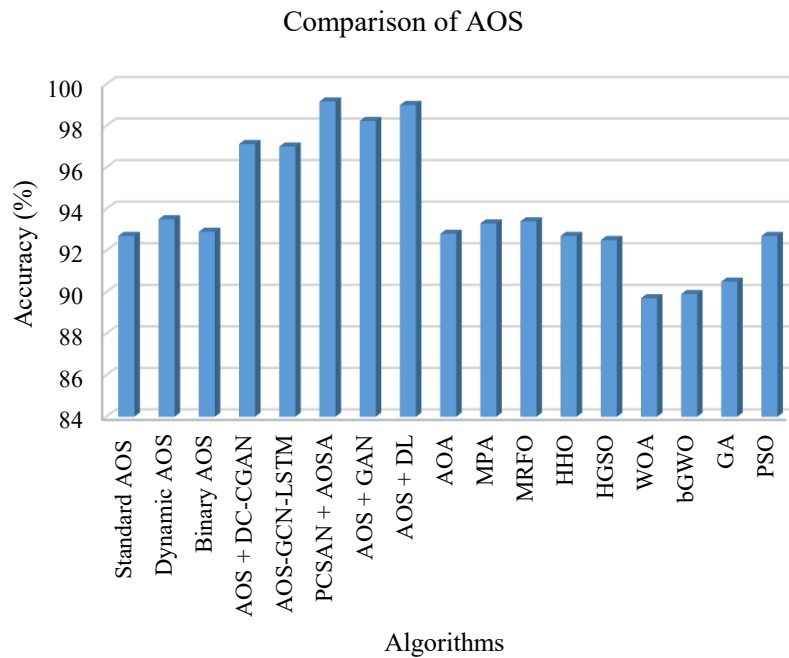


Figure 8: Performance comparison of AOS with other algorithms

6 Key Application Areas and Benchmark Problems

Many previous works applied the Atomic Orbital Search (AOS) and its derivatives to solve a range of optimization problems and benchmark instances. The objective was to prove the searching capabilities of AOS by performing tests on representative benchmark problems and implementing AOS and variants of AOS to practical optimization problems. This sub-section presents a summary of AOS-based optimization algorithms and their application, including representative benchmarking problems and results, presented in table 5.

Table 5: Applications of atomic orbital search and physics-inspired algorithms

| Study | Algorithm Type | Role of AOS | Hybridization | Baseline / Comparators | Key Search Enhancements |
|-----------------------------------|-----------------------|---------------------------|----------------------------|---------------------------------|--------------------------------|
| Durmus et al., (2024) | AOS | Parameter optimization | None | GA, PSO | Orbit energy update |
| Noman et al., (2024) | Binary AOS | Hyperparameter tuning | CNN + Lévy flight | Evolutionary CNNs | Lévy flight boosting |
| Iqbal et al., (2024) | Adaptive-AOS | Network optimization | Battery storage | GA-based NR | Adaptive layer selection |
| Hussain et al., (2023) | AOS | Control optimization | MPPT controller | PSO, INC | Fast convergence |
| Ali et al., (2023) | AOS | Parameter extraction | PV diode models | GA, ABC | Accurate fitness reformulation |
| Azizi, (2021) | Canonical AOS | Global optimization | None | PSO, DE, GWO | Multi-layer orbit search |
| Farahmand-Tabar & Shirgir, (2024) | Positron-Enabled AOS | Reliability optimization | Positron excitation | GA, PSO | Positron-enabled excitation |
| Manita et al., (2023) | O-AOS + LR | Wrapper FS | Logistic Regression | SVM, NB, DT | Orthogonal learning |
| Revanesh et al., (2023) | Hybrid-AOS | Embedded FS | Capsule GAN | CNN, LSTM | Weight tuning via AOS |
| Zhang et al., (2023) | BEA + NSGA-III | FS optimizer | Multi-objective EO | MOFS methods | Pareto clustering |
| Elaziz et al., (2021) | Dynamic- AOS | Wrapper FS | Dynamic learning | PSO, GA, GWO | Adaptive orbit update |
| Niu et al., (2025) | Improved AOS | Energy optimization | Train control | PSO | Improved exploration |
| Asna et al., (2022) | MO-QAOS | Site selection (proxy FS) | Multi-objective | GA, PSO | Quantum operators |
| Shi et al., (2023) | AOS-GCN-LSTM | Feature weighting | GCN + LSTM | ML baselines | Graph-guided tuning |
| Qin et al., (2020) | K-means + AO-based ML | Feature representation | K-Means | Classical ML | Density fitting |
| Korraï et al., (2025) | AOS-CNN | Implicit FS | Pyramid CNN | ML baselines | Attention weighting |
| Kiruthiga et al., (2024) | AOS-FATC | Control optimization | Artificial Tree Control | PID | Feedback refinement |
| Marichelvam et al., (2025) | Hybrid- AOS | Scheduling optimization | Heuristic hybrid | GA | Local–global balance |
| Najm et al., (2023) | AOS | Resource allocation | 5G scheduler | Heuristics | Fitness prioritization |
| Çakıroğlu et al., (2023) | AOS (comparative) | Parameter selection | Swarm hybrids | PSO, ABC, EO | Cross-algorithm comparison |
| Kumar et al., (2023) | AOS-PID | Controller tuning | Fractional PID | PSO-PID | Parameter sensitivity |
| Rohit et al., (2023) | Hybrid-AOS | Antenna optimization | Human Mental Search | GA | Dual-heuristic balance |
| Periakaruppan et al., (2023) | AOS-GAN | Embedded FS | Self-attention GAN | CNN, RNN | Attention-guided FS |
| Saravanan et al., (2024) | AOS-DL | Feature weighting | Deep learning | CNN | Search-driven tuning |
| Ali et al., (2023) | AOS | Parameter extraction | Metaheuristic optimization | Atomic Orbital Search Algorithm | Atomic Orbital Search |
| Zhao et al., (2019) | ASO | Parameter estimation | Metaheuristic optimization | Atom Search Optimization | Population-based search |

