

Large Language Models for Data Science: A Survey

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Abstract

Data science is an interdisciplinary field that focuses on extracting knowledge from raw data using statistical analysis and machine learning techniques. However, as data continues to grow in scale and complexity, data scientists face increasing challenges in handling unstructured data, automating workflows, and scaling analytical processes. The advancements of large language models (LLMs) present an unprecedented opportunity to enhance and streamline data science tasks by enabling automation and augmentation of key processes in the data science pipeline. This survey contributes to four core aspects: the role of LLMs in the data science cycle, specialized domain applications, challenges and limitations, and social impact and future directions. Furthermore, we introduce a structured framework defining how LLMs contribute to each stage of data science, provide an in-depth discussion on their applications in key domains such as healthcare and finance, analyze key obstacles such as data quality and model interpretability, and explore ethical concerns and future research opportunities. Serving as a comprehensive resource, this survey aims to assist researchers and practitioners in understanding and utilizing LLMs to advance modern data science methodologies.

1 Introduction

The field of data science has experienced significant advancements over the past decade, driven by the increasing availability of large-scale data and the development of sophisticated machine learning techniques (Wu, 2024; Lyko et al., 2016a; Hong et al., 2024). Data science primarily focuses on extracting knowledge from raw data, with the ultimate goal of deriving data-driven actionable insights across diverse industries, including healthcare, finance, and engineering (Cady, 2024; Sarker, 2021). For example, in healthcare, data science is revolutionizing personalized medicine and pre-

dictive diagnostics through data-driven methodologies (Goetz and Schork, 2018). Generally, traditional methods applied in data science rely on a combination of statistical analysis and machine learning techniques (Li et al., 2017; Qin et al., 2020). However, as data complexity continues to grow, researchers in data science face numerous challenges in handling unstructured data, automating workflows, and scaling analytical processes. These challenges necessitate more intelligent, flexible, and scalable solutions to support modern data science solutions.

Recently, the emergence of large language models (LLMs) has introduced a significant shift in how data science tasks are performed. LLMs, such as GPT-4 (OpenAI, 2024a) and LLaMA (Dubey et al., 2024), possess powerful capabilities in question answering (Talmor et al., 2018; Kwiatkowski et al., 2019), code generation (Ni et al., 2023; Nascimento et al., 2024), and contextual reasoning (Liu and colleagues, 2024; Hao et al., 2023). Such capabilities of LLMs have motivated researchers to explore their assistance in automating and enhancing various stages of the data science workflow. For example, LLMs can assist in data extraction (Katz et al., 2024), feature engineering (Li et al., 2024d), statistical analysis (Brugere et al., 2024), and visualization (Ko et al., 2024), as illustrated in Fig. 1. Additionally, LLMs also improve accessibility by allowing interactions based on natural language with complex data systems.

Nevertheless, despite their growing adoption in data science, LLMs also present several challenges. For example, they struggle with numerical computations in data science applications (Fang et al., 2024), limiting their reliability for tasks requiring precise quantitative reasoning. Additionally, societal biases embedded in LLMs may pose ethical concerns, potentially affecting fairness in decision-making (Wang et al., 2024). Given these limitations, there is an urgent need for a systematic re-

view of current LLM applications in data science, as well as an in-depth exploration to advance LLMs for data science.

In this survey, we investigate the role of LLMs in data science based on our proposed taxonomy and analyze their impact across workflow stages. The primary contributions of this survey are as follows:

- **Taxonomy based on the Data Science Workflow:** We systematically examine how LLMs contribute to various stages of the data science workflow, including data acquisition, preparation, analysis, and presentation. Through the taxonomy, we aim to provide a comprehensive overview of LLM-driven automation and augmentation across these critical phases.
- **Limitations of LLMs in Data Science:** We analyze key challenges associated with integrating LLMs into data science workflows, including issues related to inconsistency (e.g., sensitivity to data formats), inefficiency (e.g., difficulty in handling large data), and insecurity (e.g., bias and privacy risks).

Additionally, we highlight potential future research directions and introduce the applications of LLMs for data science in specific domains such as finance and healthcare. In concrete, this survey aims to serve as a guide for researchers and practitioners seeking to leverage LLMs for various data-driven tasks, including data processing, analysis, and communication.

Differences between This Survey and Others. Several surveys have explored various aspects of LLMs in data science (Zeng et al., 2024a, 2023; Hua et al., 2024; Zhao et al., 2023; Hadi et al., 2023). However, these surveys often lack a holistic view of LLMs’ roles across the entire data science workflow. Particularly, they tend to focus on specific stages, such as data acquisition (Liu et al., 2024d; Wang et al., 2023h; Albalak et al., 2024), or specific data types, such as tabular data (Sui et al., 2024; Ruan et al., 2024; Fang et al., 2024). Other related surveys concentrate on the application of LLMs in specific domains, including health (He et al., 2025; Goedde et al., 2023; Qiu et al., 2023; Zhou et al., 2023a; Yuan et al., 2024b), finance (Li et al., 2023d; Zhao et al., 2024c; Lee et al., 2024a; Nie et al., 2024), and education (Al-Smadi, 2023; Wang et al., 2024e; Hosseini et al., 2023; Li et al., 2023b). In contrast, this survey offers a comprehensive framework for the utilization of LLMs in four

interconnected stages of the data science workflow.

