Mathematical Models in Cryptocurrency Markets and Decentralized Finance (DeFi): Pricing, Risk, and Network Dynamics

Jairo Dote-Pardo[1,2] and María Teresa Espinosa-Jaramillo[3]

Abstract: Mathematical modeling has seen a rise in response to the increasing complexity and volatility of decentralized finance (DeFi) systems and cryptocurrencies, so helping to understand, forecast, and control risks in this developing financial scene. Examining how mathematical models have developed to meet issues in price forecasting, volatility estimation, portfolio optimization, and systemic risk analysis, this paper offers a comprehensive and up-to-date review of 96 peer-reviewed publications spanning 2019 to 2024. Using a qualitative content analysis technique, we found dominant modeling strategies such stochastic volatility models, regime-switching techniques, copulas, and deep learning-based hybrid models. While older models like GARCH stay fundamental, our results indicate that in turbulent markets newer methods—particularly those combining artificial intelligence and high-frequency data—show better performance. Nevertheless, we also underline important drawbacks

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including the lack of model interpretability, inadequate DeFi sustainability and governance consideration, and limited real-time validation. The paper ends with recommendations for future studies on explainable artificial intelligence, risk measures including environmental and cyber vulnerabilities, and models combining ethical and systematic aspects of digital finance. In the changing crypto ecosystem, developing more strong, open, and socially responsible financial tools depends on these paths.

Keywords: cryptocurrencies; Decentralized Finance (DeFi); mathematical modeling; volatility forecasting; portfolio optimization; stochastic processes; risk management; machine learning; Value-at-Risk (VaR); blockchain analytics

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1. Introduction

Driven by the emergence of cryptocurrencies and the fast rise of Decentralized Finance (DeFi), financial systems have undergone an unmatched transformation in the last ten years (Felix Adebayo Bakare et al., 2024); (Gramlich et al., 2023). These developments have brought a basic change in the way value is stored, moved, and managed across digital networks, enabled by blockchain technology and cryptographic protocols (Alzoubi and Mishra, 2023); (Tripathi et al., 2023). Originally imagined as a decentralized alternative to conventional fiat currencies, cryptocurrencies have developed into a varied and complicated asset class with particular market behaviors, volatility traits, and speculative dynamics (Kayani and Hasan, 2024); (Bennett et al., 2023); (Giudici et al., 2020). DeFi, on the other hand, has expanded the scene by means of permissionless and autonomous smart contracts duplicating and innovating upon conventional financial services—such as lending, borrowing, trading, and asset management (Adamyk et al., 2025); (Harvey and Rabetti, 2024). These changes have spawned a quickly growing digital financial ecosystem mostly operating outside of traditional regulatory systems (J. S. Dote-Pardo et al., 2025); (Vijayagopal et al., 2024).

The use of strict mathematical models becomes not only appropriate but also vital as these markets develop (Mokhov et al., 2023); (Tarka, 2018). Quantitative research finds rich ground in the high-frequency, data-rich environment of cryptocurrencies and the algorithmic character of DeFi protocols (Anas et al., 2024). Still, the inherent complexity of these systems—characterized by nonlinear interactions, endogenous feedback loops, and emergent network effects—presents major modeling difficulties (Zhao et al., 2023). Often needing significant modification to fit the distributed, trustless, and sometimes non-stationary character of these markets, traditional financial mathematics tools such as no-arbitrage pricing theory, risk-neutral valuation, and stochastic control (Tapiero, 2006). Likewise, network-based models now widely used in communication systems and epidemiology are being used to grasp how information, liquidity, and systemic risk flow across blockchain-based financial structures (Theodorakopoulos et al., 2024)(Taherdoost and Madanchian, 2023)(Tagde et al., 2021).

Emphasizing three basic dimensions—asset pricing, risk modeling, and network dynamics—this systematic literature review aims to offer a thorough synthesis of the mathematical modeling techniques created to examine cryptocurrency markets and DeFi platforms. The review not only classifies the prevailing theoretical frameworks and methodological innovations across these domains but also critically assesses their relevance, assumptions, and constraints. It does this by answering a number of important research questions: (i) How has research on mathematical models in cryptocurrency markets and DeFi evolved over time? (ii) What mathematical models have been used in this field of research? (iii) How have the relevant topics in this topic evolved? (iv) What is the conceptual framework that characterizes this field of study? (v) What are the future directions for research in this line?

By means of this study, the evaluation helps to consolidate knowledge at the crossroads of mathematics and DeFi by stressing both current in-sights and new research frontiers. The study intends to guide future mathematical questions into this changing field of finance by means of mapping the development of modeling techniques and spotting important gaps in the literature. In the end, this work hopes to promote a better knowledge of how mathematical tools can be used to model, forecast, and maybe stabilize the more complicated and powerful world of DeFi markets and cryptocurrency.

