

# Large Language Model-based Data Science Agent: A Survey

**Peiran Wang<sup>†</sup>**

*University of Illinois Urbana-Champaign*

*whilebug@gmail.com*

**Yaoning Yu<sup>†</sup>**

*University of Illinois Urbana-Champaign*

*ynn003600@gmail.com*

**Ke Chen<sup>†</sup>**

*University of Illinois Urbana-Champaign*

*kec10@illinois.edu*

**Xianyang Zhan**

*University of Illinois Urbana-Champaign*

*zhan39@illinois.edu*

**Haohan Wang**

*University of Illinois Urbana-Champaign*

*haohanw@illinois.edu*

## Abstract

The rapid advancement of Large Language Models (LLMs) has driven novel applications across diverse domains, with LLM-based agents emerging as a crucial area of exploration. This survey presents a comprehensive analysis of LLM-based agents designed for data science tasks, summarizing insights from recent studies. From the agent perspective, we discuss the key design principles, covering agent roles, execution, knowledge, and reflection methods. From the data science perspective, we identify key processes for LLM-based agents, including data preprocessing, model development, evaluation, visualization, etc. Our work offers two key contributions: (1) a comprehensive review of recent developments in applying LLM-based agents to data science tasks; (2) a dual-perspective framework that connects general agent design principles with the practical workflows in data science.

## 1 Introduction

In recent years, the rapid development of Large Language Models (LLMs) has driven significant innovations across various domains. Leveraging their remarkable capabilities in understanding and generating human-like text, LLMs have become foundational in creating intelligent agents capable of performing complex tasks autonomously. These agents have demonstrated substantial potential in diverse fields, including healthcare Qiu et al. (2024), finance Yu et al. (2024), education Zhang et al. (2025b), and software engineering Hong et al. (2023).

Among these fields, data science has emerged as a particularly critical area for applying LLM-based agents Sun et al. (2024b). Data science involves extracting meaningful insights from vast and diverse datasets, a process that traditionally requires extensive manual effort and expertise. Consequently, LLM-based data science agents (DS Agents) have attracted attention for their ability to automate and optimize data analysis, model development, and decision-making processes.

In this survey, we examine LLM-based data science agents from two complementary perspectives: agent design and data science application. From the agent design perspective, we summarize key architectural paradigms—including single-agent systems, collaborative multi-agent structures, and dynamic agent generation—and analyze core components such as agent roles, execution strategies, knowledge integration, and reflection mechanisms. From the data science perspective, we explore how LLM agents are applied across

---

<sup>†</sup> These authors contributed equally to this work.

---

major workflow stages such as data preprocessing, modeling, evaluation, and visualization. We also outline common task types, including model-building and insight-generation tasks, and characterize the iterative nature of the data science loop. Additionally, our survey goes beyond mere documentation by synthesizing insights from recent studies to identify research opportunities and future directions in this evolving field Sahu et al. (2024); Fan et al. (2023).

From the agent perspective (§3), we summarize how the agent structure is designed (§3.1), how the reasoning of LLM within agents is performed (§3.2), where the knowledge comes from (§3.3), and the reflection of the agent (§3.4). From this perspective, we provided a comprehensive analysis of the agent design of LLM-based data scientist agents.

From the data science perspective (§4), we summarize how LLM-based agents are applied across key stages of the data workflow, including data preprocessing, modeling, evaluation, and visualization. We categorize common task types such as model development and insight generation, and highlight the recurring data science loop that these agents help automate. This perspective clarifies the practical roles LLM agents play in enabling end-to-end data analysis.

In summary, this survey makes two primary contributions.

- It provides a comprehensive review of recent efforts to apply LLM-based agents to data science tasks, synthesizing work across areas such as data preprocessing, modeling, evaluation, and visualization.
- It proposes a dual-perspective framework that bridges the gap between general agent design principles—such as role allocation, execution, and reflection—and the specific operational needs of data science workflows, offering a structured lens to understand and develop LLM-based data science systems.

## 2 Related Works

Recent surveys on LLM-based multi-agent systems have introduced various taxonomies from architectural, task-specific, and coordination perspectives. We briefly review them and highlight how our approach differs.

### 2.1 Modular Architectures

Existing surveys often decompose LLM-based agents into functional modules such as planning, memory, perception, and action. For example, Guo et al. (2024b) identifies components like agent-environment interface and capability acquisition; similar structures appear in Liu et al. (2024a), Sun et al. (2024b), and others.

Our work adopts this modular view but anchors it in the context of data science workflows. Instead of listing capabilities, we emphasize how modules interact during task execution—e.g., how reasoning, planning, and knowledge access are coordinated in dynamic or static execution (§3.2), and how external knowledge sources are integrated into decision-making (§3.3). We also highlight how modularity supports runtime adaptation through reflection mechanisms (§3.4), where agents adjust behaviors based on feedback, errors, or performance signals—enabling dynamic coordination across modules.

### 2.2 Collaboration and Communication

Agent collaboration is commonly categorized by structure (centralized, decentralized) or mode (cooperation, competition, etc.), as seen in Tran et al. (2025). Related works Guo et al. (2024b), Li et al. (2024g) discuss role-based or layered designs.

However, these are mostly static views. In our work, we also examine dynamic orchestration, where agents adaptively coordinate by adjusting roles or workflows during execution. This includes settings where task allocation evolves based on feedback, or agents are restructured at runtime to respond to changing demands (§3.1.4, §3.2).

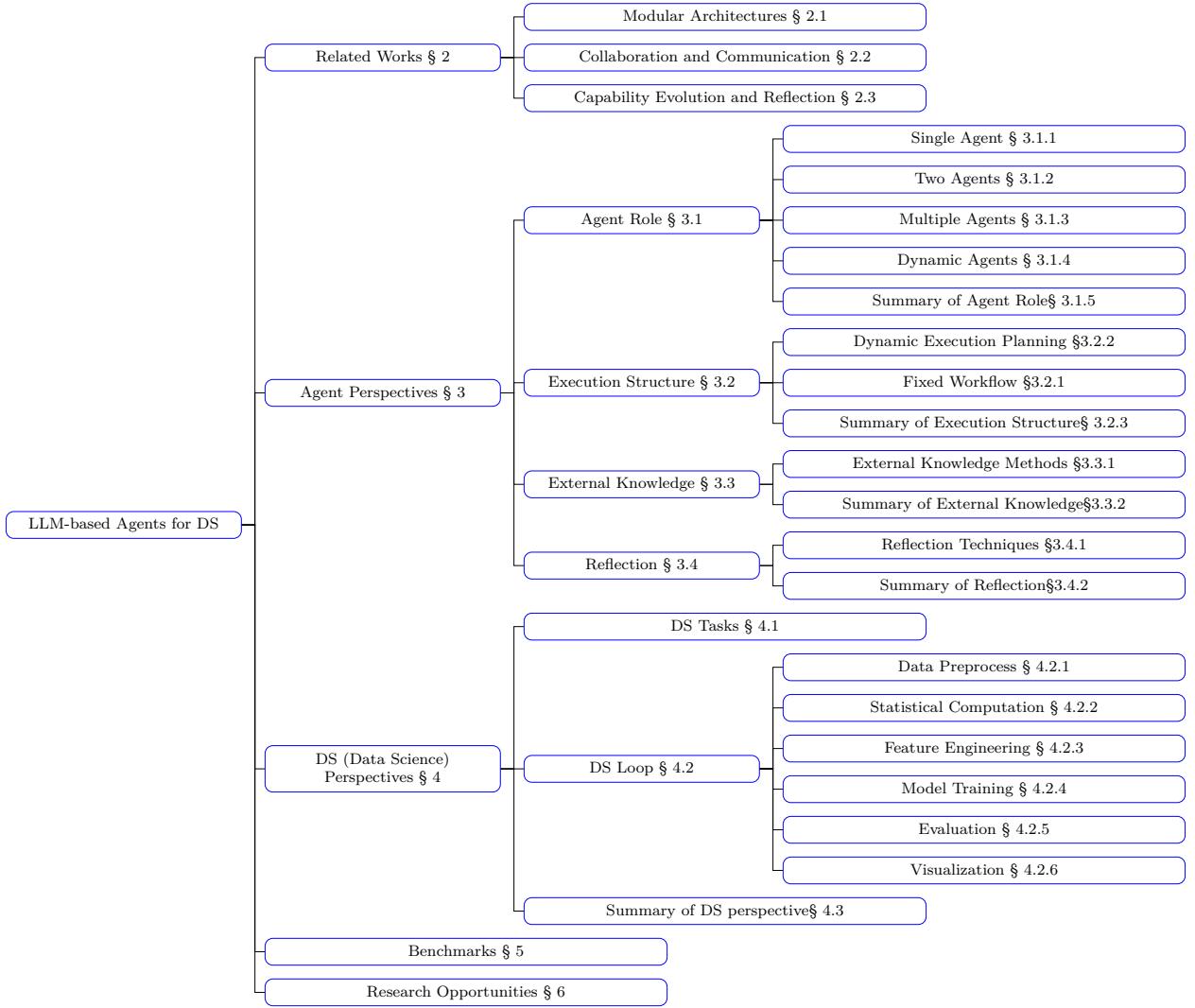


Figure 1: Structure of This Survey

## 2.3 Capability Evolution and Reflection

Several surveys recognize that agent systems can adapt via feedback, memory updates, or reflection—for example, Li et al. (2024g) includes an evolution phase with memory consolidation, and Wang et al. (2024a) discusses reflective planning. Similar notions appear in Guo et al. (2024b) and others.

In contrast to treating reflection as an auxiliary feature, we emphasize it as a cross-stage mechanism that drives dynamic execution adjustments (§3.4). We outline three key dimensions: the driver, level(scope of impact), and adaptability of reflection, framing reflection as a central control process for progress monitoring and adaptive behavior.

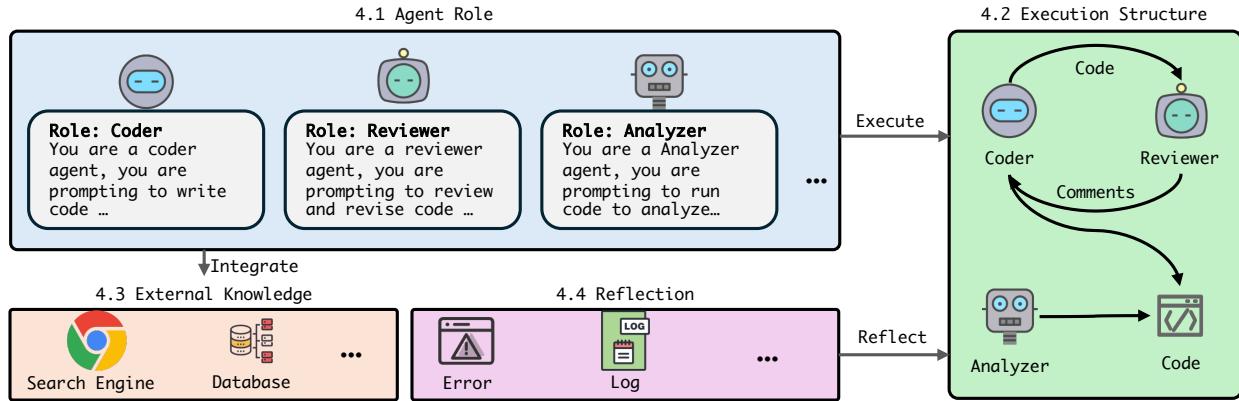


Figure 2: We illustrate the basic components for current data science agents: 1) agent role; 2) execution structure; 3) knowledge and 4) reflection.

### 3 Analysis from Agent Perspective

Large Language Model (LLM)-based agents have emerged as powerful tools in various domains, particularly in data science. The design and functionality of LLM-based agents can be understood through their basic components, which include agent role, execution structure, knowledge, and reflection.

**Agent role** (see §3.1). LLM agents are allocated different roles, which allows the agents to split the main tasks and focus on specific tasks. Diverse agent roles are presented in previous works, ranging from single-agent systems handling all tasks independently to multi-agent systems with specialized roles like developers, testers, planners, etc.

**Execution structure** (see §3.2). The execution structure designs how agents manage task allocation, task execution, user interaction, error handling, etc. The execution structure covers dynamic planning where agents adjust plans based on real-time feedback, fixed workflows with predefined task sequences, and plan-then-execute frameworks that separate strategy formulation from task execution.

**External Knowledge** (see §3.3). The knowledge sources allow agents to access and integrate external information, enhancing their ability in specific domains. LLM-based agents augment their knowledge through external databases, retrieval-based approaches, and API calls.