2 Data Science Workflow

In this work, we define the data science workflow that typically involves four interconnected stages: data acquisition, data preparation, data analysis, and data interpretation. Traditional approaches to data science often involve labor-intensive tasks that can limit scalability and adaptability (Khatri and Brown, 2010a). However, with the increasing complexity and volume of data, modern data science requires automated, scalable, and context-aware solutions to effectively manage diverse data sources. In this regard, LLMs are emerging as transformative tools in data science, offering enhancements across all phases of the workflow:

- **Data Acquisition:** This stage involves collecting raw data from various sources, including structured databases, unstructured text, and sensor streams. In this stage, LLMs can help automate the collection, annotation, and synthesis of both structured and unstructured data (Gur and colleagues, 2022).
- **Data Preparation:** This stage encompasses feature engineering, data cleaning, and storage management to ensure data quality and usability. LLMs can help refine features through semantic analysis and dynamic transformations (Choi et al., 2024).
- **Data Analysis:** In this stage, both textual (e.g., summarization and reasoning) and numerical (e.g., statistical modeling) analyses are performed to extract meaningful insights from data. LLMs can improve both quantitative and qualitative analyses by providing contextual insights and complex reasoning (Liu and colleagues, 2024).
- **Data Interpretation:** This stage involves communicating findings and insights through visualization and decision-making systems. LLMs in this stage can help create visualizations and summaries that enhance data accessibility and usability (Chen et al., 2023c).

Together, these stages form an iterative and structured pipeline that enables efficient and scalable data-driven insights. By integrating LLMs across these phases, data scientists can streamline the workflow, minimize manual effort, and improve the reliability of analytical results.

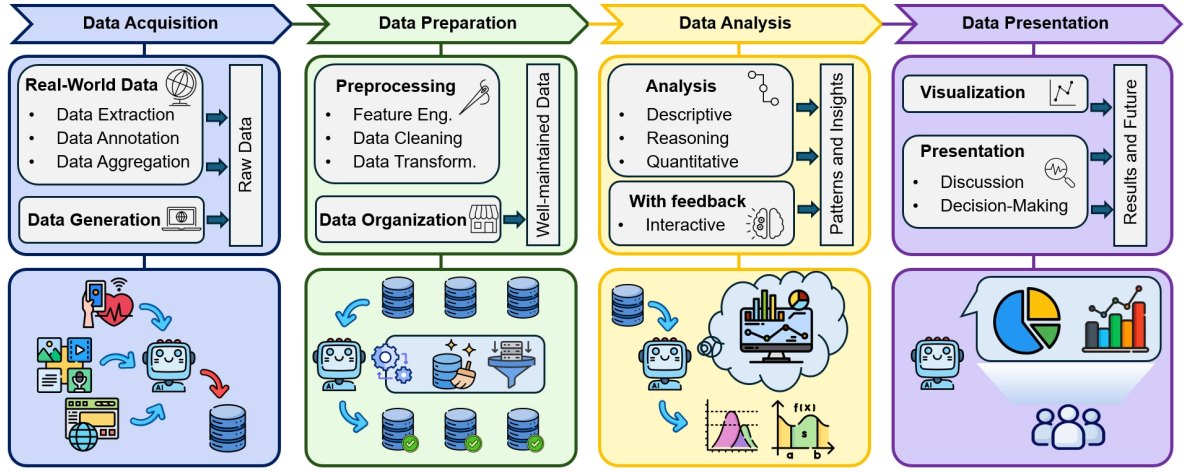


Figure 1: The proposed taxonomy of research works on LLM for data science.

3 LLMs for Data Acquisition

Data acquisition serves as a foundational stage of the data science workflow, encompassing the collection of data from diverse sources (Lyko et al., 2016b). Traditional approaches often face challenges related to data heterogeneity and quality, limiting their efficiency in handling large and complex datasets. LLMs offer promising solutions by automating data extraction, annotation, aggregation, and even generating structured data from raw inputs. In the following sections, we explore existing research on leveraging LLMs to enhance these four key aspects of data acquisition.

3.1 Data Extraction

Extracting valuable data from raw sources is often a time-consuming and domain-specific process, as it relies on rule-based or specialized machine learning approaches. LLMs can streamline this by automatically parsing data across websites, scholarly archives, and online platforms, producing summaries and structured outputs (Gur et al., 2022; Zheng et al., 2024; Dolphin et al., 2024; Jiang and Ferrara, 2023; Katz et al., 2024; Li et al., 2024o). LLMs also excel at entity recognition and meta-data generation (Sancheti et al., 2024; Kim and Lee, 2024; Harrod et al., 2024; Zhang and Soh, 2024; Gillani et al., 2024), facilitate multilingual tasks (Whitehouse et al., 2023; Li et al., 2024q; Thellmann et al., 2024; Miah et al., 2024; Kmainasi et al., 2024), and handle multimodal data (Wysocki et al., 2024; Wang et al., 2024c; Ge et al., 2024). In IoT applications, LLMs assist in detecting sensor anomalies and identifying inter-device correlations for proactive maintenance (Cui et al., 2024; Kok

et al., 2024; An et al., 2024; Shiralil et al., 2024; Abshari et al., 2024; Worae et al., 2024).

Additionally, domain-specific prompting can guide LLMs to focus on the most relevant data, which is particularly effective in medical applications (Xiao et al., 2024a; Xia et al., 2024; Carta et al., 2023; Hu et al., 2024b), leading to more accurate results. Moreover, retrieval-augmented generation (RAG) boosts factual precision and reduces errors (Ding et al., 2024b; Arslan and Cruz, 2024; Li et al., 2024f,h). By streamlining extraction, these techniques ensure that only the most relevant data progresses to subsequent steps of further refinement, such as annotation and aggregation.