2. Materials and Methods

2.1. Data

Data for this review were obtained from the Web of Science (WoS), recognized for containing the highest-impact scientific output worldwide (Birkle et al., 2020). Thus, the results obtained in this work are reliable when guiding new research and technological developments focused on the use of mathematical models to address current challenges in financial markets, in areas such as cryptocurrencies and DeFi. The search equation used (1) considers terms that are commonly used in the context of mathematical models, cryptocurrencies, and DeFi.

WoS: (TI=(cryptocurren* OR crypto-curren* OR bitcoin* OR ethereum* OR stablecoin* OR DeFi OR decentralized-finance* OR automated-market-maker* OR AMM OR liquidity-pool* OR impermanent-loss* OR DAO* OR decentralized-autonomous-organization*)) AND TI=(mathematical-model* OR stochastic-process* OR stochastic-differential-equation* OR jump-diffusion* OR Lévy-process* OR fractional-calculus* OR game-theory* OR Nash-equilibrium* OR network-theory* OR graph-theory* OR risk-measure* OR Value-at-Risk* OR CVaR* OR optimization* OR control-theory* OR mechanism-design* OR volatility-model* OR time-series-analysis* OR chaos-theory* OR algebraic-geometry* OR topological-data-analysis*)

(1)

2.2. Exclusion and inclusion criteria

To ensure the greatest possible transparency and potential replicability of the data selection process, the PRISMA framework for systematic literature reviews (Page et al., 2021) was followed (Figure 1). In the first stage, 146 results were identified in WoS, of which 33 were excluded: 28 were proceedings papers and 5 were meeting abstracts. This allowed the screening phase to begin with 113 articles, of which a total of 12 were excluded, as they were published after 2024. Thus, the eligibility phase began with 101 articles, of which 5 were removed, considering that 4 were not in the field of finance and 1 was published in a journal no longer indexed in WoS. Thus, 96 articles were included.

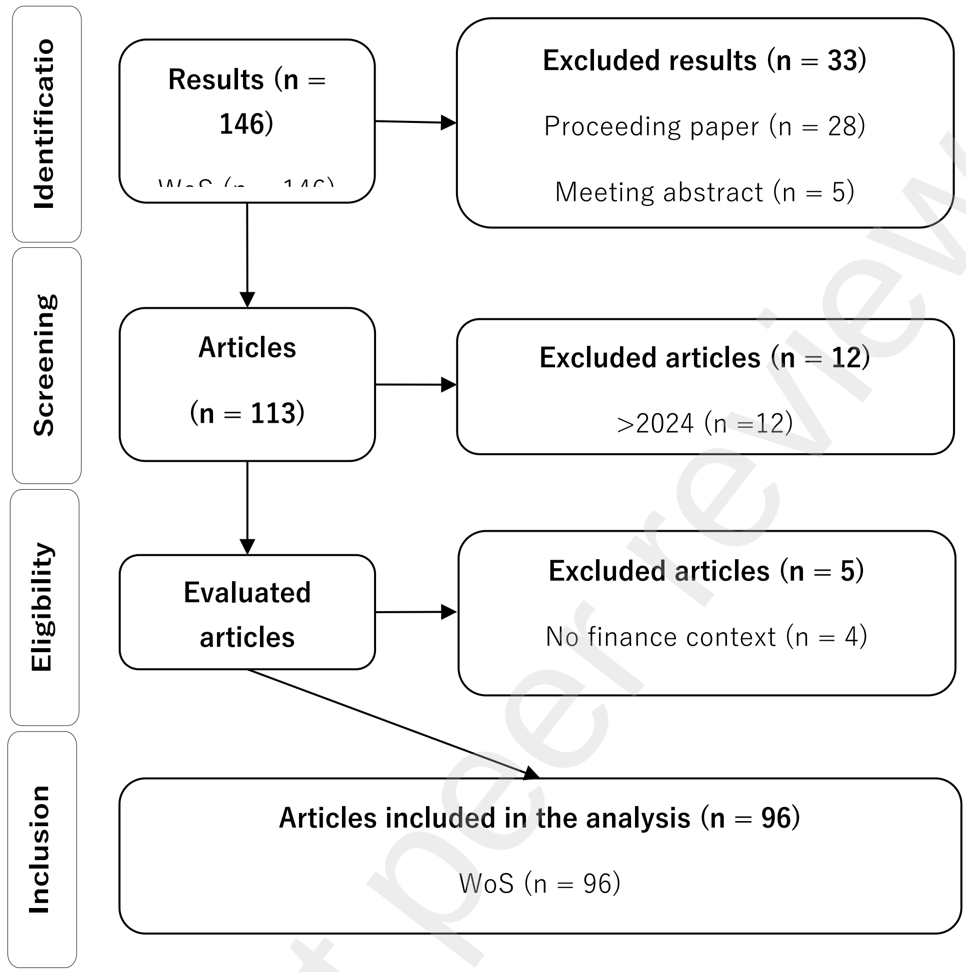

Figure 1. Inclusion and exclusion criteria of results using the PRISMA method.