**Reflection** (see §3.4). Reflection methods provide feedback information for LLM-based agents to improve performance and adapt to complex environments. Techniques include agent feedback for self-correction, model metrics feedback for optimization, code error handling for reliability, and history window mechanisms for long-term learning.

#### 3.1 Agent Role Design

In this section, we discuss the role design of LLM-based agents, focusing on their agent role specification. Starting from single-agent designs, which manage all tasks independently, we summarize the transition to two-agent systems that introduce role separation, such as planner-executor and coder-reviewer frameworks. Furthermore, we conclude different multi-agent systems, covering software engineering style systems, minimum function agents, etc. Lastly, we introduce some dynamic agent role design frameworks where agents are generated adaptively rather than predefined.

##### 3.1.1 Single Agent

The single-agent design is the simplest design structure as shown in Figure 3. Most existing single-agent works directly follow the ReAct design (a prompting technique , where LLMs are used to generate both reasoning traces and task-specific actions) Freimanis & Andersson Rhodin (2024); Chen et al. (2024a); Sun

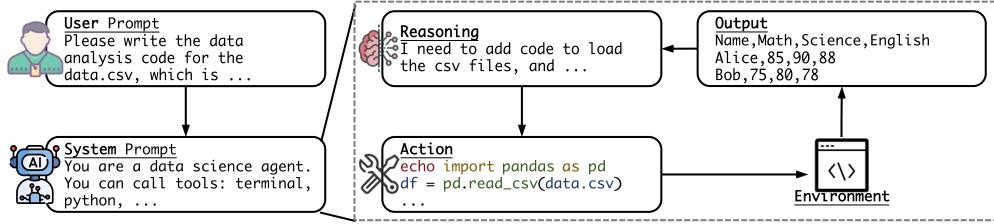


Figure 3: The basic structure for a single agent structure, with only the agent and execution environment.

et al. (2024a); Jing et al. (2024); Hu et al. (2024a); Deng et al. (2024); Le et al. (2023); Zhang et al. (2024a); Gupta et al. (2024)Bendinelli et al. (2025); Xu et al. (2025), where the single agent will perform thought, action, and observation processes iteratively on its own.

### 3.1.2 Two Agents

Evolving from the single agent, the two-agent design is introduced to decompose the single agent's functions, dividing the functions into two specialized roles, particularly either a planner&executor or code&reviewer structure.

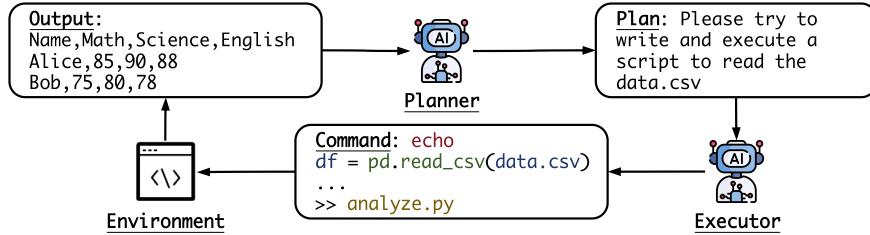


Figure 4: An example of planner and executor agent structure, where the planner generates a plan for the executor to execute in detail.

**Planner and executor.** Different from the single agent discussed previously, some works split the single agent into two agents Huang et al. (2024b); Liu et al. (2024b); Zhang et al. (2023b); Chi et al. (2024); Li et al. (2024e)Wang et al. (2025a), planner and executor. As an example shown in Figure 4, the planner will get observations from previous execution results or users' requests, and generate a next-step plan, or a whole plan in advance. Then, the executor is prompted to interact with the environments and will follow the generated plans to execute.

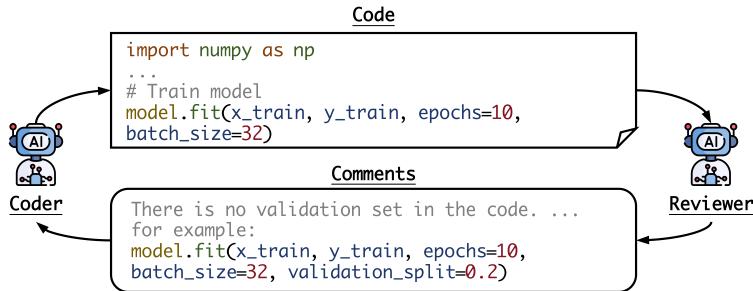


Figure 5: In the coder&reviewer structure, the coder generates the code, while the reviewer will make comments to revise the code for the coder.

**Coder and reviewer.** Another type of two-agent structure is the “coder and reviewer” style Trirat et al. (2024); Huang et al. (2023) as shown in Figure 5. In such a design, the coder is responsible for completing tasks following the typical ReAct structure. Another agent, the reviewer is introduced to check the validity of the code generated by the coder. Trirat et al. (2024) allows the reviewer to check the generated response

at each step of generation, while Huang et al. (2023) only allows the reviewer to function at the end of the entire generation process.

### 3.1.3 Multiple Agents

Multi-agent systems enhance problem-solving capabilities by enabling collaboration among multiple agents, each with distinct roles and expertise. In such systems, agents are assigned specialized responsibilities, allowing them to focus on different tasks while exchanging progress and information.

**Software engineering-style team.** The Software Engineering (SE) team-style agent design draws inspiration from traditional human software development teams Qian et al. (2024); Zhao et al. (2024b); Trirat et al. (2024); Hong et al. (2023); Tao et al. (2024); Lin et al. (2024); Nguyen et al. (2024). In an SE team-style framework, agents are typically assigned roles that correspond to key human roles in software development, here we state some example roles: The product manager defines the product vision and organizes requirements. The requirements analyst translates user needs into detailed software specifications. The scrum master facilitates task planning and sprint coordination. Hierarchical roles like team leader, module Leader, and function coordinator handle task decomposition at varying levels of granularity. The executor for the task is the developer, who is responsible for implementing the code, while the senior developer refines it. Finally, the QA engineer ensures quality through rigorous testing, and the tester validates specific functionalities. Some SE team-style agents also perform hierarchical roles which allow some agents with high permissions to manage others.

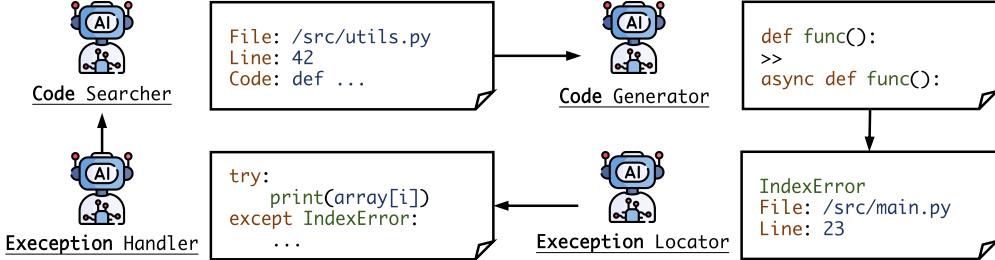


Figure 6: For agents with minimum functions, each agent is only responsible for a minimum function, such as search code, run code, etc.

**Minimum function agents.** Minimum function agents are designed to handle narrowly scoped and atomic tasks separately, as shown in Figure 6. Across existing frameworks, minimum function agents are given very small and specific functions to handle. For instance, code search agents locate relevant files, classes, or methods within a repository, while fault localization agents identify buggy code sections using debugging techniques like spectrum-based fault localization Zhang et al. (2024e). Other agents specialize in generating patches to fix identified issues, executing tests to validate code correctness, or systematically building repository structures from high-level descriptions Zan et al. (2024); Arora et al. (2024). In the context of exception handling, some agents detect fragile code, identify exception types, and implement robust handling mechanisms to enhance code reliability Zhang et al. (2024b). All works emphasize task decomposition and modularity, with outputs from one agent often serving as inputs for another, forming structured and collaborative workflows Zan et al. (2024); Phan et al. (2024); Arora et al. (2024); Seo et al. (2025); You et al. (2025); Ou et al. (2025).

**Client-server design.** Client-server agents, adopt a hierarchical architecture where a central controller agent manages and coordinates the operations of multiple specialized client agents Zhang et al. (2023a); Yang et al. (2024a); Gandhi et al. (2024); Zhao et al. (2024a). The controller or server agent functions as a project manager, planning entire workflows of the given tasks, and allocates the tasks to the client agents. Client agents perform as roles like software engineers or testers, focusing on executing specific subtasks such as data analysis, modeling, or feedback generation. These roles allow for clear separation of tasks, while also enabling dynamic adjustments based on task requirements or external feedback Zhang et al. (2023a); Bai et al. (2024); Zhao et al. (2024a); Shen et al. (2024).

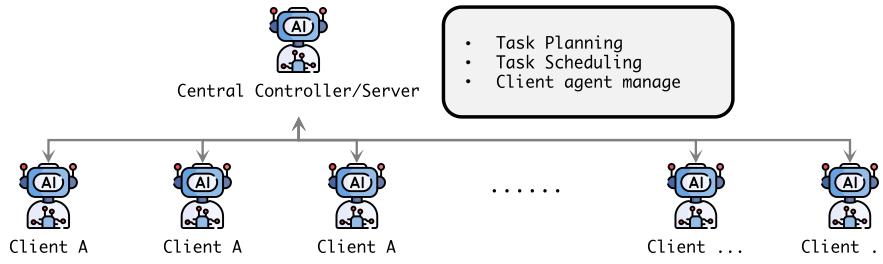


Figure 7: In the client-server agent structure, normally there will be a central server controls all the other clients.

### 3.1.4 Dynamic Agents

Dynamic agents represent a class of multi-agent systems that emphasize adaptability by dynamically creating, modifying, or expanding agents during runtime. Unlike static agents, which follow predefined workflows and configurations, dynamic agents are designed to respond to the complexity or variability of tasks by adjusting the agents' internal structure (prompt, etc.) or introducing new agents Hu et al. (2024b); Ishibashi & Nishimura (2024). Current frameworks for dynamic agent creation adopt two primary paradigms:

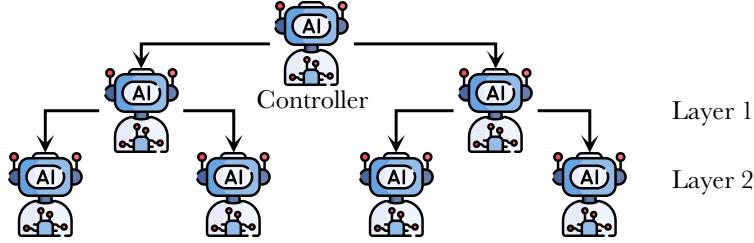


Figure 8: Hierarchical agent generation.

**Hierarchical agent generation.** This paradigm involves a parent agent or a high-level controller (e.g., Mother Agent in SoA Ishibashi & Nishimura (2024)) that decomposes complex tasks into subtasks. Each child agent operates independently on its specific subtask. It is particularly effective in managing tasks with clear functional divisions, such as modular code generation or system-level software design Ishibashi & Nishimura (2024).

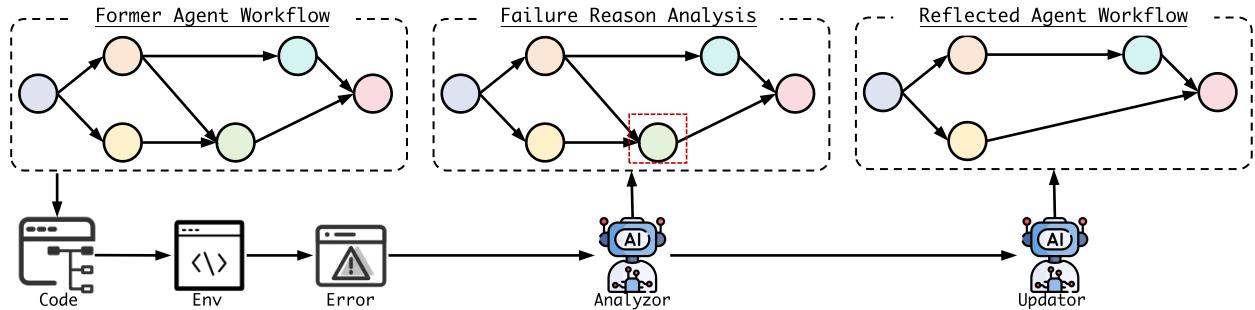


Figure 9: Iterative agent generation through feedback.