3.2 Data Annotation

After data extraction, refining the data through annotation is typically required for effective model training and evaluation. However, this process is often labor-intensive, particularly for large-scale or multimodal datasets (Sorokin and Forsyth, 2008). LLMs reduce this overhead by automatically generating labels for data in tasks such as sentiment analysis, object detection, and transcription (Tan et al., 2024; Wang et al., 2024b; Shvetsova et al., 2025), demonstrating strong performance in zero- and few-shot settings (Sapkota et al., 2024; Zhang et al., 2023a; Sainz et al., 2023; Chen et al., 2024h). Techniques such as advanced prompting (e.g., self-correction, multi-agent debates) and domain-specific fine-tuning further improve label quality (Kamoi et al., 2024; Chen and Si, 2024; Li et al., 2024c; Alizadeh et al., 2025; Bansal and Sharma, 2023; Tang et al., 2023). Additionally, human-in-the-loop and active learning techniques

help refine or verify labels, ensuring reliability for downstream training (Li et al., 2023a; Tang et al., 2024; Kim et al., 2024b; Pangakis and Wolken, 2024; Ming et al., 2024).

3.3 Data Aggregation

After annotation, data is generally aggregated into a unified format for efficient analysis and decision-making. Traditional methods often rely on rigid schemas or structured databases, which can falter with semi-structured or unstructured content (Orcutt et al., 1968; Jesus et al., 2014; Bloodgood, 2025). On the other hand, LLMs offer greater flexibility by processing both structured data (e.g., tables) and unstructured (e.g., text, images), enabling seamless integration (Das et al., 2024b; Su et al., 2024; Le et al., 2024). Additionally, LLMs can generate concise summaries of trends and correlations (Kurisinkel and Chen, 2023; Kuang et al., 2024; Li et al., 2024a), producing reports or dashboards that guide decision-making (John et al., 2023; Weng et al., 2024b,a).

3.4 Data Generation

Although LLMs excel at extracting, annotating, and aggregating data, they still face challenges when raw data is scarce in specific scenarios, such as disease modeling and low-resource languages (Yuan et al., 2023a; Whitehouse et al., 2023; Song et al., 2024). This data scarcity can severely hinder model development (Zhou et al., 2024e; Ding et al., 2024a). Nevertheless, LLMs help mitigate these limitations by generating synthetic datasets across various domains. For example, LLMs can simulate diverse IoT sensor conditions (Zhou et al., 2024c,d; An et al., 2024) and impute missing values across numerical, categorical, and textual fields (Little and Rubin, 2019; He et al., 2024; Chen et al., 2024g; Wang et al., 2025). Furthermore, by adhering to domain-specific distributions, LLMs generate specialized datasets for applications in finance, healthcare, and transportation (Nie et al., 2024; Belyaeva et al., 2023; Zhang et al., 2024h,i). These capabilities enable LLMs to produce high-fidelity synthetic data, ensuring dataset availability and enhancing model robustness even in data-scarce environments.

4 LLMs for Data Preparation

Effective data preparation is crucial for ensuring the quality, accessibility, and usability of data for downstream steps (Khatri and Brown, 2010b).

Data preparation generally aims to transform extracted data into a structured and analyzable format. Traditional approaches often struggle with labor-intensive workflows, making automation a pressing need. More recently, LLMs offer transformative solutions by automating feature extraction and streamlining data cleaning, thereby enhancing the efficiency and scalability of data preparation.

4.1 Feature Engineering

In the data preparation stage, feature engineering focuses on selecting, transforming, and generating data features to facilitate data analysis or improve model training (Li et al., 2017; Kusiak, 2001). LLMs automate and optimize feature engineering by analyzing dataset descriptions (e.g., column names, sample values) and adaptively selecting relevant features based on semantic or statistical cues (Choi et al.; Jeong et al., 2024; Lee et al., 2024b; Jia et al., 2024b; Toufiq et al., 2023; Li et al., 2024d; Luo et al., 2024; Yang et al., 2024a). Beyond selection, LLMs generate new features through arithmetic operations (Han et al.; Lee et al., 2024b; Zhang et al., 2024g; Küken et al., 2024; Wang et al., 2024d) and leverage advanced prompting techniques, such as evolutionary algorithms (Gong et al., 2024), code generation (Hollmann et al., 2024), and Monte Carlo Tree Search (Zhang et al., 2024f), to create more complex and dynamic feature transformations. By automating these processes, LLMs reduce the reliance on manual intervention and enhance the efficiency and adaptability of feature engineering.

4.2 Data Cleaning

Data cleaning ensures that raw inputs are accurate and consistent, addressing issues such as missing and noisy values, duplicate entries, and inconsistencies across data sources. LLMs can help automate data cleaning tasks, including repairing and imputing missing values in text (Hassan et al., 2023; Bolding et al., 2023; Zhang et al., 2024c; Choi et al., 2024), structured (Yan et al., 2024b; Li et al., 2024j; Zhu et al., 2024a; Ding et al., 2024a; Luo et al., 2024), and semi-structured data (Jain et al., 2023; Mondal et al., 2024; Huang et al., 2024d; Biester et al., 2024; Ni et al., 2024). Their effectiveness is further enhanced by retrieval augmentation (Ahmad et al., 2023), code-driven methods (Huynh and Lin), and efficient tuning approaches (Zhang et al., 2024j). Beyond fixing errors, LLMs help filter out irrelevant or low-quality samples, improv-

ing dataset integrity and ensuring cleaner training data for downstream applications. They play a crucial role in maintaining the quality of synthetic data pipelines by automatically detecting and removing noisy or unreliable samples (Li et al., 2024c; Wang et al., 2024b; Yasunaga et al., 2024; Tong et al., 2024; Liang et al., 2024).