2.3. Data analysis

Three tools were used for data analysis: Microsoft Excel, VOSviewer, and R Studio with its Bibliometrix package (Dote-Pardo et al., 2025). These tools enabled the bibliometric analysis, focusing on the evolution of publications and journals over time, the identification of collaborative networks between countries, the identification of collaborative networks between relevant authors on the subject, and the mapping of keyword co-occurrences, which allowed for the construction of thematic clusters.

3. Results

3.1. Characterization and evolution of research

Figure 2 showing the worldwide distribution and cooperative networks in academic research connected to mathematical modeling in cryptocurrency markets and DeFi. Darker hues indicate more academic output or more active participation in the research area; countries are shaded in different tones of blue. Especially, nations like China, India, and Iran show in the darkest tones, suggesting notable contributions to the literature on DeFi and cryptocurrency modeling.

The lines linking nations show patterns of worldwide co-authorship and cooperation. Particularly across Asia and Europe, these lines are concentrated, implying a dense and active research network in these areas. The visual density of connections suggests that countries in these areas not only significantly contribute on their own but also participate regularly in cross-border academic cooperation. On the other hand, lighter-colored or gray areas on the map suggest little or no representation in the dataset examined, so suggesting areas where academic activity in this field might still be developing.

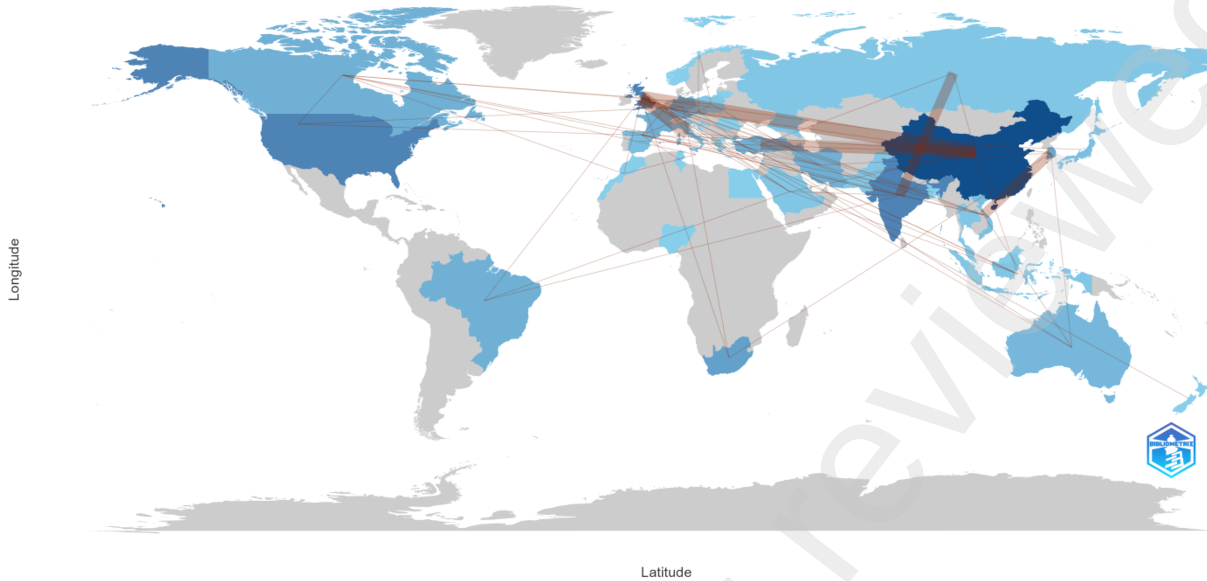

Figure 2. Country collaboration map.

Figure 3 shows the annual evolution of the number of articles, journals, and authors related to mathematical models in research on cryptocurrencies and DeFi. The left vertical axis represents articles (white bars) and journals (black line above the bars). Both variables show an upward trend between 2018 and 2022, with a sustained increase in the number of published articles and the number of scientific journals addressing this topic. This growth reflects an expansion in editorial and academic interest in mathematical models applied to crypto and DeFi markets.

On the other hand, the right vertical axis shows the evolution of the number of authors (purple line), which also shows continued growth, especially significant between 2019 and 2021. This suggests a progressive incorporation of researchers into the field, which not only expands scientific output but also contributes to greater diversity in methodological and thematic approaches.

Overall, the figure demonstrates a consolidation of the area as an object of study, with an increase in academic production, in the diversity of scientific publications involved, and in the number of researchers actively participating in the development of knowledge about cryptocurrencies and decentralized finance.