**Iterative agent generation through feedback.** Dynamic agents adjust their structures and behaviors iteratively based on real-time feedback from their environment or other agents (Figure 9). EvoMAC Hu et al. (2024b) exemplifies this paradigm, employing a collaborative rather than hierarchical approach, where agents refine their outputs and workflows through mechanisms analogous to backpropagation—such as a loss agent computing errors and an update agent adjusting agent workflows accordingly. This textual feedback enables the dynamic creation or reconfiguration of agents, supporting adaptability for tasks with evolving requirements, such as changing software specifications (Figure 9) Hu et al. (2024b).

### 3.1.5 Summary of Agent Role

Beyond specific agent role design, we summarize the key features of agent roles, including agent structure, agent relationship, role task allocation, and task granularity. These key features reveal the core thoughts through the design of agent roles.

Framework	CS	FL	PG	VA	RI	ED	EH
AutoCodeRover	✓	✓	✓	✓			
CODES					✓		
HYPERAGENT	✓			✓			
MASAI	✓	✓	✓	✓			
Seeker					✓	✓	

Table 1: This table summarizes the roles of Minimum Function Agents in different frameworks. The columns represent specific functions: Code Search (CS), Fault Localization (FL), Patch Generation (PG), Validation (VA), Repository Initialization (RI), Exception Detection (ED), and Exception Handling (EH). A checkmark (✓) indicates that the framework supports the corresponding function.

Role	PM	RA	AR	SM	TL	ML	FC	DE	SD	QA	TE
AgileCoder	✓			✓				✓	✓		✓
AutoML-Agent	✓									✓	
ChatDev		✓						✓			✓
FlowGen		✓	✓	✓				✓			✓
MetaGPT	✓		✓					✓		✓	✓
MAGIS	✓							✓		✓	
VisionCoder					✓	✓	✓	✓			✓

Table 2: Summary of SE Team Roles in Agent Designs: Product Manager (PM), Requirements Analyst (RA), Architect (AR), Scrum Master (SM), Team Leader (TL), Module Leader (ML), Function Coordinator (FC), Developer (DE), Senior Developer (SD), QA Engineer (QA), Tester (TE).

**Agent structure.** The structure of LLM-based agents can be categorized into several types, each with its advantages and challenges:

1. With a manager: In this structure, a central agent manages and controls all agents. Software engineering-style agents and Client-server agents mainly have this structure. For example, in the AutoML-GPTTrirat et al. (2024) framework, a central LLM serves as the controller, managing the entire pipeline by integrating specialized agents for subtasks such as model design and hyperparameter tuning.
2. Without a manager: Each agent operates independently and solves tasks autonomously. Minimum function agents mainly pose this structure, since all the agents with minimum function share the same position. An example of this is the MASAI Arora et al. (2024) framework, which utilizes decentralized agents that collaborate on machine learning and data science tasks by sharing results but not a central management system.
3. Hierarchical managers: A higher-level agent controls lower-level agents in a layered structure. Hierarchically generated agents and part of software engineering style agents mainly pose such structure. An example of this can be found in Hierarchical agent generation, such as in EvoMAC Hu et al. (2024b), where a parent agent dynamically creates child agents to handle specific subtasks during runtime.

**Agent relationship.** The relationship between agents within the system can vary significantly depending on the design philosophy:

1. Compete: Agents work against each other to complete a task, often in the coder-reviewer paradigm (similar to the adversarial concept in GAN). In frameworks like MASAI Arora et al. (2024), agents engage in competitive strategies to address machine learning and data science challenges. The competition

---

between reviewers and coders allows the iterative refinement of the code. Some works also allow multiple agents to propose multiple plans to compete.

2. **Collaborate**: Agents work together toward a shared objective. For example, in the MAGIS Tao et al. (2024) framework, agents assume different roles like Manager, Developer, and QA Engineer to collaborate on resolving GitHub issues. Their tasks are divided to ensure modular development, with continuous collaboration between agents.
3. **Hybrid**: Agents alternate between competing and collaborating based on the task requirements. For instance, in AutoCodeRover Zhang et al. (2024e), agents work together to localize faults and generate patches, but may compete in terms of optimizing solutions or strategies based on the specific issue at hand.

**Agent role task allocation.** LLM-based agents can allocate tasks in either a static or dynamic manner:

1. **Static Task Allocation**: In some systems, agents are assigned a fixed set of tasks that they perform. For example, in the Data Director Hong et al. (2024) framework, agents follow a static task allocation, where the tasks are predefined and agents work through structured stepwise execution.
2. **Dynamic Task Allocation**: Tasks are allocated based on the real-time needs and feedback from the system or environment. An example of dynamic task allocation can be seen in the EvoMAC Hu et al. (2024b) framework, where agents adjust dynamically based on environmental feedback, creating or dismissing agents as needed to refine or expand their tasks.

**Agent Role Task Granularity.** The granularity of tasks assigned to agents influences both the precision and complexity of their execution:

1. **Coarse Granularity**: Some agents are given broader, less detailed tasks. For example, in AutoML-GPT Trirat et al. (2024), the central controller agent coordinates the entire machine learning pipeline, handling coarse-grained tasks such as managing the overall workflow rather than focusing on the details of each individual task.
2. **Fine Granularity**: In other cases, tasks are broken down into smaller units for more specific execution. For example, in MapCoder Islam et al. (2024a), multiple agents collaborate, each handling a fine-grained task such as code generation, debugging, or retrieval. This detailed task assignment ensures high accuracy but requires more computation overhead.

## 3.2 Execution Structure

In this section, we summarize the execution strategies of LLM-based agents, emphasizing their approaches how to complete the tasks.

### 3.2.1 Static Execution

Static execution refers to a workflow-style structure where agents follow a predefined sequence of actions to accomplish tasks. In this paradigm, the workflow is rigidly designed, ensuring that each step is executed deterministically without deviations. This type of workflow is particularly useful in scenarios where tasks require consistent, repeatable processes or involve complex subtasks that must be systematically handled. By defining clear workflows, these systems ensure reliability, transparency, and ease of evaluation, as agents operate within well-defined boundaries. A common feature of static execution structures is the division of tasks into sequential, predefined stages Seo et al. (2025); Li et al. (2025); Xu et al. (2025); Ou et al. (2025). These workflows often start with data or task interpretation, followed by intermediate processing steps such as feature selection, data transformation Qi & Wang (2024), or subtask decomposition Luo et al. (2024), and conclude with result generation Gu et al. (2024) or validation Shen et al. (2024).

### 3.2.2 Dynamic Execution

**Just-in-time plan.** The “just-in-time” planning approach represents a dynamic and iterative execution strategy widely adopted by modern LLM-based agents (see Figure 10). Unlike pre-defined static workflows,

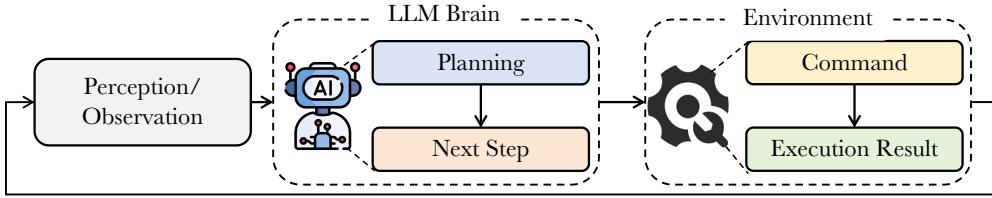


Figure 10: In just-in-time planning, one agent is responsible for planning and execution simultaneously.

this structure enables agents to generate and refine plans based on real-time feedback from previous execution steps Rasheed et al. (2024); Yang et al. (2024a)Bendinelli et al. (2025). Specifically, agents observe the outcomes of each executed step, use these observations to reevaluate the task’s context, and then dynamically devise the next step Cao et al. (2024); Zhao et al. (2024a). Just-in-time planning is particularly effective in domains where the environment or task requirements are dynamic Zhao et al. (2024a), as it reduces redundancy and enhances precision by continuously aligning actions with the latest data or results Zhang et al. (2024d); Liu et al. (2024b).

**Plan then execute.** The “plan-then-execute” framework is a widely adopted structure in LLM agent systems, particularly for tasks requiring complex reasoning and multi-stage problem-solving (see Figure 4 for an example). This framework divides the agent’s workflow into two distinct phases. In the planning phase, the agent formulates a high-level strategy by breaking down the overarching task into smaller, manageable sub-tasks. In the execution phase, the agent performs these sub-tasks sequentially or iteratively, strictly adhering to the initial plan while refining the process based on intermediate results or environmental feedback. Such a design mirrors human problem-solving strategies, offering modularity, scalability, and adaptability for diverse tasks, from software development Qian et al. (2024) to program repair Zhang et al. (2024e) and exception handling Zhang et al. (2024b).

**Hierarchy execution.** Hierarchy execution is a structured approach where agents decompose complex tasks into smaller, manageable subtasks organized hierarchically. While the core principle of decomposing tasks into subtasks and refining them when needed remains consistent across implementations, structural details and execution strategies vary significantly among frameworks. For example, SELA uses tree-based hierarchies and Monte Carlo Tree Search (MCTS) to optimize AutoML workflows Chi et al. (2024), CodeTree employs explicit task decomposition to identify and evaluate coding strategies with execution feedback for dynamic optimization Li et al. (2024d), and LATS integrates MCTS into a language-agent-driven framework using model-driven value functions and self-reflection Zhou et al. (2023). Meanwhile, MapCoder and AGILE-CODER introduce collaborative multi-agent systems for task decomposition Islam et al. (2024a); Nguyen et al. (2024), Data Interpreter uses dynamic graph-based hierarchies for flexible task management Hong et al. (2024), VisionCoder adopts role-based decomposition mirroring traditional software engineering workflows Zhao et al. (2024b), and ScienceAgentBench and Self-Organized Agents incorporate feedback-driven planning to refine subsequent cycles Chen et al. (2024c); Ishibashi & Nishimura (2024).

### 3.2.3 Summary of Execution Structure

This section provides a summary of the execution structures employed by LLM-based agents, highlighting detailed execution dimensions including task execution, task routing, user interaction, and error handling. These execution dimensions significantly affect how agents adapt to dynamic environments and handle complex tasks. Below are the key execution dimensions with specific examples from §3 of the survey.

**Execution flexibility.** Execution flexibility describes how agents handle task allocation during execution, ranging from static to dynamic allocation:

1. **Static Execution:** In this case, task allocation is predefined before execution and remains unchanged throughout the process. An example is the Data Director Hong et al. (2024) framework, where agents follow a fixed workflow with predefined tasks and are not dynamically adjusted during the execution.

Framework	Tree	Graph	Role	Dynamic Adjust	Feedback	Multi-Agent	MCTS
SELA	✓						✓
VisionCoder			✓				
AGILECODER			✓	✓			
MASAI			✓	✓		✓	
Data Interpreter		✓		✓			
MapCoder	✓				✓	✓	
CodeTree	✓			✓			
ScienceAgentBench					✓		
LATS	✓				✓		✓

Table 3: Summary of Hierarchy Planning in Different Frameworks. The columns represent the type of planning structure employed, including Tree-Based, Graph-Based, Role-Based, Dynamic Adjustment, Feedback-Driven, Multi-Agent Collaboration, and Monte Carlo Tree Search (MCTS). A checkmark (✓) indicates the framework supports the corresponding structure.

2. Dynamic Execution: The task allocation changes during execution as the agent receives feedback or as the environment evolves. EvoMAC Hu et al. (2024b) employs a dynamic execution strategy where agents adjust their internal structure, adding or removing agents based on real-time feedback and task complexity.
3. Hybrid Execution: This approach combines both static and dynamic task allocation. For example, in AutoML-GPT Zhang et al. (2023a), task allocation is primarily managed by the central controller but can dynamically adjust based on the results from specialized agents performing tasks like hyperparameter tuning or model design.

**Task routing.** Task routing governs how tasks are passed between agents in a multi-agent system:

1. Rule-based Routing: Tasks follow a specific rule or sequence to move from one agent to another. For instance, in MASAI Arora et al. (2024), tasks follow predefined rules based on the nature of the task, with each agent handling tasks according to a strict order.
2. Agent-based Routing: In this type, one central agent controls the flow of tasks, deciding which agent will handle each task. An example is found in AutoML-GPT Zhang et al. (2023a), where the central LLM oversees task assignment and ensures tasks are routed to the appropriate agents based on the task requirements.
3. Role-based Routing: Agents handle tasks according to their predefined roles. In MAGIS Tao et al. (2024), for instance, different agents like Manager, Developer, and QA Engineer assume roles in the task flow, with each agent taking task when its role is responsible for the incoming part.