4.3 Data Transformation

Data transformation converts raw data into structured, analyzable formats, making it more suitable for modeling and analysis. LLMs facilitate data transformation by converting unstructured data into structured formats such as graphs (Li et al., 2024e; Zhou et al., 2024a), trees (Yuan et al., 2024a), and executable code (Rajkumar et al., 2022a; Sharma et al., 2023; Mayer et al., 2024). They also assist in handling cross-modal data transformations, such as image captioning (Hu et al., 2022) and text-to-image generation (Brade et al., 2023). By automating these transformations, LLMs reduce the manual effort required to preprocess diverse data types, enhancing efficiency and scalability in data pipelines.

4.4 Data Organization

Data organization ensures structured storage, management, and retrieval of information. LLMs enhance various aspects of data organization, including database tuning (Giannankouris and Trummer, 2024; Fan et al., 2024; Huang et al., 2024e; Li et al., 2024n; Lao et al.), query optimization (Akioyamen et al., 2024; Li et al., 2024g; Sun et al., 2024b), system diagnosis (Zhou et al., 2023b; Chen et al., 2024d; Singh et al., 2024; Giannakouris and Trummer, 2024), and pipeline orchestration (Hoseini et al., 2024; Shetty et al., 2024), leveraging their broad generalization capabilities (Fernandez et al., 2023; Weng et al., 2024a; Junior et al., 2024; Kim and Ailamaki, 2024; Li et al., 2024p). Recently, as LLMs continue to scale in parameter size, researchers have been exploring efficient memory management and storage strategies to optimize data organization (Bang, 2023; Li et al., 2024b; Xu et al., 2024a; Wang et al., 2024a; Yuan et al., 2024c; Kim et al., 2024c; Lee et al., 2024c). Additionally, efforts are also focused on improving vector storage for retrieval-augmented generation (RAG) applications, ensuring scalable and efficient retrieval (Zhang et al., 2023d; Jing et al., 2024; Tareaf et al., 2024; Rochan et al., 2024).

5 LLMs for Data Analysis

Data analysis is a crucial stage in the data science workflow, bridging data preparation and data interpretation to extract meaningful patterns and insights. Traditional data analysis methods depend on predefined statistical techniques and limited prior knowledge. In contrast, LLMs enhance data analysis by leveraging their advanced reasoning and contextual awareness. LLMs can systematically interpret structured and unstructured data, uncover hidden relationships, and provide deeper insights beyond conventional approaches.

5.1 Descriptive Analysis

Descriptive analysis focuses on summarizing and exploring data patterns to extract meaningful patterns and insights. This step is fundamental to data analysis, serving as a foundation for more advanced inferential and predictive techniques. Traditional approaches, often relying on smaller models (e.g., BERT), struggle to capture complex semantics and contextual nuances (Jin et al., 2024a). More recently, LLMs have demonstrated exceptional capabilities in extracting valuable insights across diverse data types. Their ability to process large and unstructured datasets makes them particularly effective in uncovering patterns that might be difficult to detect using conventional methods.

Summarization. Recent research highlights the significant potential of LMs in extracting key insights from textual data. Direct extraction strategies aim to identify and retrieve key phrases or sentences directly from raw text (Viswanathan et al., 2023; Zhang et al., 2023e). LLMs have also demonstrated proficiency in abstractive summarization, such as generating TL;DR for academic papers (Zhang et al., 2024d), summarizing key sentences from documents and news articles (Zhao et al., 2023; Bražinskas et al., 2022), and obtaining descriptions for visual data (Yu et al., 2021) and tabular data (Zeng et al., 2024b). Notably, the effectiveness of these methods often relies heavily on prompt design. Recent advancements, such as automatic prompt discovery (Narayan et al., 2021), chain-of-thought (Wang et al., 2023e), and agent-based approaches (Xiao et al., 2023), have further enhanced LLMs' ability to generate structured and contextually rich summaries.

Exploratory Text Mining. Beyond summarization, LLMs enhance exploratory text mining for the discovery of latent patterns and insights from large

text corpora. LLMs aid in topic modeling (Pham et al., 2023; Yang et al., 2024b; Mu et al., 2024) and sentiment analysis (Sun et al., 2023b; Xing, 2024), tackling challenges like incomplete topics and hallucinations. Furthermore, cross-lingual (Miah et al., 2024) and multimodal frameworks (Wang et al., 2024a; Yu et al., 2022) extend LLMs’ scope beyond text, integrating diverse data modalities and multiple languages.

5.2 Analytical Reasoning

Analytical reasoning in data analysis involves using deductive techniques to extract meaningful insights from raw data. LLMs enhance this process by integrating pre-trained knowledge (e.g., commonsense and logical reasoning) with new data, enabling them to uncover high-level patterns and relationships across diverse modalities. For example, LLMs can effectively interpret patterns in complex textual data by understanding the contextual nuances (Chowdhery et al., 2023; Wyatte et al., 2024; Chae and Davidson, 2023). For images and videos, LLMs combined with vision encoders (e.g., CLIP (Radford et al., 2021), GPT-4V (Yang et al., 2023a)) exhibit strong reasoning capabilities in identifying objects, scenes, and abstract concepts (Wu et al., 2025; Cooper et al., 2024; Naeem et al., 2023). In audio analysis, LLMs enhance emotion recognition, speaker identification, and music genre detection when combined with audio embeddings (Zhang and Poellabauer, 2024; Dhingra et al., 2024; Meguenani et al., 2024; Li et al., 2021). Their ability to process graph-based data also extends to structural pattern recognition, transforming complex relationships into interpretable insights on graphs (Liu et al., a; Ye et al., 2023a; Guo et al., 2023; Srinivas and Runkana, 2024).