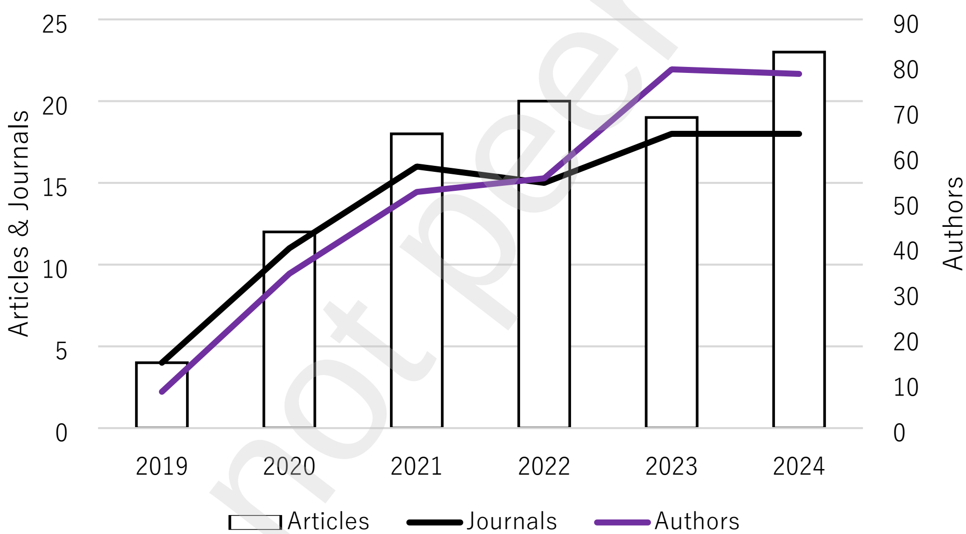

Figure 3. Research evolution over years: articles, journals and authors.

3.2. Main mathematic models

The annual development of the application of various mathematical models in scientific papers connected to cryptocurrencies and DeFi is shown in Figure 4. The vertical axis shows the number of papers that used each type of mathematical model in a given year, between 2019 and 2022. This representation lets us see how academic interest in each methodological approach has changed over time.

Though it has since dropped, statistical models' (gray line) early dominance was clear, peaking in 2020. By contrast, the use of machine learning models (orange line) has increased consistently since 2019, exceeding other methods in 2022, mirroring the growth of automated predictive analysis in DeFi platforms and crypto markets.

With a significant recovery in 2022, econometric models (blue line) have remained consistently important, suggesting their ongoing usefulness for the study of prices, volatility, and interactions between economic factors. Other methods, including neural networks, game theory, simulation models, and optimization, show more erratic patterns with sporadic appearances that imply a more specialized use or application to particular problems.

The graph shows a general methodological diversification in the field: although some traditional models are still relevant, newer and more computationally demanding techniques like machine learning are fast catching up. This variety shows the growing complexity of the events examined in distributed markets and the demand for flexible and strong mathematical tools to handle them.