Convergence speed, solution accuracy, algorithm robustness, and optimization reliability have been extensively verified for the Atomic Orbital Search (AOS) and all the modified algorithms using the aforementioned standard benchmark functions, particularly those in the test sets of Congress on Evolutionary Computation (CEC). Apart from benchmark testing, extensive studies have also been conducted regarding feature selection and classification, in which binary and hybrid forms of AOS algorithms are capable of identifying important features in high-dimensional spaces. UCI datasets, Enron spam datasets, and biological datasets have been applied to analyse UCI performance, and it is found that UCI can achieve better classification performance compared to traditional optimizers such as GA and PSO. AOS has also been successful in many other problems, such as scheduling and industrial optimization problems, such as flexible job shop scheduling, where hybrid approaches have been shown to improve the makespan, completion time, and job tardiness while preserving the computational efficiency. In energy and power engineering applications, AOS has proven successful in the field of maximum power point tracking, renewable energy forecasting, smart grid optimization, and enhancement of power quality, and in many cases has been found to have a better convergence rate and stability than traditional optimization techniques. In addition, AOS has been used in applications of engineering design and control, including antenna array synthesis, structure optimization, digital filter design, and controller tuning, successfully achieving competitive solutions for complex constrained problems. Multi-objective AOS can balance conflicting objectives, such as energy consumption and delay, and is applied to emerging applications in IoT and wireless sensor networks (WSN) for clustering, routing, congestion control, and network planning. Most of the studies, however, have been simulation oriented, which translates to the need for large-scale real-world validation and scalability studies.

In figure 9 illustrates that feature selection and classification constitute the majority of applications, followed by engineering design and energy systems. Although AOS and its hybrids have already been successfully applied to a wide variety of problem types, only a few implementations for scheduling and industrial optimization problems have been done so far. The very specific nature of scheduling and optimization problems generally requires specialized solution techniques, and while AOS and its hybrids can be used for real-time scheduling and for optimization problems in general, more specialized methods exist for these particular domains. AOS and its hybrids are excellent solution techniques for all applications.