**User interaction.** User interaction defines the extent to which users are involved in task execution:

1. Fully-auto: In this case, no user intervention is required. For example, AutoCodeRover Zhang et al. (2024e) operates entirely automatically, with no need for human input during task execution.
2. Human intervene: User interaction is frequent, and users must intervene with the system regularly. MAP-Coder Islam et al. (2024a) requires user feedback to ensure that agents are following the correct task path, especially in error-prone stages of task execution.
3. Hybrid: Some systems balance user input with autonomous execution. In MetaGPT Hong et al. (2023), for instance, the system functions autonomously but allows users to step in for oversight or specific corrections when needed, such as when a complex decision-making process requires a human touch.

**Plan execution.** This dimension describes whether planning and execution are integrated or separated:

1. Plan-Execution in One: One agent handles both planning and execution. In EvoMAC Hu et al. (2024b), for example, the same agent can dynamically plan the next steps and execute them without relying on separate agents for each task.
2. Plan-Execution Separate: The planning and execution roles are handled by separate agents. Parsel Zelikman et al. (2023), for example, separates the planning phase (where tasks are decomposed and strategized) from the execution phase (where the steps are carried out by different agents based on the plan generated).

**Task decomposition.** Task decomposition determines how tasks are broken down and managed:

1. Not Decomposed: In some systems, tasks are handled in their entirety without decomposition. AutoCodeRover Zhang et al. (2024e) may process some high-level tasks as a whole without further division, especially in simple workflows
2. Vertical Decomposition: Tasks are broken down hierarchically, with agents responsible for different levels of the task. This is seen in EvoMAC Hu et al. (2024b), where tasks are decomposed into sub-tasks at various levels, with parent agents overseeing child agents performing specific subtasks
3. Horizontal Decomposition: Tasks are divided into equal parts that are handled concurrently by multiple agents. MASAI Arora et al. (2024) employs horizontal decomposition, dividing a task into multiple smaller subtasks which are handled one following another.
4. Hybrid Decomposition: Some systems use a combination of vertical and horizontal decomposition. AutoML-GPT Trirat et al. (2024), for example, combines both hierarchical task breakdowns (for overseeing large workflows) and parallel execution (for handling repetitive tasks such as data preprocessing)

**Error handling.** Error handling determines how a system deals with problems encountered during execution:

1. Solve in Next Steps: Errors are handled in subsequent steps, either by a different agent or in the following phase of execution. For instance, AutoML-GPT Trirat et al. (2024) might handle errors in model design or tuning by adjusting parameters in later steps of the pipeline.
2. Traceback: The error is traced back to the previous steps to regenerate or correct the output. In MASAI Arora et al. (2024), if an error occurs during task execution, the system might trace back to earlier stages of the task to identify and resolve the root cause before continuing with execution.

### 3.3 External Knowledge

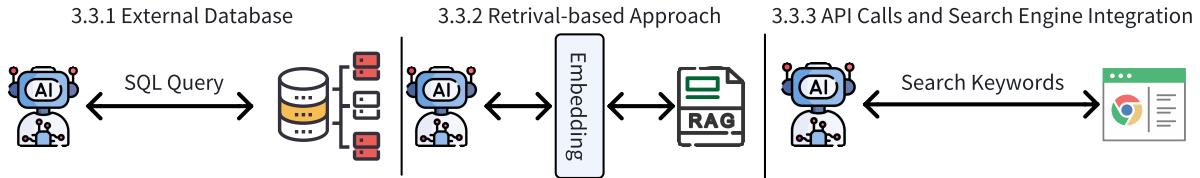


Figure 11: Overview of common external knowledge sources for DS agents.

In this section, we summarize current methods for external knowledge acquisition in LLM-based agents. While pretrained LLMs have extensive internal knowledge, external sources are often needed to address outdated or domain-specific information. We specifically discuss external databases, retrieval-based approaches, API calls, and search engine integration, as well as hybrid methods that combine these techniques.

#### 3.3.1 External Knowledge Methods

**External Database** External databases are collections of organized information stored independently of LLMs, designed to serve as reliable sources of well-defined external knowledge for LLM-based agents Gu et al. (2024); Zhang et al. (2023a); Li et al. (2024e;f); Jing et al. (2024); Liu et al. (2024b); Pietruszka et al. (2024); Hassan et al. (2023); Chen et al. (2024a). For example, some utilize historical logs and past experimental

---

results as a structured knowledge base Liu et al. (2024b); Xu et al. (2025), while Hassan et al. (2023) incorporates user-provided datasets with structured databases to enhance contextual understanding. This method provides structured and consistent data, particularly useful for domain-specific tasks that require precision and stability.

**Retrieval-based Approach** Beyond external databases, LLM-based agents employ different retrieval-based approaches to dynamically obtain external knowledge from unstructured sources. For example, Tang et al. (2023) leverages the BM25 retriever, which uses ranking search to identify the most relevant code and documentation based on word frequency and importance, to extract relevant segments based on given instructions. Meanwhile, Li et al. (2024c) uses RAG(Retrieval-Augmented Generation) to improve response accuracy and reduce hallucination by retrieving relevant external data and integrating it into the generation process. Furthermore, Guo et al. (2024a) extends Case-Based Reasoning, which retrieves and adapts past cases rather than just ranking or generating text, and Cao et al. (2024) employs LlamaIndex, a data framework for RAG, to efficiently structure, retrieve, and inject knowledge into LLMs. Retrieval-based approaches, especially RAG, are widely used in applications, such as bias detection Li et al. (2025), geospatial analysis Chen et al. (2024b), and financial forecasting Yang et al. (2024a), supporting broader contextual understanding and enhancing adaptability in handling structured and unstructured information.

**API Calls and Search Engine Integration** Another widely adopted approach involves direct interaction with external repositories and search engines, allowing LLM-based agents to directly interact with external repositories or retrieve real-time data from the internet. For instance, Liao et al. (2024) integrates API calls to handle time series analysis by retrieving Prophet models, a statistical forecasting tool that models trends and seasonal variations in time-series data, while Bogin et al. (2024) accesses GitHub repositories and datasets from platforms like Hugging Face. By enabling agents to retrieve external knowledge on demand, API calls and search engine integration provide critical flexibility and responsiveness in dynamic environments.

**Hybrid Approach** To enhance knowledge acquisition, many systems adopt hybrid approaches by combining multiple methods. A common strategy is integrating both API calls and external databases to agents' accessible knowledge sources Merrill et al. (2024); Huang et al. (2024c); Li et al. (2024b); Zhang et al. (2023b); Luo et al. (2024). For example, Merrill et al. (2024) employs Google Search API alongside anonymized wearable health data for retrieving relevant health information. Moreover, some works combine retrieval approaches with an external databases to equip the system with expert-level knowledge Ou et al. (2025). Additionally, several works combine API calls and search engines with retrieval-based approaches for dynamic retrieval Grosnit et al. (2024); Chen et al. (2024b); Tang et al. (2023), while others adopt a fully hybridized approach incorporating all three strategies Guo et al. (2024a); Cao et al. (2024). For instance, Yang et al. (2024a) utilizes third-party APIs for financial data retrieval, applies RAG for financial sentiment analysis, and manages an external database for knowledge storage and retrieval.

### 3.3.2 Summary of External Knowledge

External database, retrieval-based approach, and external API and search engine integration represent three primary methodologies adopted by LLM-based agents for external knowledge acquisition. External databases provide structured and reliable domain-specific information, ensuring precision and stability for targeted tasks. Retrieval-based approaches dynamically extract relevant segments from sources, enhancing contextual comprehension and adaptability. API calls and search engines deliver real-time and frequently updated data, supporting immediate responsiveness in dynamic scenarios. Collectively, these methods enable LLM-based agents to cover a wide range of external knowledge and, moreover, empower LLMs to gauge, verify, enrich, or even refine their internal knowledge, thereby significantly improving their overall accuracy and reliability of their responses.

## 3.4 Reflection

LLM multi-agent systems rely on reflection mechanisms to iteratively refine their performance, enhance robustness, and adapt to complex environments. Reflection, in this context, refers to a system's ability to evaluate its past outputs, identify errors or inefficiencies, and adjust its strategies accordingly—enabling

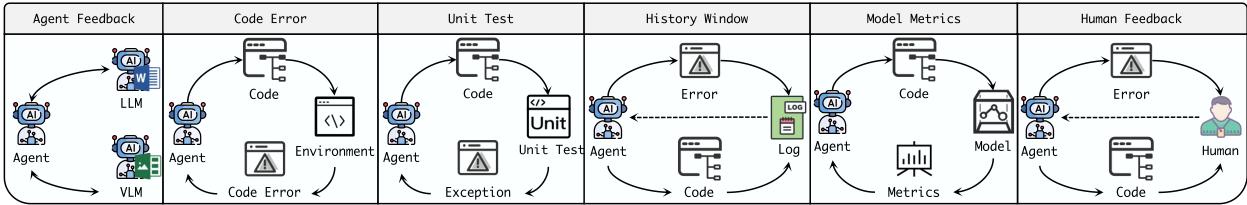


Figure 12: Overview of common reflection techniques in LLM multi-agent systems.

continuous self-improvement. In this section, we discuss how LLM multi-agent systems employ various reflection mechanisms to improve output quality and system reliability. These mechanisms enable automated agents to iteratively refine their responses based on execution outcomes, predefined evaluation metrics, or external feedback.

### 3.4.1 Reflection Methods

**Agent Feedback:** Many LLM multi-agent systems rely on agent feedback mechanisms, where one or more agents review the outputs of other agents and provide corrective guidance. In code generation tasks, for instance, DA-Code Huang et al. (2024c), BIASINSPECTOR Li et al. (2025), and AUTOMIND Ou et al. (2025) applies a reviewer agent to evaluate generated scripts, detect syntax or logical errors, and suggest improvements. Similarly, in multimodal tasks, visual language models (VLMs) serve as reviewers to assess image-based outputs for correctness and coherence. MatPlotAgent Yang et al. (2024b) exemplifies this by evaluating visualizations generated from inputs.

**Code Error Handling:** Automated error-handling mechanisms are essential for ensuring reliability of systems that generate and execute code, such as BudgetMLAgent Gandhi et al. (2024), WaitGPT Xie et al. (2024), and DatawiseAgent You et al. (2025). These mechanisms monitor execution failures, capture error messages, and diagnose potential causes. Upon detecting an error, systems analyze faulty outputs and refine code iteratively without external intervention. This allows systems to mimic human programmers—reflecting on errors, identifying root causes, and progressively improving the solution.

**Unit Testing:** Unit testing is a structured validation mechanism where an agent generates test cases and evaluates whether the system’s output meets predefined functional requirements. If a test fails, the agent refines the output and reruns the tests iteratively until all test cases pass. This method is widely used in LLM-driven programming tasks, where models generate executable code Guo et al. (2024a). By automatically verifying whether the generated code meets expected functionality, unit testing helps to detect syntax errors, logical flaws, and compatibility issues before execution.

**Model Metrics Feedback:** In tasks with clear quantitative performance indicators, model metrics feedback enables systematic, data-driven optimization. Rather than relying on external evaluations, systems refine their outputs using predefined performance thresholds, such as accuracy, F1 score, or loss reduction. Some implementations use threshold-based optimization, iteratively revising until desired metrics are met. For example, FinRobot Yang et al. (2024a) uses a composite scoring system that integrates normalized performance metrics with weighted evaluation criteria to select or fine-tune models until the target score is achieved. Others adopt exploratory search strategies, such as Monte Carlo Tree Search (MCTS) Chen et al. (2024b), to explore different refinement paths and select the most effective one. This structured approach allows LLM multi-agent systems to self-improve efficiently without requiring human or agent-based feedback at each step.

**History Window:** Unlike mechanisms that focus on immediate corrections, history window mechanisms enable long-term learning by maintaining a log of past outputs and errors Hong et al. (2024) Wang et al. (2025a); Seo et al. (2025); Xu et al. (2025). These logs help systems track recurring mistakes and recognize patterns across multiple iterations. Some implementations enhance this capability with checkpointing, periodically saving stable system states Zhao et al. (2024a). If a later refinement degrades performance, the system can revert to a previous checkpoint. By leveraging historical insights, history window mechanisms

---

prevent repeated failures, allowing systems to refine their decision-making over time and avoid ineffective adjustments.

**Human Feedback:** Despite advancements in automated reflection, human feedback remains indispensable in high-stakes applications. For example, TableAnalyst Freimanis & Andersson Rhodin (2024), a Human-in-the-loop system, allows experts to review and refine outputs, particularly when LLM-generated responses require contextual understanding or ethical considerations. Reinforcement learning from human feedback (RLHF) is a prominent example, where human reviewers assess model-generated responses and provide corrective guidance. Although more interactions required, human feedback mechanisms ensure that outputs align with domain-specific expectations and maintain interpretability in critical applications.