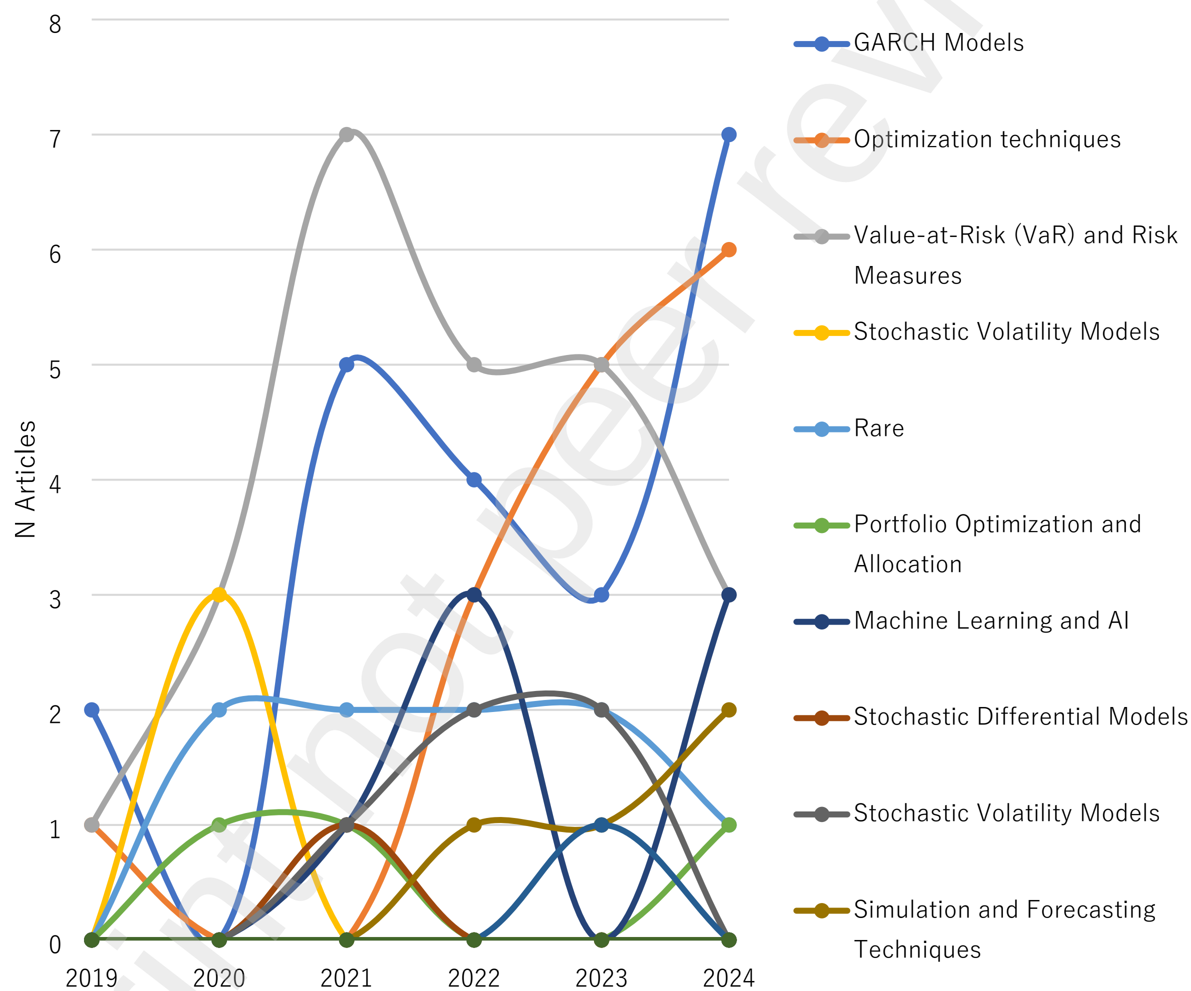

Figure 4. Mathematical models used in number of articles per year.

3.3. Topic evolution

Comparing two periods—1919–2022 and 2023–2024—Figure 5 shows the topic evolution in the titles of scientific papers on mathematical models in cryptocurrencies and DeFi. A Sankey diagram shows how certain first-period title keywords link to the main second-period keywords.

Reflecting an early emphasis on the analysis of conventional financial data, market behavior, and the dangers connected with the use of Bitcoin, the most often used words in the 2019–2022 period were bitcoin, risk, market, series, prediction, modeling, and optimization.

Beginning in 2023, a shift toward words like model, cryptocurrencies, deep, and once more bitcoin is seen, but now with more relative weight. This implies that, although Though Bitcoin stays a central theme, the emphasis is shifting toward a more general handling of cryptocurrencies and an increasing interest in advanced optimization methods and deep learning.

The term based shows up in both eras, suggesting ongoing use of model- or data-based methods. The inclusion of the word deep, which was not formerly present, is also significant since it indicates a larger incursion of more advanced artificial intelligence technologies into recent literature.

Research in DeFi and cryptocurrencies has evolved from a more conventional, technical emphasis on Bitcoin and time series analysis to a larger, more modern scene that includes several cryptocurrencies, advanced modeling techniques, and deep learning tools, so reflecting the maturation and diversification of the academic field. Figure 5 shows this evolution.

Figure 5. Thematic evolution.

3.4. Keywords mapping

Based on the keywords provided by authors on mathematical models in cryptocurrencies and DeFi, Figure 6 shows a conceptual structure map. Thematically grouping the most often used words using Multiple Correspondence Analysis (MCA) method exposes the intellectual structure of the field.

The graph reveals two significant clusters. Left in blue are words linked to quantitative and computerized methods. Here we discover ideas related to technical analysis, price forecasting, risk management, and the heavy use of algorithms. Words like “machine learning,” “deep learning,” “copula,” “GARCH,” “volatility,” “portfolio diversification,” and “option pricing” reflect an approach focused on modeling com-plex crypto market dynamics using advanced statistical, artificial intelligence, and optimization tools.

Red on the right list’s words connected to applied financial studies, asset management, and investment strategies. Words like “investment,” “asset management,” “digital currency,” “ensemble learning,” and “artificial neural network” stand out. This field emphasizes studying the economic effect of cryptocurrencies and the application of computational models to assist financial choices.

The spatial distribution of these groups indicates a distinct theme: on the one hand, a line of research concentrating on mathematical modeling and, on the other, one emphasizing financial and strategic uses. This graphic captures the multidisciplinary character of the sector uniting mathematicians, engineers, economists, and management specialists all adding from various perspectives to the research of decentralized markets.