5.3 Interactive Analysis

Interactive analysis enables dynamic and user-driven data exploration by integrating iterative feedback, query-driven interpretation, and adaptive learning. LLMs enhance this process by engaging with data and user queries interactively, refining insights based on external feedback, and autonomously guiding analytical workflows. While traditional reinforcement learning can acquire experience from environmental rewards, it often lacks prior knowledge and exhibits poor generalization. **Feedback-Driven Analysis.** LLMs leverage external annotations and user feedback to iteratively analyze data, improving accuracy and adaptability

over time. LLMs have demonstrated the ability to reflect on external feedback for raw data (Hong et al., 2024; Ji et al., 2023b). Through memory retention and retrieval, LLMs store valuable analytical experiences, enabling more effective analysis of future data (Kim et al., 2024a; Shinn et al., 2024; Huang et al., 2022; Zhao et al., 2024a). These reflective capabilities extend beyond text, improving image generation (Yang et al., 2023b; Goswami et al., 2025) and personalized recommendation systems, where user feedback optimizes predictions and interactions over time (Xi et al., 2024; Wang et al., 2023f; Zhu et al., 2025).

Query-Driven Analysis. LLMs further support interactive analysis through query-answering interpretation, allowing users to extract insights from data intuitively. LLMs can answer questions on data across charts (Li et al., 2024r; Cheng et al., 2023; Han et al., 2023; Zhang et al., 2024a; Masry et al., 2023), tables (Li et al., 2024l; Zhou et al., 2024b; Zhu et al., 2024b), diagrams (Hu et al., 2024a; Wang et al., 2024d), and graphs (Xu et al., 2024b; Guo et al., 2023; Zhang et al., 2024i). For higher-level and more abstract questions, LLMs can dynamically select analytical techniques (Ma et al., 2023; Guo et al., 2024b; Zhu et al., 2024c; Liu et al., b; Zhang et al., 2023b) and autonomously generate exploration goals, queries, and interpretative answers without explicit prompts (Manatkar et al., 2024; Dibia, 2023).

5.4 Quantitative Analysis

Quantitative analysis focuses on extracting numerical insights from structured data using various techniques, including statistical methods, predictive modeling, and causal inference. LLMs generally enhance this process by automating calculations and improving model selection.

Statistical Analysis. LLMs assist in descriptive tasks, such as computing means and variances, across charts (Masry et al., 2023; Huang et al., 2024b; Liu et al., 2023a; Masry et al., 2024; Meng et al., 2024a; Do et al., 2023), tabular data (Brugere et al., 2024; Liu et al., 2023b), and time series (Jin et al., 2024b). Agent-based LLMs decompose multi-step calculations (Wang et al., 2023c; Huang et al., 2024c; Ye et al., 2023b; Wang et al., 2024h; Guo et al., 2024a) and invoke external tools and code for statistical modeling (Choe et al., 2024; Xia et al., 2023b; Wang et al., 2024f; Yuan et al., 2023b; Hong et al., 2024; Zhang et al., 2023b; Nascimento et al., 2024; Sun et al., 2024a). More-

over, LLMs facilitate hypothesis testing and correlation analysis (Qiu et al., 2024; Paruchuri et al., 2024; Zhu et al., 2024d; Liu et al., 2024c), offering interpretable approaches to statistical analysis.

Predictive Analysis. LLMs contribute to predictive modeling by assisting in the selection, development, and evaluation of models like linear regression and random forests (Nascimento et al., 2023; Junior et al., 2024; Hong et al., 2024). LLMs can also generate code for advanced tasks like time series forecasting (Morales-García et al., 2024; Ye et al., 2024), and adapt their reasoning across diverse data modalities, including text (Xiao et al., 2024b; Jacobs et al., 2024), time series (Jin et al., 2023; Chang et al., 2023; Jia et al., 2024a; Yu et al., 2023), charts (Masry et al., 2024; Wang et al., 2023g), tables (Yang et al., 2024c; Hamman et al., 2024; Wang et al., 2023d), and graphs (Wang et al.; Lin et al., 2024). Since LLMs are not intrinsically optimized for structured data, many frameworks combine LLMs with specialized deep learning techniques to enhance predictive performance (Zhang et al., 2024b; Bogahawatte et al., 2024; Moghadas et al., 2024; Liu et al., 2024a; Nam et al., 2024).

Causal Analysis. LLMs can uncover cause-and-effect relationships by refining Bayesian network structures and collaborating with causal discovery algorithms (Cohrs et al., 2024; Long et al., 2023; Ban et al., 2023b,a; Li et al., 2024p,k; Hu et al., 2024c; Liu et al., 2024c). Tool-augmented LLMs also invoke specialized causal discovery packages to improve inference (Shen et al., 2024).

6 Data Presentation

Data presentation is the final stage in the data science workflow, where processed and analyzed data is transformed into interpretable insights. This stage ensures that findings are effectively conveyed to users, enabling better comprehension. While traditional data presentation relies on manual scripting and specialized visualization tools, LLMs revolutionize the process by allowing users to generate and refine visual representations through natural language interaction, making data-driven insights more accessible and adaptable (Qin et al., 2020; Alvarez et al., 2021).

6.1 Human-Centric Visualization Generation

LLMs can output code, structural specifications, and chart queries based on user input to generate visualizations (Maddigan and Susnjak, 2023; Chen

et al., 2024c; Ko et al., 2024; Li et al., 2024m; Wang et al., 2023b). Users provide dataset details and analysis goals, iteratively refining visual outputs when necessary (Tian et al., 2024; Dibia, 2023). Users can also interactively modify LLM-generated visualizations through adaptive interfaces (Chen et al., 2022).