### 3.4.2 Summary of Reflection

Beyond specific implementations, reflection mechanisms can be understood in terms of three fundamental dimensions: the **driver**, the **level**, and the **adaptability** of reflection. These dimensions help contextualize the broader implications of reflection in multi-agent systems, providing insights into how different strategies contribute to long-term performance improvements.

**Drivers of Reflection.** Reflection in LLM multi-agent systems is driven by different mechanisms that shape how the system refines its performance. Some systems improve through internal Hong et al. (2024) or external feedback Merrill et al. (2024), either from agents or human reviewers. Others adopt goal-driven approaches, continuously optimizing their outputs based on predefined performance criteria without relying on explicit external feedback Chen et al. (2024b).

1. Feedback-driven reflection operates based on internal or external evaluation and corrective feedback, where agents or human evaluators assess outputs and provide improving guidance. For example, in agent feedback mechanisms, LLM agents critique one another's outputs, engaging in cycles of feedback and revision Trirat et al. (2024). This process is particularly common in multi-agent collaborations where specialized agents, such as debugging agents in code generation tasks Huang et al. (2024c), verify and refine responses. Human feedback mechanisms introduce expert oversight, ensuring model outputs align with qualitative expectations Luo et al. (2024). While feedback-driven reflection allows flexibility and adaptation to dynamic environments, it also introduces challenges such as response latency and inconsistency in external evaluations.
2. Goal-driven reflection, in contrast, follows a more quantitative optimization approach, where systems refine their outputs based on predefined performance criteria rather than external evaluation. Many multi-agent systems employ metric-based optimization, where refinements are guided by quantitative performance indicators such as BLEU scores in machine translation or loss minimization in model training. Some implementations, such as reinforcement learning and self-play strategies, enable systems to optimize through iterative self-improvement. For instance, AlphaGo Granter et al. (2017) refines its strategies without relying on external critique by playing against itself. The key advantage of goal-driven reflection lies in its predictability and efficiency, allowing systems to make systematic progress without requiring continuous human or agent-based feedback loops. However, it also risks overfitting to specific metrics, which can reduce generalization and overlook qualitative aspects of task performance.

**Levels of Reflection.** Reflection does not operate uniformly across all components of a system; rather, it varies in scope, with some mechanisms focusing on fine-grained, localized improvements, while others engage in system-wide analysis and optimization.

1. Local reflection focuses on refining individual task iterations, ensuring immediate performance improvements. Common techniques include unit testing Guo et al. (2024a), execution error diagnosis Zhang et al. (2023b), and targeted debugging routines Huang et al. (2024c). The primary advantage of local reflection lies in efficiency, as it enables rapid refinement without requiring the system to analyze historical data or restructure workflows. Additionally, it enhances precision by addressing specific issues within isolated tasks, preventing minor errors from propagating. However, because these mechanisms operate in isolation, they may fail to detect systematic inefficiencies. For example, in code generation Liao et al. (2024), a debugging agent may repeatedly fix syntax errors in isolated function calls without recognizing an un-

---

derlying flaw in the model’s broader logic generation capabilities. As a result, errors may be corrected in the short term but persist across different tasks.

2. Global reflection analyzes patterns across multiple iterations, extracting insights that guide long-term optimization. History window mechanisms exemplify this approach by enabling systems to track recurring mistakes and refine their responses accordingly Bogin et al. (2024). Some implementations further enhance global reflection through checkpointing Hong et al. (2024), where stable system states are periodically saved. If a newer version fails to improve performance, the system can revert to a prior state instead of reinforcing ineffective updates. This method is particularly valuable in preventing cyclical failures, such as a conversational agent repeatedly generating redundant responses due to misaligned reinforcement signals. However, implementing global reflection requires sophisticated memory management and comes with higher computational costs, making it more suitable for large-scale, complex multi-agent systems.

**Adaptability of Reflection.** Another essential consideration is the degree of flexibility and adaptability within the reflection process. While some methods follow fixed, predefined correction strategies, others adjust dynamically based on performance patterns observed during execution.

1. Structured reflection mechanisms operate according to fixed evaluation criteria, ensuring a stable and repeatable refinement process. This category includes unit testing, where outputs must pass predefined test cases Guo et al. (2024a), and threshold-based metric optimization Yang et al. (2024a), where refinements continue until performance metrics such as accuracy or loss reach a set threshold. The primary benefit of structured reflection is its predictability, making it particularly useful in well-defined problem spaces requiring strict correctness—such as automated hyperparameter tuning in machine learning, where models are optimized based on predefined performance metrics. However, its rigidity limits adaptability, making it unsuitable for handling unexpected edge cases or unstructured, open-ended tasks, where predefined evaluation criteria may not capture qualitative aspects of performance.
2. Adaptive reflection mechanisms dynamically adjust their evaluation strategies based on previous attempts or insights gathered from different parts of the system. Systems employing adaptive agent feedback Hong et al. (2024), self-modifying history windows Qi & Wang (2024), or reinforcement learning refine their reflection processes as they accumulate more information. This flexibility allows LLM multi-agent systems to not only correct mistakes but also optimize their refinement strategies over time. For example, in dialogue systems, such as SageCopilot Liao et al. (2024), an adaptive reflection mechanism may modify its response-generation strategy if users repeatedly indicate dissatisfaction, shifting towards more context-aware replies rather than just fixing specific errors. Despite its advantages, adaptive reflection introduces challenges in complexity and computational overhead. Dynamically evolving strategies require greater processing power and careful tuning to prevent unintended biases or instability in the reflection process.

## 4 Analysis from Data Science Perspective

### 4.1 Data Science Tasks

Data science agents are increasingly being integrated into diverse workflows to automate and optimize data-centric tasks. These tasks can be broadly categorized based on their objectives, this section outlines two representative types of tasks where AI agents are commonly deployed: (i) tasks that focus on building and refining machine learning models, and (ii) tasks centered on the generation of insights and outputs from data.

**Building Machine Learning Models** Building machine learning models is a core objective within data science, focusing on creating predictive, explanatory, or generative models to solve domain-specific problems. These tasks typically aim to maximize the accuracy, efficiency and generalizability of the model across datasets by automating key processes such as feature engineering, hyperparameter optimization, and model selection Tang et al. (2023). The automation of ML model building uses iterative workflows, where each stage—data preprocessing, model evaluation, and refinement—is informed by prior outputs, often through multi-agent collaborations or tree-based optimization strategies Chi et al. (2024). Additionally, they are characterized by robust integration of tools , alongside domain-specific libraries tailored for computer vision,

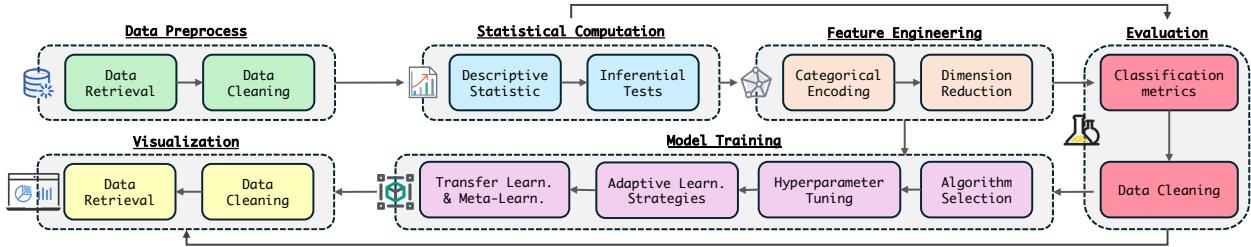


Figure 13: Typical data science loop

NLP, and tabular data analysis Grosnit et al. (2024); Xue et al. (2025). These features enable efficient scaling and adaptation to diverse data environments, providing robust solutions to challenges in domains ranging from financial analysis to biomedical research Yang et al. (2024a); Gandhi et al. (2024); Chen et al. (2024a).

**Output Analysis Tasks** Output analysis tasks focus on extracting, interpreting, and communicating insights derived from data. These tasks aim to generate clear and actionable narratives through visualization, summarization, or benchmarking while prioritizing interpretability and relevance Zhao et al. (2024a). LLM-based agents are often used to annotate visualizations and generate and refine textual explanations. For example, output analysis tasks leverage sophisticated tools like Vega-Lite for visualization and natural language models for insight generation, to enhance communication of data-driven findings Xie et al. (2024). In addition, agents are used for data storytelling through automated animated videos that transform raw data into engaging narratives by coordinating visual, textual, and auditory elements Shen et al. (2024).

Analysis tasks such as data cleaning output evaluation focus on quality dimensions like completeness, accuracy, and consistency Li et al. (2024f). Agents typically employ rule-based metrics or statistical heuristics to assess whether cleaned datasets meet project-specific requirements Li et al. (2024f). These evaluations often integrate automated validation pipelines, where agents verify the success of cleaning operations (e.g., deduplication, missing value imputation) and provide reports summarizing detected issues and corrective actions taken Huang et al. (2024c).

## 4.2 Data Science Loop

The data science loop serves as a structured blueprint for how LLM-based agents can systematically enhance and automate key phases of data workflows. Each step from initial data retrieval and cleaning to advanced statistical analysis, model development, and visualization can be augmented by LLM-based agents to improve the efficiency and quality of decision-making. As shown in Figure 13, this loop captures the full lifecycle of a data-driven project and provides a framework for understanding where agent-based systems integrate into and optimize the process.

### 4.2.1 Data Preprocess

The data preprocessing phase includes steps for getting, cleaning, and preparing data. It starts with collecting data from different sources like databases, APIs, web scraping, sensor logs, and research repositories Guo et al. (2024a). Structured data comes from relational databases using SQL, while unstructured text is gathered through APIs or web crawlers Huang et al. (2024c). Some systems combine different types of data, such as tables, images, audio, or text Luo et al. (2024); Cao et al. (2024). Automated pipelines use retrieval-augmented generation (RAG) to find and pull useful data, making sure that it is high quality and relevant for later steps. Li et al. (2024h); Sun et al. (2024a); Rasheed et al. (2024); Yang et al. (2024a). After collection, the data is cleaned to improve accuracy and consistency. This step fixes missing values, duplicates, outliers, and inconsistencies that could cause problems in later analysis. If important values are missing, agents will fill gaps or remove incomplete rows based on their domain knowledge and pre-defined rules. Duplicates are found and removed using hashing or fuzzy matching methods like Levenshtein distance for text. Outliers are detected using basic statistical methods like Z-score and IQR filtering, while more

---

advanced techniques like isolation forests and autoencoders handle complex cases. Hong et al. (2024); Li et al. (2024h).

#### 4.2.2 Statistical Computation

The statistical computation phase uses statistical methods to analyze data, find patterns, and show relationships. These methods help understand distributions and correlations in the data. Basic techniques include descriptive statistics (mean, median, variance), inferential tests (e.g., t-tests, chi-square tests), and correlation analysis are widely employed to establish baselines and validate data integrity Gu et al. (2024). Methods like hypothesis testing and parametric or non-parametric methods are also utilized to derive insights under uncertainty Zhang et al. (2023b). Parallelized frameworks like Dask or Spark are used to improve computational efficiency for large-scale or distributed datasets Jing et al. (2024).

#### 4.2.3 Feature Engineering

In the feature engineering phase, raw data is transformed into meaningful representations that improve model performance. This phase involves creating, selecting, and refining features to ensure they are both relevant and discriminative for the underlying predictive task Pietruszka et al. (2024). A well-designed feature engineering process enables machine learning models to capture patterns effectively while mitigating overfitting and reducing noise. The core techniques in feature engineering include handling missing values, categorical encoding, numerical transformations, and dimensionality reduction. Standard approaches such as one-hot encoding and label encoding allow categorical variables to be numerically represented, while scaling techniques like min-max normalization and standardization ensure consistent feature magnitudes Tang et al. (2023). Advanced feature engineering techniques involve feature construction and selection strategies. Polynomial feature expansion, interaction terms, and domain-specific transformations (e.g., log transformations for skewed distributions) enhance a model's ability to capture complex relationships. Additionally, methods like Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbor Embedding (t-SNE) facilitate dimensionality reduction, improving computational efficiency and reducing redundant information. Feature importance techniques, such as SHAP (SHapley Additive exPlanations) and permutation importance, guide the selection of the most predictive variables Chi et al. (2024).