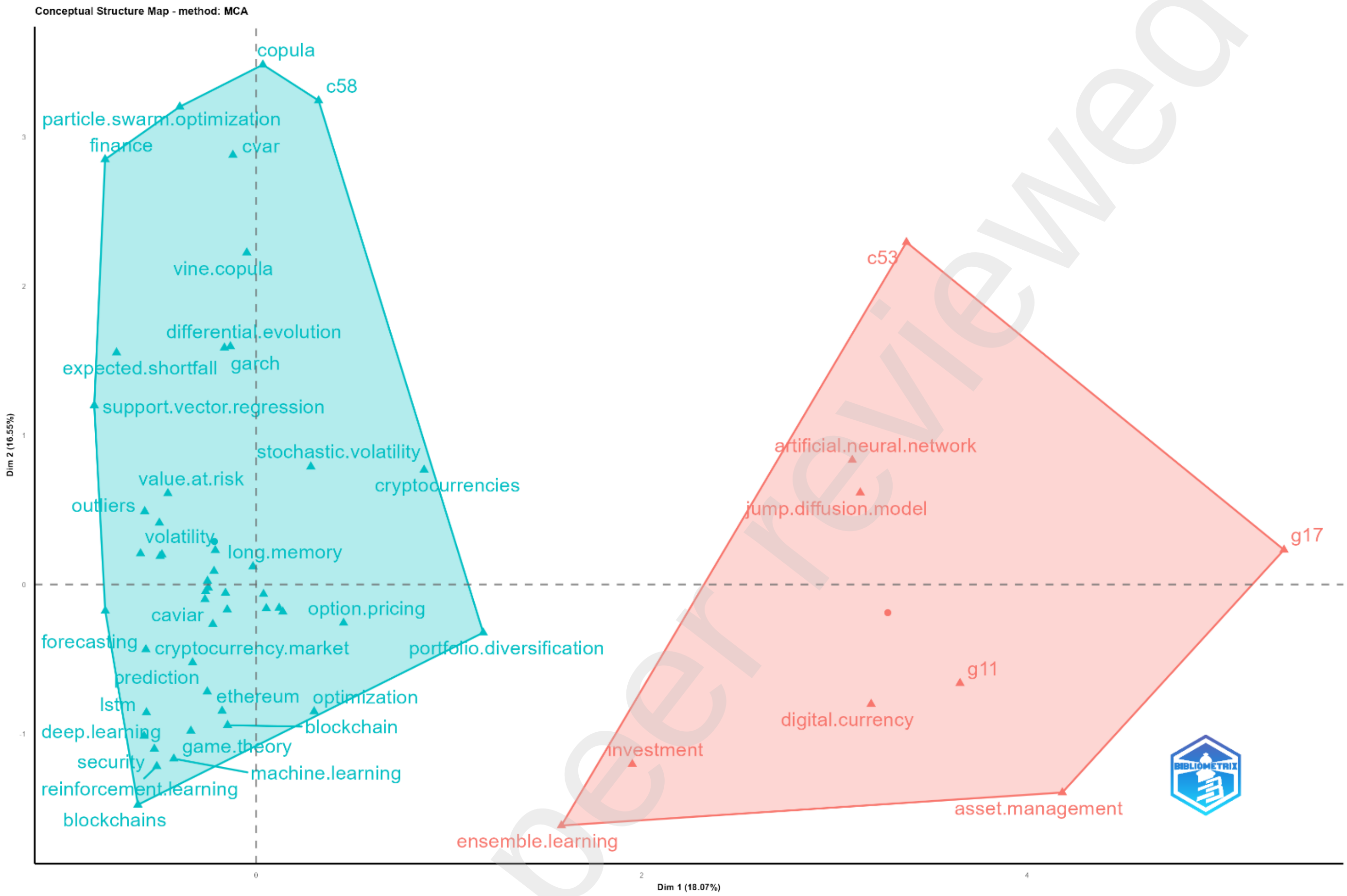

Figure 6. Author keywords' Factorial analysis.

3.5. State of the art

One of the most notable aspects of the evolution of the state-of-the-art in cryptocurrencies is the growing sophistication and effectiveness of the mathematical models used to understand and anticipate the behavior of these assets. As the crypto market has consolidated as a highly volatile and structurally complex system, traditional methods have given way to models capable of capturing nonlinear dynamics, extreme dependency structures, and regime shifts.

GARCH models and their extensions have historically been one of the most common tools for modeling the conditional volatility of cryptocurrencies. Their initial effectiveness lay in their simplicity and ability to capture heteroskedasticity, although it quickly became apparent that they were insufficient to reflect fat tails and the occurrence of extreme events. Therefore, subsequent studies incorporated asymmetric t-distributions, scaled variance functions, and regime-switching GARCH models (Maciel, 2021), which considerably improved the forecast quality of risk measures such as VaR and Expected Shortfall (ES).

Another family of mathematical models that has shown remarkable effectiveness are stochastic volatility (SV) models, especially those with jumps and t-distributed components, which have been shown to outperform conventional GARCH models in both volatility adjustment and prediction (Zahid and Iqbal, 2020). The integration of jumps allows for better capturing abrupt market reactions to news or regulatory changes, a common phenomenon in the crypto space.

On the other hand, the combination of statistical techniques with copula theory tools, such as vine copulas or copulas in the context of COGARCH and

MSCOGARCH (Trucíos et al., 2020); (Mba and Mwambi, 2020), has made it possible to effectively model the nonlinear dependence between crypto assets, which is crucial for portfolio optimization and multivariate risk management. These methodologies have proven superior to traditional linear correlations, especially in the context of crises or simultaneous price declines.