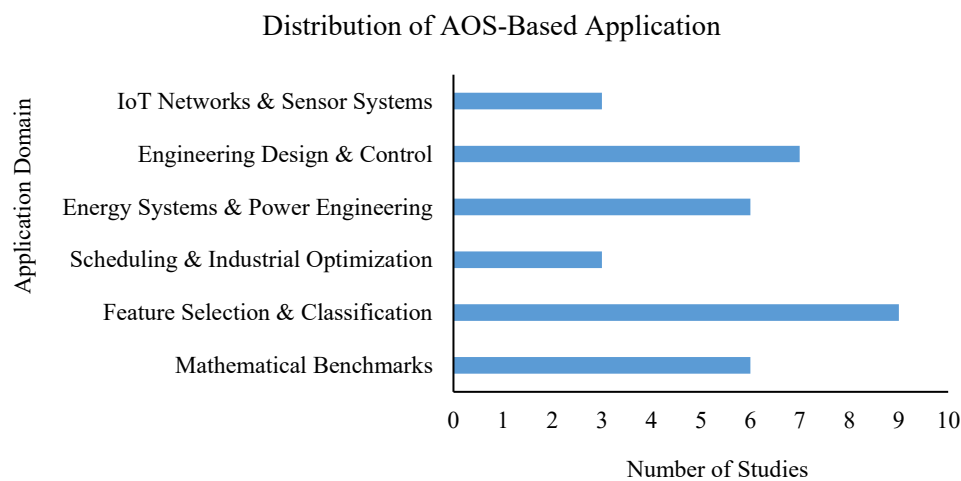


Figure 9: Distribution of AOS-based applications across different domains

7 Discussion and Open Issues

The literature surveyed revealed that the modified, hybrid, and multi-objective Atomic Orbital Search (AOS) algorithms were found to have better convergence speed, better solutions, more accurate search, and performed better optimization than the Atomic Orbital Search (AOS) and a number of conventional metaheuristics. Hybrid AOS methods that combine methods like opposition-based learning, orthogonal learning, dynamic adaptation, and machine learning models generally achieve better classification performance and better feature reduction in feature selection and classification problems. The improvements, however, usually come at the cost of greater complexity in calculation and careful adjustment of the transition rates of photons, population size, and number of layers in the orbits. AOS has demonstrated high accuracy in energy systems and power engineering solutions like maximum power point tracking, renewable energy forecasting, power system control, and energy optimization problems. Comparative studies often show that algorithms such as PSO and GA are slower to converge, less stable, and less effective at optimizing than comparative studies. However, the majority of assessments are based on simulations and benchmark datasets and limited testing in long-term, operational field environments. In addition, hybrid AOS methods have been shown to be successful in other problems, such as scheduling and industrial optimization problems, in which problem-specific heuristics improve the quality of the solutions and computational efficiency. Although good results have been achieved from the various methods to minimize makespan, completion time, and resource utilization, there is not much research on their scalability in large-scale industrial environments. In the same way, AOS and the multi-objective variants have been used in the engineering design field and are competitive with existing methods like NSGA-II. Studies focusing on low and medium-dimensional benchmark applications, however, are largely limited to a few high-dimensional and expensive design situations that have not been investigated that much. The flexibility of AOS to solve clustering, routing, congestion control, and network planning issues is further illustrated by emerging applications in IoT networks and wireless sensor systems. For balancing conflicting objectives like energy, delay, and coverage, multi-objective variants are especially beneficial. Even with these developments, most of the studies are still simulation-based and concentrate on small – to – medium-scale networks. Future research should focus on scalability analysis, adaptive parameter-control mechanisms, real-time implementation, validation on large-scale practical applications, and open-source implementation.

8 Conclusions

This paper summarizes and classifies physics-inspired feature selection algorithms from a systematic review perspective, concentrating on those belonging to the AOS class to gain a better understanding. The study also classifies variants based on PRISMA and analyses their bibliometric features and identifies research themes, authoritative authors, and AOS algorithm breakthroughs. Experimental results indicate that AOS variants based on binary classification, opposition classification, and learning mostly outperform the original AOS in high-dimensional classification tasks. Experimental results demonstrate that the variants of AOS, such as binary classification, opposition classification, and learning, perform better than the original AOS in high-dimensional classification tasks in most cases. Moreover, the multi-objective AOS is a compromise on both accuracy and feature sparsity. Based on quantitative data, there was a rise in the number of AOS research citations from 1 in 2019 to 11 in 2024, with the most citations in 2021 (336). The accuracy of several experiments is more than 95%, and the number of reductions is more than 50% without affecting the performance. There are also a few disadvantages that need to be considered. Poor benchmarking, algorithmic settings, and scalability testing in the high-dimensional data space can cause these results to vary from one study to another,

reducing reproducibility. Therefore, future studies should focus on scalability, adaptive parameter-control approaches, multi-objective feature selection formulations, AOS with understandable AI and deep learning frameworks, open-source implementations, and benchmarking. For more widespread practical implementation, real-time and online AOS-based feature selection must be advanced. All things considered, AOS shows promise as a versatile, physics-inspired feature selection optimizer with significant potential for future theoretical advancement and practical application once the present issues are resolved.

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