6.2 Interactive Presentation

Discussion. Beyond single-instance visualizations, multi-agent systems extend LLM-driven visualization by enabling collaborative generation and refinement (Chugh et al., 2023; Guan et al., 2024). For instance, one agent may write or debug visualization scripts (ALMutairi et al., 2024), while another creates graphs or serves as a task planner (Islam et al., 2024; Li et al., 2024i; Xue et al., 2024). LLM can also convert natural language instructions into structured commands for visualization agents (Huang et al., 2024a).

Human-Driven Decision-Making. LLMs assist by offering expert-like suggestions or collaborating with human users (Ma et al., 2024; Cao et al., 2024a). In healthcare, they can improve diagnostic accuracy while aligning with professional guidelines (Umerenkov et al., 2023; Benary et al., 2023; Goh et al., 2023; Eigner and Händler, 2024).

7 Social Impact and Future Work

Despite the remarkable capabilities, LLMs also exhibit crucial shortcomings that can hinder data science projects. In this section, we introduce the ethics concerns, limitations, and future work of LLMs in data science.

7.1 Ethics Consideration

Bias & Fairness. LLMs can embed implicit biases that skew results and violate fairness principles (Dai et al., 2024a; Gallegos et al., 2024; Li et al., 2023c). For instance, LLM-generated content may be over-ranked by certain IR or RAG systems (Dai et al., 2024b; Chen et al., 2024e; Bao et al., 2023), while inaccuracies, irrelevancies, or instruction deviations go unchecked (Liu et al., 2024b; Lee et al., 2022; Min et al., 2023; Durmus et al., 2020; Maynez et al., 2020). Moreover, LLM-based evaluators have displayed favoritism toward specific tokens or group attributes (Hou et al., 2024; Chen et al., 2024b; Wang et al., 2024c; Liu et al., 2023c; Zhang et al., 2024k), necessitating careful mitigation strategies.

Privacy. LLMs pose privacy risks by potentially exposing sensitive user data in prompts or inferred attributes (Yan et al., 2024a; Neel and Chang, 2024; Das et al., 2024a). Cloud-hosted services may log personally identifiable information (PII)(Iqbal et al., 2024), and the models themselves can accurately infer unobserved traits such as occupation or location(Staab et al., 2024). Recent surveys highlight the roles of model size, data duplication, and prompt length in such leaks (Neel and Chang, 2024), prompting research into differential privacy (Dwork, 2006), federated learning (McMahan et al., 2017), multi-level privacy evaluations (Shao et al., 2024), and privacy-preserving synthetic data generation (Wang et al., 2024e; Ramesh et al., 2024) to mitigate these threats.

7.2 Limitations and Future Work

Sensitivity to Dataset Formats. LLMs often exhibit inconsistent performance across different serialization formats, making it hard to automate tasks on tabular or semi-structured data. Some studies show superior fact-searching accuracy when data is presented as DFLoader or JSON, yet better table-specific tasks (e.g., partitioning, cell lookup) emerge in HTML or XML formats—especially notable for GPT-4 (Fang et al., 2024; Singha et al., 2023; Sui et al., 2024; OpenAI, 2024a). These findings reveal that minor changes in data format alone can lead to sizable variations in LLM performance, complicating development pipelines.

Reasoning over Numerical Operations. LLMs are also known to have reasoning limitations, especially over numerics. Competitive LLMs such as GPT-4o (OpenAI, 2024b) can easily output incorrect number comparison $9.11 > 9.9$ if the generation order between thought and conclusion is reversed (Xie, 2024), while other evidences show LLMs easily making mistakes on symbolic operations when processing tabular data (Chen, 2023). These LLMs can also frequently struggle with primitive operations such as letter counting within a word, whose error rate strongly correlates with the total (and individual) number of tokens in a word (Fu et al., 2024) and tokenization design (Zhang et al., 2024e).

Test-time Overthinking. Models specialized with extended test time compute or long reasoning such as OpenAI O1 (OpenAI, 2024c), QWQ (Qwen, 2024) and DeepSeek R1 (DeepSeek, 2024) are known to overthink on simpler mathematic questions, causing unnecessarily long reasoning chain

and incorrect results that cannot be addressed by length-adjusted preference optimization (Meng et al., 2024b) and only partially mitigated by solution filtering in conjunction with reflection (Chen et al., 2024f).

Token Inefficiency. When raw tables become large (even as small as 30 rows), LLMs often fail to parse the data effectively, leading to inflated token usage and increased computational costs (Chen, 2023; Fang et al., 2024). This token inefficiency often forces external execution strategies, such as Python scripts (Chen et al., 2023b; Gao et al., 2023), SQL queries (Rajkumar et al., 2022b), verifier programs (Ni et al., 2023), or dynamic decomposition (Ye et al., 2023c; Wang et al., 2024g), to reduce context size and limit hallucinations (Ji et al., 2023a).

Tokenizer-Free Representation. Conventional tokenization methods (Schuster and Nakajima, 2012; Sennrich et al., 2016; Kudo and Richardson, 2018) often split numbers into multiple fragments (e.g., “digit chunking”), encouraging memorization rather than true algorithmic processing (Spathis and Kawsar, 2024). Systems like Byte Pair Encoding (BPE) (Sennrich et al., 2016) can produce inconsistently tokenized numerals, whereas LLaMA retains numbers intact (Fang et al., 2024). Recently, Byte Latent Transformers (BLT) (Pagnoni et al., 2024) propose a more flexible approach by treating tokenization as an inference-time byte-grouping problem driven by lightweight encoding-decoding models and byte-level entropies, rather than a fixed, pre-trained vocabulary. This shift promises greater adaptability and performance comparable to conventional tokenizers.