#### 4.2.4 Model Training

In the model training phase, refined data and features are input into machine learning algorithms to create predictive models. This phase encompasses algorithm selection, hyperparameter tuning, and iterative validation to optimize performance. Commonly used algorithms range from traditional methods like linear regression and decision trees to modern neural architectures designed for high-dimensional and multi-modal data Huang et al. (2024a). Agents in training pipelines integrate and use ML libraries and tools to facilitate model creation, while hyperparameter optimization frameworks such as Optuna and Ray Tune enhance the search for optimal configurations Liu et al. (2024b). Real-time monitoring and adaptive learning strategies are often employed to refine models, particularly in dynamic environments where data evolves over time Chen et al. (2024b). Advanced techniques, such as transfer learning and meta-learning, enable models to leverage knowledge from pre-trained networks, reducing training time and improving performance Luo et al. (2024). The model training phase is iterative by nature, with feedback loops that refine both the model and its underlying assumptions, ensuring robustness and generalizability across unseen data Zhang et al. (2024d).

#### 4.2.5 Evaluation

The evaluation phase is to assess the performance and reliability of machine learning models. This step involves the use of metrics tailored to the task at hand, such as accuracy, precision, recall, and F1 score for classification tasks, or RMSE (Root Mean Squared Error) and MAE (Mean Absolute Error) for regression analyses Li et al. (2024e). For unsupervised tasks, metrics like silhouette score and Davies-Bouldin index are employed to evaluate clustering quality Jing et al. (2024). Cross-validation techniques, such as k-fold or leave-one-out, are widely used to estimate model performance on unseen data, ensuring that results generalize

---

beyond the training set Chen et al. (2024c). The integration of automated evaluation frameworks allows for streamlined reporting and comparison, enabling iterative improvement and enhancing the credibility of the final model Xie et al. (2024).

#### 4.2.6 Visualization

The visualization phase turns data into easy-to-understand images that help with decision-making. Clear visuals change complex data into simple forms like charts, plots, and dashboards. These help people see patterns, trends, and unusual points. This step uses both fixed and interactive visuals, letting users explore the data in different ways.

Modern data science agents leverage a variety of visualization libraries and tools to create visualizations tailored to different analytical needs Hong et al. (2024); Li et al. (2024h); Liao et al. (2024). In addition to traditional visualizations like line plots and histograms, more advanced visualizations, such as model interpretability plots (e.g., SHAP values), are used to explain model outputs in a transparent manner.

### 4.3 Summary of Data Science Perspective

**Fixed Data Science Pipeline** Data science agents typically follow structured workflows in different stages such as data preprocessing, feature selection, and model training You et al. (2025). LLM-based agent systems like Qi & Wang (2024) and Li et al. (2024f) automate data preprocessing strategies and address data quality issues like missing values, inconsistencies, and duplications. Feature selection mechanisms Li et al. (2024b) further enhance model performance by identifying the most data features, thus optimizing capabilities. Additionally, advanced agent systems, such as Chi et al. (2024); Trirat et al. (2024), dynamically generate optimized data science pipelines.

**Self-planning Training** Data science agents exhibit self-planning training capabilities, autonomously selecting optimal algorithms, configuring hyperparameters, and iteratively validating model performance during the training phase Seo et al. (2025). This methodology parallels traditional Neural Architecture Search (NAS), an automated process that optimizes neural network designs, but significantly leverages agent-driven decision-making frameworks Liu et al. (2024b). By systematically exploring and refining model configurations based on ongoing feedback, these agents ensure robust and adaptive performance tailored to specific contexts.

**Metrics-based Feedback** In contrast to traditional coding-oriented agents, data science agents utilize rigorous model-based metrics feedback for iterative improvement. FairOPT Jung et al. (2025) leverages quantitative metrics such as accuracy, precision, recall, and F1 scores to assess model outputs and systematically enhance their performance through structured refinement cycles. This metrics-driven feedback mechanism ensures continuous performance enhancement and enables agents to maintain consistent accuracy across diverse analytical scenarios.

**Visualization Analysis** Data science agents distinctly emphasize the visualization of analytical outcomes, recognizing its critical role in data interpretation and communication. Visualization-focused systems Zhao et al. (2024a) generate clear, insightful visual representations that facilitate a comprehensive understanding of complex analytical results. Furthermore, specialized agents like MatplotAgent Yang et al. (2024b) employ visualization explicitly as an informative feedback mechanism for detecting and correcting analytical errors. By integrating visual feedback into their error-handling processes, these agents significantly enhance the interpretability, accuracy, and overall effectiveness of data-driven decision-making.

## 5 Benchmark

Table 4 presents a summary of curated benchmarks designed for evaluating LLM-based agents from a data science perspective. Notable examples include ML-Bench Tang et al. (2023) for multimodal and time-series tasks and DS-Bench Jing et al. (2024) for data analysis and modeling. Specialized benchmarks such as GeoAgent-

---

Bench Liao et al. (2024) provide evaluation frameworks for geospatial analysis, while MatPlotAgent-Bench Yang et al. (2024b) focuses on visualization.

Beyond general data science, several benchmarks target specialized domains. FoodPuzzle Huang et al. (2024b) explores computational approaches to understanding flavor profiles at the molecular level. Merrill et al. (2024) evaluates LLM capabilities in personal health reasoning with wearable data. AgentClinic Schmidgall et al. (2024) assesses patient interactions and multimodal clinical data processing. GenoTEX Liu & Wang (2024) benchmarks LLMs in genomics, covering dataset selection, preprocessing, and statistical analysis.

Additionally, TheAgentCompany Xu et al. (2024) serves as a practical evaluation framework for AI-driven automation in corporate environments, covering tasks in data science, software engineering, and business operations. These benchmarks provide a foundational dataset and evaluation standard for LLM-based agent systems.

## 6 Future Research Opportunity

In this section, we outline future directions inspired by recent advancements and existing challenges identified to stimulate subsequent research in LLM-based data science agents.

### 6.1 Trainable architecture

Inspired by pioneering works such as EvoMACHu et al. (2024b), there is substantial potential in exploring dynamically refine agent architecture. This approach facilitates continuous optimization of system efficacy across varying data science domains. Emerging methodologies Yuksekgonul et al. (2024); Hu et al. (2025) propose leveraging backpropagation-inspired textual gradients to systematically adjust and improve agent architectures. Future research might investigate automated structural generation methods capable of autonomously deriving optimal agent architectures tailored explicitly to domain-specific requirements, significantly enhancing both scalability and adaptability of LLM-based agents.

### 6.2 Advanced Reflection Mechanisms

Current reflection strategies predominantly address short-term corrections through immediate feedback mechanisms. Expanding these mechanisms to include comprehensive long-term reflective processes, such as history-window-based learning and unsupervised self-correction, presents significant opportunities. Implementing iterative refinement methodologies and advanced error-tracing capabilities can substantially enhance the robustness and reliability of agents over extended operational periods. Furthermore, an in-depth examination of the underlying reasons behind reflective failures Cemri et al. (2025) could provide crucial insights. Such research may lead to the development of sophisticated reflective frameworks capable of proactively identifying and mitigating systematic inefficiencies.

### 6.3 Multimodal Processing

Integrating vision-language models (VLMs) with LLM-based agents offers a substantial opportunity to enhance their interpretative capabilities, particularly in analyzing visual data prevalent in statistical and analytical reports. The incorporation of specialized multimodal agents demonstrates a clear potential for effectively interpreting visual information, generating relevant feedback, and correcting inaccuracies Yang et al. (2024b). Future research may explore hybrid models that fuse textual and visual modalities more seamlessly, leveraging cross-modal embeddings to improve the precision of visual data interpretation. Additionally, developing specialized visual-feedback agents capable of autonomously interpreting and refining graphical data could significantly improve the accuracy, reliability, and utility of insights derived from visual analytics within complex data-driven environments.

Benchmark	Source	# of Tasks	Task Types
BLADE Gu et al. (2024)	Literature	714	multiple-choice and ground truth-analysis studies
InfiAgent-DABench Hu et al. (2024a)	GitHub	257	Data Analysis and ML
ML-Bench Tang et al. (2023)	GitHub	9641(168)	Multimodal, time series, audio, LLM, vision, biomedical, graphs
DevBench Li et al. (2024a)	Github	22	DL, CV, and NLP
SUPER Bogin et al. (2024)	GitHub	799	Research data science challenges
DA-Code Huang et al. (2024c)	Kaggle, GitHub	500	Data wrangling, EDA, ML
FeatEng Pietruszka et al. (2024)	Kaggle	103	Classification, regression, feature engineering
Tapilot Li et al. (2024e)	Kaggle	1024	Data analysis, request clarification
MLE-Bench Chan et al. (2024)	Kaggle	75	Modelling Tasks(image, video, LLMs, tabular)
DSBench Jing et al. (2024)	ModelOff, Kaggle	540	Data analysis, modeling
PyBench Zhang et al. (2024c)	Kaggle, Arxiv, multimedia files	143	Data Analysis, ML, image, text, and audio analysis
DSEval Zhang et al. (2024d)	Tutorials, StackOverflow, Kaggle	825	Data analysis
Spider2-V Cao et al. (2024)	Tutorials, enterprise applications	494	Warehousing, transformation, visualization
MatPlotAgent-Bench Yang et al. (2024b)	Matplotlib, OriginLab	100	Standard and advanced visualization
ScienceAgentBench Chen et al. (2024c)	Peer-reviewed publications	102	Data processing, modeling, visualization
SagePilot Liao et al. (2024)	External datasets	276	SQL-related tasks
Text2Analysis He et al. (2024)	LLM and human-generated	2249	Data analysis, modeling
DataNarrative Islam et al. (2024b)	Pew Research, Tableau Public, GapMinder	1449	Data-driven visualization, storytelling
Insigt-Bench Sahu et al. (2024)	ServiceNow platform	100	Data Analysis tasks
MMAU Yin et al. (2024)	In-house, Kaggle, DeepMind-Math	20	DS/ML, contest-level coding, math
GeoAgent-Bench Liao et al. (2024)	GitHub, tutorials, LLM generation	19,504	Single-turn, multi-turn in Geo-spatial analysis
MLAgentBench Huang et al. (2023)	Kaggle, canonical datasets	13	Research Image, text, graph, tabular, time series ML tasks
Merrill et al. (2024)	Human experts, wearable data	4172	Numerical, open-ended reasoning in personal health
AgentClinic Schmidgall et al. (2024)	USMLE, MIMICIV, NEJM, MedAQ	535	Patient interaction, multimodal data collection in clinics
GenoTEX Liu & Wang (2024)	GEO, TCGA, NCBI Gene Database	1146	Dataset selection, processioning, statistical analysis in Genomics
TheAgentCompany Xu et al. (2024)	Company websites, human examples	175	DS tasks in company settings
FoodPuzzle Huang et al. (2024b)	FlavorDB	2744	Molecular prediction and profile completion in flavor science
MLGym Nathani et al. (2025)	Publications and datasets	13	DS, CV, NLP, RL, and game theory
DataSciBench Zhang et al. (2025a)	CodeGeeX, BCB, and human	519	Data Analysis, modeling, data Visualization
Chen et al. (2024a)	CREEDS and GEO		GEO Database and Drug Repurposing Database in medical fields
BIODSA-1K Wang et al. (2025b)	Publications	1029	Biomedical hypothesis and analysis
DS-1000Lai et al. (2023)	Stackoverflow	1000	Code generation in DS
BioDSBench Wang et al. (2024b)	Published studies, TCGA-type genomics, and clinical data	293	Biomedical coding tasks
ML-Dev-Bench Padigela et al. (2025)	Unknown	30	Data processing, modeling, API integration
TimeSeriesGym Cai et al. (2025)	Kaggle, Github, publications, hand-crafted	34	Time-series problem

Table 4: Summary of Benchmarks in Data Science Perspective

## 7 Conclusion

This survey provides a comprehensive analysis of Large Language Model (LLM)-based agents in data science, addressing key aspects from both agent design and data science perspectives. It systematically explores

---

different agent roles, execution structures, external knowledge acquisition methods, and reflection techniques. The study introduces a dual-perspective framework bridging general agent design principles with specific data science requirements, covering structures from single-agent to dynamic multi-agent systems and execution methods from dynamic planning to static workflows. Overall, this paper offers a comprehensive summary of existing work on LLM-based data science agents.