Regarding prediction models, the use of neural networks—such as LSTM, BiLSTM, and their hybrid versions with attention mechanisms—has demonstrated high accuracy in estimating future prices and detecting trends using multivariate time series (Ladhari and Boubaker, 2024); (Jung et al., 2024). Their ability to handle nonlinearities, long temporal dependencies, and heterogeneous data has consolidated their position as one of the most effective approaches in highly uncertain environments.

Furthermore, optimization approaches such as Particle Swarm Optimization, genetic algorithms, and multi-objective optimization techniques have been incorporated to improve model calibration and portfolio construction, demonstrating high adaptability and computational efficiency, even in markets with high dimensionality and noise (Omran et al., 2023); (Shirvani et al., 2024).

Thus, the effectiveness of mathematical models in cryptocurrency analysis has increased substantially over time. From robust, nonparametric econometric models to advanced machine learning and artificial intelligence techniques, current literature shows a clear trend toward combining quantitative tools that more accurately capture the complexities of the behavior of these digital assets. This methodological progression not only improves predictive accuracy but also strengthens decision-making in investment and regulatory contexts.

4. Discussion

Research on cryptocurrencies and DeFi has grown exponentially in recent years, generating a substantial body of literature highlighting the use of increasingly complex and sophisticated mathematical models (Alamsyah and Muhammad, 2024). The 96 studies reviewed in this research clearly demonstrate how the state of the art in this area has evolved, and how mathematical models have proven not only effective but also necessary for understanding, predicting, and managing the behavior of digital assets characterized by high volatility, interdependence, and structural uncertainty.

One of the first fields where models have shown greater maturity is in volatility analysis. Traditionally, GARCH models and their extensions have dominated this space, providing a solid foundation for evaluating the conditional variance of returns for cryptocurrencies such as Bitcoin, Ethereum, or Litecoin (Chu et al., 2017). However, multiple studies, such as those by (Tiwari et al., 2019), demonstrate that the GARCH model is insufficient to capture the abrupt changes and extreme behaviors that characterize these markets. In response, more flexible models have begun to be used, such as stochastic volatility models with heavy-tailed distributions, long-memory models, and regime-switching models like MS-GARCH. These techniques allow for more accurate capture of phenomena such as abrupt jumps, volatility persistence, and structural changes in price time series. Furthermore, recent proposals such as range models combined with methods robust to outliers have proven particularly useful during periods of crisis and high uncertainty, as observed in (Fiszeder et al., 2024).

Regarding price forecasting, there is a clear transition from classical econometric models to deep learning approaches. While ARIMA models and traditional neural networks still have their place, LSTMs and their bidirectional variants (BiLSTMs) have demonstrated outstanding performance. Studies such as those by (Berger and Koubová, 2024), (Ladhari and Boubaker, 2024), and (Tripathi and Sharma, 2023) have integrated these models with evolutionary optimization algorithms—such as particle swarm, cuckoo search, and mechanical attention—to improve forecast accuracy. This combination has made it possible to predict price behavior with minimal margins of error, which represents a significant advance for investors and fund managers.

Risk measurement constitutes another essential pillar of financial analysis in cryptocurrencies. Here, metrics such as VaR and ES have been widely used, although their effectiveness depends on the underlying model. The incorporation of novel approaches such as the LSTM-joint-combined model (Lu et al., 2023) and models based on generalized autoregressive scoring processes (TVM-aGAS) has allowed for more realistic estimates. In an innovative way, some authors have extended these models to non-financial contexts, developing metrics such as Climate VaR and Climate ES to assess the environmental impact of the energy use of cryptocurrencies, particularly in the case of Bitcoin. Similarly, credible models based on fuzzy theory have been proposed to address the structural uncertainty of these assets, offering more adaptive and accurate alternatives to tail risks.

Regarding portfolio optimization, the literature reflects an evolution from traditional approaches based on Markowitz theory (Markowitz, 1952) to advanced dynamic optimization techniques. While classical models remain relevant due to their clarity and theoretical soundness, recent research has incorporated deep reinforcement learning models to construct portfolios that dynamically adjust to changes in return distribution. Similarly, the use of copula structures (vine copulas) and metaheuristic techniques such as swarm optimization has made it possible to capture cross-dependencies between cryptocurrencies and build more resilient portfolios, as illustrated by studies by (Mba and Mwambi, 2020), (Cui et al., 2023) and others.

No less important are emerging applications that integrate mathematical models with topical themes, such as sustainability, sentiment analysis, and consensus mechanisms in DeFi environments. Some works have used data series extracted from social media, Google Trends, and platforms such as YouTube and Twitter to feed predictive models that incorporate user behavior as a key explanatory variable. (Dipple et al., 2020) and (Fay et al., 2024) stand out for their integration of social media activities and market prices using stochastic differential equations. Other studies have developed models that evaluate the energy efficiency of cryptocurrency mining, proposing solutions to reduce energy consumption through hardware redesign or changes to consensus algorithms (Koutra and Tenentes, 2024). Furthermore, in the DeFi field, game-theoretic frameworks have been used to analyze incentive logic and radical uncertainty management, as (Langenohl, 2022) explains. These approaches not only broaden the application horizon of mathematical models but also contribute to better governance of these ecosystems.