8 Conclusion

In this survey, we examined the role of large language models (LLMs) in enhancing data science workflows, focusing on their applications across various stages, from data acquisition to analysis and presentation. While LLMs offer significant potential to automate and streamline tasks, challenges such as model reliability, data quality, and ethical concerns like bias and privacy risks remain. Future research should aim to address these limitations by improving model robustness, interpretability, and integration with traditional methods. Ultimately, LLMs can transform data science practices, offering more efficient, accessible, and automated solutions for a wide range of industries and domains.

Limitation

While this survey provides a broad overview of the role of LLMs in data science, there are several limitations to consider. First, the rapid pace of developments in LLMs means that some of the discussed techniques, applications, and challenges may quickly become outdated. Additionally, the survey primarily focuses on high-level applications and concepts, which may not capture the full technical depth or domain-specific nuances of LLM usage in data science. Furthermore, given the vast scope of data science, the survey may not address every potential application of LLMs in all subfields, and certain interdisciplinary applications might have been underrepresented. Finally, due to the complexity of LLMs, certain challenges such as model biases and ethical implications may require more focused, in-depth exploration than what this survey can provide.

Ethics Statement

This survey acknowledges the importance of ethical considerations in the use of LLMs within data science. The applications discussed in this work are subject to potential ethical concerns, including but not limited to bias in model predictions, privacy risks, and fairness in decision-making. LLMs, being trained on vast and often uncensored datasets, may unintentionally perpetuate societal biases, which can influence data science workflows and lead to inequitable outcomes. Furthermore, the use of LLMs in sensitive domains, such as healthcare and finance, requires strict adherence to ethical guidelines to safeguard user privacy and ensure transparency in automated decision-making processes. Researchers and practitioners are encouraged to prioritize the ethical implications of deploying LLMs in data science applications and to strive for solutions that mitigate bias, enhance model interpretability, and uphold privacy and fairness standards. This survey aims to raise awareness of these challenges and advocates for continued research into the responsible use of LLMs in data science.

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A Bridging Traditional Data Science with LLM Capabilities

The integration of LLMs into data science represents a paradigm shift in how data is processed and analyzed. Traditional approaches often rely on rigid rules and extensive feature engineering. LLMs, however, can generalize across tasks and domains by leveraging extensive pre-trained knowledge and contextual understanding (Dai and colleagues, 2024). Particularly, LLMs reduce dependency on predefined schemas and enable more adaptive and flexible data workflows. For instance, they can generate synthetic data to address gaps in existing datasets (Zhou, 2024), clean and structure raw data, and support complex analytical tasks using natural language interfaces (Chen and Si, 2024). Moreover, LLMs democratize data science by allowing non-experts to engage with data via conversational interfaces. This capability lowers barriers to data-driven decision-making and encourages collaboration between technical and non-technical stakeholders (Zhang, 2024).

In conclusion, the evolution of data science reflects a continuous progression towards greater automation, scalability, and accessibility. LLMs are instrumental in this transformation, offering unprecedented opportunities to enhance every stage of the data science life cycle.

B Applications

LLMs have transformed specialized fields by automating complex language tasks, streamlining domain-specific workflows, and supporting more informed decision-making (Shu et al., 2017; Li et al., 2017; Zafarani, 2014). Applications extend beyond generic data science processes to include social science, medical research, finance, legal analysis, education, and environmental sciences.

B.1 Social Science

In social science, LLMs analyze large volumes of unstructured data to uncover human behavior, societal trends, and policy impacts.

Sentiment Analysis. By processing texts from platforms like Twitter or Reddit, LLMs detect emerging issues, predict social shifts, and inform policymaking (Törnberg, 2023; Zeng et al., 2024a; Zhang et al., 2023c; Jiang et al., 2024). Their ability to handle slang, dialects, and multilingual inputs makes them invaluable for studying diverse populations (Törnberg, 2024; Broekens et al., 2023;

Shaikh et al., 2023; Dudy et al., 2024; Bian et al., 2023).

Policy Making. LLMs streamline policy research by analyzing government documents, academic literature, and public feedback. They identify key themes, summarize large text corpora, and highlight policy outcomes, allowing real-time evaluation of effectiveness and reducing manual effort (Chen et al., 2024a; Ishimizu et al., 2024; Kasztelnik and Branch, 2024; Ziems et al., 2024; Weber and Reichardt, 2023).

B.2 Medical

In healthcare, LLMs enhance clinical decision-making, patient care, and drug discovery, offering structured insights from vast clinical records and scientific literature.

Clinical Diagnostics. LLMs extract critical information from unstructured patient data—such as symptoms and test results—to assist with diagnosis recommendations and risk detection (Wang et al., 2023a; McPeak et al., 2024; Lorenzoni et al., 2024; Xia et al., 2023a). This reduces clinicians' workload while improving diagnostic accuracy (Xie et al., 2024; Bannett et al., 2024; Panagoulas et al., 2024).

Drug Discovery. In pharmaceutical research, LLMs parse scientific articles and experimental data to identify promising compounds, predict molecular interactions, and accelerate drug development timelines (Xu and Elemento, 2024; Tripathi et al., 2024; Sallam, 2023; Bran et al., 2023; Cao et al., 2023).

B.3 Finance

Financial applications of LLMs include risk analysis, fraud detection, and market prediction, all benefiting from their ability to handle large, domain-specific datasets.