---

## References

- Daman Arora, Atharv Sonwane, Nalin Wadhwa, Abhay Mehrotra, Saiteja Utpala, Ramakrishna Bairi, Aditya Kanade, and Nagarajan Natarajan. Masai: Modular architecture for software-engineering ai agents. *arXiv preprint arXiv:2406.11638*, 2024.
- Tianyi Bai, Ling Yang, Zhen Hao Wong, Jiahui Peng, Xinlin Zhuang, Chi Zhang, Lijun Wu, Jiantao Qiu, Wentao Zhang, Binhang Yuan, et al. Multi-agent collaborative data selection for efficient llm pretraining. *arXiv preprint arXiv:2410.08102*, 2024.
- Tommaso Bendinelli, Artur Dox, and Christian Holz. Exploring llm agents for cleaning tabular machine learning datasets. *arXiv preprint arXiv:2503.06664*, 2025.
- Ben Beglin, Kejuan Yang, Shashank Gupta, Kyle Richardson, Erin Bransom, Peter Clark, Ashish Sabharwal, and Tushar Khot. Super: Evaluating agents on setting up and executing tasks from research repositories. *arXiv preprint arXiv:2409.07440*, 2024.
- Yifu Cai, Xinyu Li, Mononito Goswami, Michał Wiliński, Gus Welter, and Artur Dubrawski. Time-seriesgym: A scalable benchmark for (time series) machine learning engineering agents. *arXiv preprint arXiv:2505.13291*, 2025.
- Ruisheng Cao, Fangyu Lei, Haoyuan Wu, Jixuan Chen, Yeqiao Fu, Hongcheng Gao, Xinzhuang Xiong, Hanchong Zhang, Yuchen Mao, Wenjing Hu, et al. Spider2-v: How far are multimodal agents from automating data science and engineering workflows? *arXiv preprint arXiv:2407.10956*, 2024.
- Mert Cemri, Melissa Z. Pan, Shuyi Yang, Lakshya A. Agrawal, Bhavya Chopra, Rishabh Tiwari, Kurt Keutzer, Aditya Parameswaran, Dan Klein, Kannan Ramchandran, Matei Zaharia, Joseph E. Gonzalez, and Ion Stoica. Why do multi-agent llm systems fail?, 2025. URL <https://arxiv.org/abs/2503.13657>.
- Jun Shern Chan, Neil Chowdhury, Oliver Jaffe, James Aung, Dane Sherburn, Evan Mays, Giulio Starace, Kevin Liu, Leon Maksin, Tejal Patwardhan, et al. Mle-bench: Evaluating machine learning agents on machine learning engineering. *arXiv preprint arXiv:2410.07095*, 2024.
- Haoran Chen, Shengxiao Zhang, Lizhong Zhang, Jie Geng, Jinqi Lu, Chuandong Hou, Peifeng He, and Xuechun Lu. Multi role chatgpt framework for transforming medical data analysis. *Scientific Reports*, 14(1):13930, 2024a.
- Yuxing Chen, Weijie Wang, Sylvain Lobry, and Camille Kurtz. An llm agent for automatic geospatial data analysis. *arXiv preprint arXiv:2410.18792*, 2024b.
- Ziru Chen, Shijie Chen, Yuting Ning, Qianheng Zhang, Boshi Wang, Botao Yu, Yifei Li, Zeyi Liao, Chen Wei, Zitong Lu, et al. Scienceagentbench: Toward rigorous assessment of language agents for data-driven scientific discovery. *arXiv preprint arXiv:2410.05080*, 2024c.
- Yizhou Chi, Yizhang Lin, Sirui Hong, Duyi Pan, Yaying Fei, Guanghao Mei, Bangbang Liu, Tianqi Pang, Jacky Kwok, Ceyao Zhang, et al. Sela: Tree-search enhanced llm agents for automated machine learning. *arXiv preprint arXiv:2410.17238*, 2024.
- Gelei Deng, Yi Liu, Víctor Mayoral-Vilches, Peng Liu, Yuekang Li, Yuan Xu, Tianwei Zhang, Yang Liu, Martin Pinzger, and Stefan Rass. {PentestGPT}: Evaluating and harnessing large language models for automated penetration testing. In *33rd USENIX Security Symposium (USENIX Security 24)*, pp. 847–864, 2024.
- Gang Fan, Xiaoheng Xie, Xunjin Zheng, Yinan Liang, and Peng Di. Static code analysis in the ai era: An in-depth exploration of the concept, function, and potential of intelligent code analysis agents. *arXiv preprint arXiv:2310.08837*, 2023.
- Andris Freimanis and Patrick Andersson Rhodin. Tableanalyst: an llm-agent for tabular data analysis-implementation and evaluation on tasks of varying complexity. 2024.

- 
- Shubham Gandhi, Manasi Patwardhan, Lovekesh Vig, and Gautam Shroff. Budgetmlagent: A cost-effective llm multi-agent system for automating machine learning tasks. *arXiv preprint arXiv:2411.07464*, 2024.
- Scott R Granter, Andrew H Beck, and David J Papke Jr. Alphago, deep learning, and the future of the human microscopist. *Archives of Pathology & Laboratory Medicine*, 141(5):619–621, 2017.
- Antoine Grosnit, Alexandre Maraval, James Doran, Giuseppe Paolo, Albert Thomas, Refinath Shahul Hameed Nabeezath Beevi, Jonas Gonzalez, Khyati Khandelwal, Ignacio Iacobacci, Abdelhakim Benechehab, et al. Large language models orchestrating structured reasoning achieve kaggle grandmaster level. *arXiv preprint arXiv:2411.03562*, 2024.
- Ken Gu, Ruoxi Shang, Ruien Jiang, Keying Kuang, Richard-John Lin, Donghe Lyu, Yue Mao, Youran Pan, Teng Wu, Jiaqian Yu, et al. Blade: Benchmarking language model agents for data-driven science. *arXiv preprint arXiv:2408.09667*, 2024.
- Siyuan Guo, Cheng Deng, Ying Wen, Hechang Chen, Yi Chang, and Jun Wang. Ds-agent: Automated data science by empowering large language models with case-based reasoning. *arXiv preprint arXiv:2402.17453*, 2024a.
- Tianyu Guo, Xiaozhi Chen, Yujia Wang, et al. Large language model based multi-agents: A survey of progress and challenges, 2024b. URL <https://arxiv.org/abs/2402.01680>.
- Tanmay Gupta, Luca Weihs, and Aniruddha Kembhavi. Codenav: Beyond tool-use to using real-world codebases with llm agents. *arXiv preprint arXiv:2406.12276*, 2024.
- Md Mahadi Hassan, Alex Knipper, and Shubhra Kanti Karmaker Santu. Chatgpt as your personal data scientist. *arXiv preprint arXiv:2305.13657*, 2023.
- Xinyi He, Mengyu Zhou, Xinrun Xu, Xiaojun Ma, Rui Ding, Lun Du, Yan Gao, Ran Jia, Xu Chen, Shi Han, et al. Text2analysis: A benchmark of table question answering with advanced data analysis and unclear queries. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 38, pp. 18206–18215, 2024.
- Sirui Hong, Xiawu Zheng, Jonathan Chen, Yuheng Cheng, Jinlin Wang, Ceyao Zhang, Zili Wang, Steven Ka Shing Yau, Zijuan Lin, Liyang Zhou, et al. Metagpt: Meta programming for multi-agent collaborative framework. *arXiv preprint arXiv:2308.00352*, 2023.
- Sirui Hong, Yizhang Lin, Bang Liu, Bangbang Liu, Biniao Wu, Ceyao Zhang, Chenxing Wei, Danyang Li, Jiaqi Chen, Jiayi Zhang, et al. Data interpreter: An llm agent for data science. *arXiv preprint arXiv:2402.18679*, 2024.
- Shengran Hu, Cong Lu, and Jeff Clune. Automated design of agentic systems, 2025. URL <https://arxiv.org/abs/2408.08435>.
- Xueyu Hu, Ziyu Zhao, Shuang Wei, Ziwei Chai, Qianli Ma, Guoyin Wang, Xuwu Wang, Jing Su, Jingjing Xu, Ming Zhu, et al. Infiagent-dabench: Evaluating agents on data analysis tasks. *arXiv preprint arXiv:2401.05507*, 2024a.
- Yue Hu, Yuzhu Cai, Yixin Du, Xinyu Zhu, Xiangrui Liu, Zijie Yu, Yuchen Hou, Shuo Tang, and Si-heng Chen. Self-evolving multi-agent collaboration networks for software development. *arXiv preprint arXiv:2410.16946*, 2024b.
- Qian Huang, Jian Vora, Percy Liang, and Jure Leskovec. Benchmarking large language models as ai research agents. In *NeurIPS 2023 Foundation Models for Decision Making Workshop*, 2023.
- Qian Huang, Jian Vora, Percy Liang, and Jure Leskovec. Mlagentbench: Evaluating language agents on machine learning experimentation. In *Forty-first International Conference on Machine Learning*, 2024a.

---

Tenghao Huang, Donghee Lee, John Sweeney, Jiatong Shi, Emily Steliotes, Matthew Lange, Jonathan May, and Muhaoo Chen. Foodpuzzle: Developing large language model agents as flavor scientists. *arXiv preprint arXiv:2409.12832*, 2024b.

Yiming Huang, Jianwen Luo, Yan Yu, Yitong Zhang, Fangyu Lei, Yifan Wei, Shizhu He, Lifu Huang, Xiao Liu, Jun Zhao, et al. Da-code: Agent data science code generation benchmark for large language models. *arXiv preprint arXiv:2410.07331*, 2024c.

Yoichi Ishibashi and Yoshimasa Nishimura. Self-organized agents: A llm multi-agent framework toward ultra large-scale code generation and optimization. *arXiv preprint arXiv:2404.02183*, 2024.

Md Ashraful Islam, Mohammed Eunus Ali, and Md Rizwan Parvez. Mapcoder: Multi-agent code generation for competitive problem solving. *arXiv preprint arXiv:2405.11403*, 2024a.

Mohammed Saidul Islam, Md Tahmid Rahman Laskar, Md Rizwan Parvez, Enamul Hoque, and Shafiq Joty. Datanarrative: Automated data-driven storytelling with visualizations and texts. *arXiv preprint arXiv:2408.05346*, 2024b.

Liqiang Jing, Zhehui Huang, Xiaoyang Wang, Wenlin Yao, Wenhao Yu, Kaixin Ma, Hongming Zhang, Xinya Du, and Dong Yu. Dsbench: How far are data science agents to becoming data science experts? *arXiv preprint arXiv:2409.07703*, 2024.

Minseok Jung, Cynthia Fuentes Panizo, Liam Dugan, Yi R., Fung, Pin-Yu Chen, and Paul Pu Liang. Group-adaptive threshold optimization for robust ai-generated text detection, 2025. URL <https://arxiv.org/abs/2502.04528>.

Yuhang Lai, Chengxi Li, Yiming Wang, Tianyi Zhang, Ruiqi Zhong, Luke Zettlemoyer, Wen-tau Yih, Daniel Fried, Sida Wang, and Tao Yu. Ds-1000: A natural and reliable benchmark for data science code generation. In *International Conference on Machine Learning*, pp. 18319–18345. PMLR, 2023.

Hung Le, Hailin Chen, Amrita Saha, Akash Gokul, Doyen Sahoo, and Shafiq Joty. Codechain: Towards modular code generation through chain of self-revisions with representative sub-modules. *arXiv preprint arXiv:2310.08992*, 2023.

Bowen Li, Wenhan Wu, Ziwei Tang, Lin Shi, John Yang, Jinyang Li, Shunyu Yao, Chen Qian, Binyuan Hui, Qicheng Zhang, et al. Devbench: A comprehensive benchmark for software development. *arXiv preprint arXiv:2403.08604*, 3, 2024a.

Dawei Li, Zhen Tan, and Huan Liu. Exploring large language models for feature selection: A data-centric perspective. *arXiv preprint arXiv:2408.12025*, 2024b.

Guoliang Li, Xuanhe Zhou, and Xinyang Zhao. Llm for data management. *Proceedings of the VLDB Endowment*, 17(12):4213–4216, 2024c.

Haoxuan Li, Mingyu Derek Ma, Jen-tse Huang, Zhaotian Weng, Wei Wang, and Jieyu Zhao. Biasinspector: Detecting bias in structured data through llm agents. *arXiv preprint arXiv:2504.04855*, 2025.

Jierui Li, Hung Le, Yinbo Zhou, Caiming Xiong, Silvio Savarese, and Doyen Sahoo. Codetree: Agent-guided tree search for code generation with large language models. *arXiv preprint arXiv:2411.04329*, 2024d.

Jinyang Li, Nan Huo, Yan Gao, Jiayi Shi, Yingxiu Zhao, Ge Qu, Yurong Wu, Chenhao Ma, Jian-Guang Lou, and Reynold Cheng. Tapilot-crossing: Benchmarking and evolving llms towards interactive data analysis agents. *arXiv preprint arXiv:2403.05307*, 2024e.