The synthesis of these contributions suggests multiple future directions for research in this area. A promising first line of research is the integration of explainable artificial intelligence (XAI) models, which allows us to understand how and why deep learning models make certain decisions, essential in markets where transparency is key. Likewise, there is an urgent need to develop risk metrics that consider the specificities of the DeFi ecosystem, such as the composability of smart contracts and code vulnerabilities. Another relevant line of research is the incorporation of environmental, social, and governance (ESG) factors into optimization models, which would pave the way for the creation of crypto ESG portfolios. The possibility of combining quantitative methods with human behavioral models is also emerging, considering that many cryptocurrency investors are retail investors and respond more to emotional than rational stimuli. Finally, the development of blockchain simulators connected to reinforcement learning environments would allow investment strategies to be trained and tested in real time under realistic and constantly evolving market conditions.

In conclusion, mathematical models applied to cryptocurrencies and decentralized finance have demonstrated a remarkable ability to capture the complexity of these digital assets. Their evolution has been rapid, moving from traditional approaches to robust and adaptive systems that integrate big data, artificial intelligence algorithms, and nonlinear dependency structures. Despite the progress made, significant challenges remain that require new interdisciplinary solutions, combining economic theory, data science, sustainability, and technological ethics. This convergence will shape future research and determine the effectiveness of models in an increasingly digital, decentralized, and interconnected market.

5. Conclusions

This work has explored in depth the evolution and effectiveness of mathematical models applied to the analysis of cryptocurrencies and DeFi, based on a systematic review of 96 scientific articles published between 2019 and 2024. The findings lead to the conclusion that mathematical models have played a fundamental role in understanding the dynamic and highly volatile behavior of cryptoassets, enabling substantial advances in key areas such as price prediction, risk measurement, and portfolio optimization.

An initial important conclusion is that volatility models have evolved considerably. While GARCH models remain widely used, they have been complemented and, in many cases, surpassed by more complex models such as stochastic volatility models with heavy tails, MS-GARCH, and those that incorporate jumps or long memory. This evolution responds to the need to capture the extreme and nonlinear dynamics of cryptocurrencies, especially in contexts of high uncertainty.

Second, the paper notes the rise of deep learning methods and hybrid models for price prediction. Algorithms such as LSTM, BiLSTM, convolutional neural networks, and models optimized with evolutionary techniques have demonstrated superior predictive capabilities, especially when integrating unconventional variables such as social media sentiment or Google search data.

Third, regarding risk measurement, increasing sophistication is observed in the use of metrics such as VaR and ES, which have been estimated with greater precision thanks to the use of robust models, Vine copulas, neural networks, and high-frequency data structures. Likewise, approaches that incorporate environmental and energy risks are beginning to emerge, expanding the concept of risk beyond the purely financial realm.

Fourth, advances in portfolio optimization include the use of artificial intelligence algorithms, swarm optimization, reinforcement learning, and dynamic strategies that integrate multiple data sources. These techniques allow for more precise management of highly volatile portfolios with nonlinearly correlated assets.

However, this work also identifies important limitations in the current literature. First, many models, especially deep learning models, lack interpretability, which hampers their validation and practical application in regulated environments. Second, most studies focus on historical data and lack validation in real-time or disruptive market conditions. Furthermore, there remains a poor integration of sustainability criteria, ESG factors, or ethical considerations in model design for the crypto ecosystem.

Finally, an underrepresentation of DeFi-specific technological risks, such as smart contract vulnerabilities or market manipulation attacks, is detected. This highlights the need to develop models that integrate cybersecurity components, automated code auditing, and decentralized governance analysis.

Overall, this research reaffirms the value of mathematical models as indispensable tools for analyzing cryptoassets, but also highlights the need to move toward more explanatory, ethical, sustainable, and resilient approaches in the face of extreme environments and new digital threats.

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Abbreviations

The following abbreviations are used in this manuscript:

ANN	Artificial Neural Network

ARIMA	Autoregressive Integrated Moving Average
ARMA	Autoregressive Moving Average
BEV	Blockchain Extractable Value
BTC	Bitcoin
CNN	Convolutional Neural Network
CVaR	Conditional Value at Risk
DeFi	Decentralized Finance
DNN	Deep Neural Network
ETH	Ethereum
GARCH	Generalized Autoregressive Conditional Heteroskedasticity
LSTM	Long Short-Term Memory
MAE	Mean Absolute Error
MSE	Mean Squared Error
MS-GARCH	Markov-Switching GARCH
RMSE	Root Mean Square Error

SV	Stochastic Volatility
SVR	Support Vector Regression
VaR	Value at Risk
VAR	Vector Autoregression

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