Risk Management. LLMs analyze financial statements, regulatory documents, and news feeds to identify market volatility, credit risk, and other threats (Cao et al., 2024b,c; Xiao et al., 2024c; Pankajakshan et al., 2024), enabling proactive strategies in fast-paced markets.

Fraud Prevention. By examining transactional data for anomalies, LLMs help financial institutions mitigate fraud risks and ensure regulatory compliance (Yin et al., 2023; Chakraborty et al., 2024; Gregory and Vito, 2024; Sun et al., 2023a; Chang et al., 2022).

B.4 Other Domains

Beyond social science, medicine, and finance, LLMs also support legal, educational, and environmental sectors by automating core data-related tasks.

Legal. LLMs extract and structure case law, identify critical clauses, and compare precedents to forecast legal outcomes (Shui et al., 2023; Fei et al., 2023; Zhao et al., 2024d; Shu et al., 2024; Kalra et al., 2024; Harasta et al., 2024).

Education. In academic settings, LLMs preprocess student interaction data from learning platforms to reveal engagement patterns, generate personalized learning features, and boost predictive models for performance (Wang et al., 2024e; Leinonen et al., 2024; Gan et al., 2023; Zhao et al., 2024b; Alhafni et al., 2024; Li et al., 2023b).

Environmental Sciences. LLMs ingest climate reports, track environmental indicators, and produce actionable insights, helping policymakers develop strategies for climate change mitigation (Kraus et al., 2023; Thulke et al., 2024; Oliver et al., 2024; Chen et al., 2023a).

By applying LLM-based techniques to domain-specific challenges, practitioners gain deeper insights, streamline workflows, and make data-driven decisions that span multiple fields.

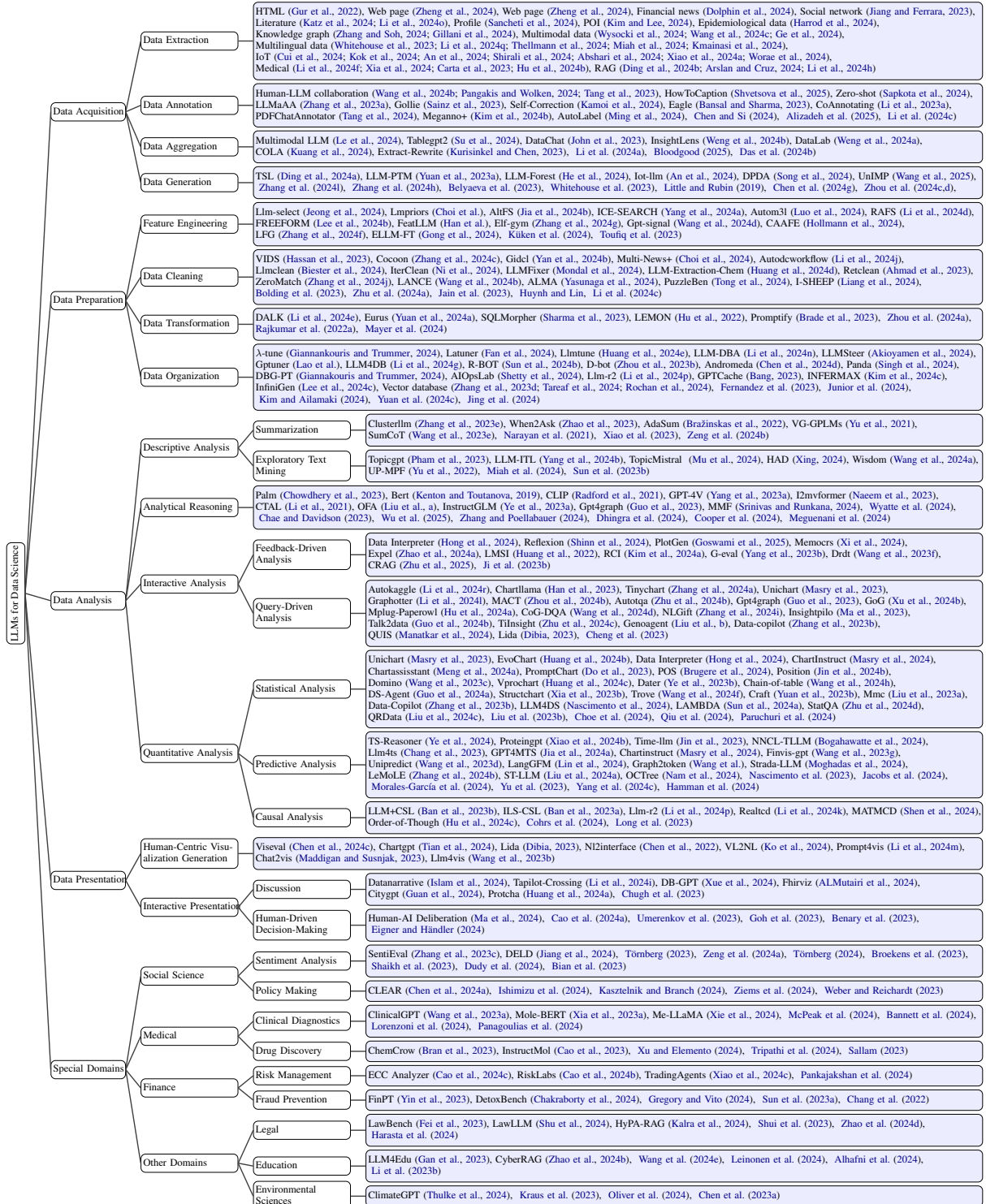


Figure 2: LLMs for Data Science