Lan Li, Liri Fang, and Vetele I Torvik. Autodcworkflow: Llm-based data cleaning workflow auto-generation and benchmark. *arXiv preprint arXiv:2412.06724*, 2024f.

Xinyu Li, Shihan Wang, Siyang Zeng, et al. A survey on llm-based multi-agent systems: Workflow, infrastructure, and challenges. *Vicinagearth*, 1(1):9, 2024g.

- 
- Ziming Li, Qianbo Zang, David Ma, Jiawei Guo, Tuney Zheng, Minghao Liu, Xinyao Niu, Yue Wang, Jian Yang, Jiaheng Liu, et al. Autokaggle: A multi-agent framework for autonomous data science competitions. *arXiv preprint arXiv:2410.20424*, 2024h.
- Yuan Liao, Jiang Bian, Yuhui Yun, Shuo Wang, Yubo Zhang, Jiaming Chu, Tao Wang, Kewei Li, Yuchen Li, Xuhong Li, et al. Towards automated data sciences with natural language and sagecopilot: Practices and lessons learned. *arXiv preprint arXiv:2407.21040*, 2024.
- Feng Lin, Dong Jae Kim, Tse-Husn, and Chen. Soen-101: Code generation by emulating software process models using large language model agents, 2024. URL <https://arxiv.org/abs/2403.15852>.
- Haoyang Liu and Haohan Wang. Genotex: A benchmark for evaluating llm-based exploration of gene expression data in alignment with bioinformaticians. *arXiv preprint arXiv:2406.15341*, 2024.
- Jiaqi Liu, Kening Wang, Yuxuan Chen, et al. Large language model-based agents for software engineering: A survey, 2024a. URL <https://arxiv.org/abs/2409.02977>.
- Siyi Liu, Chen Gao, and Yong Li. Large language model agent for hyper-parameter optimization. *arXiv preprint arXiv:2402.01881*, 2024b.
- Daqin Luo, Chengjian Feng, Yuxuan Nong, and Yiqing Shen. Autom3l: An automated multimodal machine learning framework with large language models. In *Proceedings of the 32nd ACM International Conference on Multimedia*, pp. 8586–8594, 2024.
- Mike A Merrill, Akshay Paruchuri, Naghmeh Rezaei, Geza Kovacs, Javier Perez, Yun Liu, Erik Schenck, Nova Hammerquist, Jake Sunshine, Shyam Tailor, et al. Transforming wearable data into health insights using large language model agents. *arXiv preprint arXiv:2406.06464*, 2024.
- Deepak Nathani, Lovish Madaan, Nicholas Roberts, Nikolay Bashlykov, Ajay Menon, Vincent Moens, Amar Budhiraja, Despoina Magka, Vladislav Vorotilov, Gaurav Chaurasia, et al. Mlgym: A new framework and benchmark for advancing ai research agents. *arXiv preprint arXiv:2502.14499*, 2025.
- Minh Huynh Nguyen, Thang Phan Chau, Phong X Nguyen, and Nghi DQ Bui. Agilecoder: Dynamic collaborative agents for software development based on agile methodology. *arXiv preprint arXiv:2406.11912*, 2024.
- Yixin Ou, Yujie Luo, Jingsheng Zheng, Lanning Wei, Shuofei Qiao, Jintian Zhang, Da Zheng, Huajun Chen, and Ningyu Zhang. Automind: Adaptive knowledgeable agent for automated data science. *arXiv preprint arXiv:2506.10974*, 2025.
- Harshith Padigela, Chintan Shah, and Dinkar Juyal. MI-dev-bench: Comparative analysis of ai agents on ml development workflows. *arXiv preprint arXiv:2502.00964*, 2025.
- Huy Nhat Phan, Tien N Nguyen, Phong X Nguyen, and Nghi DQ Bui. Hyperagent: Generalist software engineering agents to solve coding tasks at scale. *arXiv preprint arXiv:2409.16299*, 2024.
- Michał Pietruszka, Łukasz Borchmann, Aleksander Jedrosz, and Paweł Morawiecki. Can models help us create better models? evaluating llms as data scientists. *arXiv preprint arXiv:2410.23331*, 2024.
- Danrui Qi and Jiannan Wang. Cleanagent: Automating data standardization with llm-based agents. *arXiv preprint arXiv:2403.08291*, 2024.
- Chen Qian, Wei Liu, Hongzhang Liu, Nuo Chen, Yufan Dang, Jiahao Li, Cheng Yang, Weize Chen, Yusheng Su, Xin Cong, et al. Chatdev: Communicative agents for software development. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 15174–15186, 2024.
- Jianing Qiu, Kyle Lam, Guohao Li, Amish Acharya, Tien Yin Wong, Ara Darzi, Wu Yuan, and Eric J Topol. Llm-based agentic systems in medicine and healthcare. *Nature Machine Intelligence*, 6(12):1418–1420, 2024.

---

Zeeshan Rasheed, Muhammad Waseem, Aakash Ahmad, Kai-Kristian Kemell, Wang Xiaofeng, Anh Nguyen Duc, and Pekka Abrahamsson. Can large language models serve as data analysts? a multi-agent assisted approach for qualitative data analysis. *arXiv preprint arXiv:2402.01386*, 2024.

Gaurav Sahu, Abhay Puri, Juan Rodriguez, Amirhossein Abaskohi, Mohammad Chegini, Alexandre Drouin, Perouz Taslakian, Valentina Zantedeschi, Alexandre Lacoste, David Vazquez, et al. Insightbench: Evaluating business analytics agents through multi-step insight generation. *arXiv preprint arXiv:2407.06423*, 2024.

Samuel Schmidgall, Rojin Ziae, Carl Harris, Eduardo Reis, Jeffrey Jopling, and Michael Moor. Agent-clinic: a multimodal agent benchmark to evaluate ai in simulated clinical environments. *arXiv preprint arXiv:2405.07960*, 2024.

Wonduk Seo, Juhyeon Lee, and Yi Bu. Spio: Ensemble and selective strategies via llm-based multi-agent planning in automated data science. *arXiv preprint arXiv:2503.23314*, 2025.

Leixian Shen, Haotian Li, Yun Wang, and Huamin Qu. From data to story: Towards automatic animated data video creation with llm-based multi-agent systems. In *2024 IEEE VIS Workshop on Data Storytelling in an Era of Generative AI (GEN4DS)*, pp. 20–27. IEEE, 2024.

Maojun Sun, Ruijian Han, Binyan Jiang, Houduo Qi, Defeng Sun, Yancheng Yuan, and Jian Huang. Lambda: A large model based data agent. *arXiv preprint arXiv:2407.17535*, 2024a.

Maojun Sun, Ruijian Han, Binyan Jiang, Houduo Qi, Defeng Sun, Yancheng Yuan, and Jian Huang. A survey on large language model-based agents for statistics and data science, 2024b. URL <https://arxiv.org/abs/2412.14222>.

Xiangru Tang, Yuliang Liu, Zefan Cai, Yanjun Shao, Junjie Lu, Yichi Zhang, Zexuan Deng, Helan Hu, Kaikai An, Ruijun Huang, et al. Ml-bench: Evaluating large language models and agents for machine learning tasks on repository-level code. *arXiv e-prints*, pp. arXiv–2311, 2023.

Wei Tao, Yucheng Zhou, Yanlin Wang, Wenqiang Zhang, Hongyu Zhang, and Yu Cheng. Magis: Llm-based multi-agent framework for github issue resolution. *arXiv preprint arXiv:2403.17927*, 2024.

Khai T. Tran, Duy Dao, Minh D. Nguyen, et al. Multi-agent collaboration mechanisms: A survey of llms, 2025. URL <https://arxiv.org/abs/2501.06322>.

Patara Trirat, Wonyong Jeong, and Sung Ju Hwang. Automl-agent: A multi-agent llm framework for full-pipeline automl. *arXiv preprint arXiv:2410.02958*, 2024.

He Wang, Alexander Hanbo Li, Yiqun Hu, Sheng Zhang, Hideo Kobayashi, Jiani Zhang, Henry Zhu, Chung-Wei Hang, and Patrick Ng. Dsmentor: Enhancing data science agents with curriculum learning and online knowledge accumulation. *arXiv preprint arXiv:2505.14163*, 2025a.

Lingchen Wang, Chao Ma, Xiaohan Feng, et al. A survey on large language model based autonomous agents. *Frontiers of Computer Science*, 18(6):186345, 2024a.

Zifeng Wang, Benjamin Danek, Ziwei Yang, Zheng Chen, and Jimeng Sun. Can large language models replace data scientists in clinical research? *arXiv preprint arXiv:2410.21591*, 2024b.

Zifeng Wang, Benjamin Danek, and Jimeng Sun. Biodsa-1k: Benchmarking data science agents for biomedical research. *arXiv preprint arXiv:2505.16100*, 2025b.

Liwenhan Xie, Chengbo Zheng, Haijun Xia, Huamin Qu, and Chen Zhu-Tian. Waitgpt: Monitoring and steering conversational llm agent in data analysis with on-the-fly code visualization. In *Proceedings of the 37th Annual ACM Symposium on User Interface Software and Technology*, pp. 1–14, 2024.

Frank F Xu, Yufan Song, Boxuan Li, Yuxuan Tang, Kritanjali Jain, Mengxue Bao, Zora Z Wang, Xuhui Zhou, Zhitong Guo, Murong Cao, et al. Theagentcompany: benchmarking llm agents on consequential real world tasks. *arXiv preprint arXiv:2412.14161*, 2024.

- 
- Wenyi Xu, Yuren Mao, Xiaolu Zhang, Chao Zhang, Xuemei Dong, Mengfei Zhang, and Yunjun Gao. Dagent: A relational database-driven data analysis report generation agent. *arXiv preprint arXiv:2503.13269*, 2025.
- Eric Xue, Zeyi Huang, Yuyang Ji, and Haohan Wang. Improve: Iterative model pipeline refinement and optimization leveraging llm agents, 2025. URL <https://arxiv.org/abs/2502.18530>.
- Hongyang Yang, Boyu Zhang, Neng Wang, Cheng Guo, Xiaoli Zhang, Likun Lin, Junlin Wang, Tianyu Zhou, Mao Guan, Runjia Zhang, et al. Finrobot: An open-source ai agent platform for financial applications using large language models. *arXiv preprint arXiv:2405.14767*, 2024a.
- Zhiyu Yang, Zihan Zhou, Shuo Wang, Xin Cong, Xu Han, Yukun Yan, Zhenghao Liu, Zhixing Tan, Pengyuan Liu, Dong Yu, et al. Matplotagent: Method and evaluation for llm-based agentic scientific data visualization. *arXiv preprint arXiv:2402.11453*, 2024b.
- Guoli Yin, Haoping Bai, Shuang Ma, Feng Nan, Yanchao Sun, Zhaoyang Xu, Shen Ma, Jiarui Lu, Xiang Kong, Aonan Zhang, et al. Mmau: A holistic benchmark of agent capabilities across diverse domains. *arXiv preprint arXiv:2407.18961*, 2024.
- Ziming You, Yumiao Zhang, Dexuan Xu, Yiwei Lou, Yandong Yan, Wei Wang, Huaming Zhang, and Yu Huang. Datawiseagent: A notebook-centric llm agent framework for automated data science. *arXiv preprint arXiv:2503.07044*, 2025.
- Yangyang Yu, Zhiyuan Yao, Haohang Li, Zhiyang Deng, Yuechen Jiang, Yupeng Cao, Zhi Chen, Jordan Suchow, Zhenyu Cui, Rong Liu, et al. Fincon: A synthesized llm multi-agent system with conceptual verbal reinforcement for enhanced financial decision making. *Advances in Neural Information Processing Systems*, 37:137010–137045, 2024.
- Mert Yuksekgonul, Federico Bianchi, Joseph Boen, Sheng Liu, Zhi Huang, Carlos Guestrin, and James Zou. Textgrad: Automatic "differentiation" via text, 2024. URL <https://arxiv.org/abs/2406.07496>.
- Daoguang Zan, Ailun Yu, Wei Liu, Dong Chen, Bo Shen, Wei Li, Yafen Yao, Yongshun Gong, Xiaolin Chen, Bei Guan, et al. Codes: Natural language to code repository via multi-layer sketch. *arXiv preprint arXiv:2403.16443*, 2024.
- Eric Zelikman, Qian Huang, Gabriel Poesia, Noah Goodman, and Nick Haber. Parsel: Algorithmic reasoning with language models by composing decompositions. *Advances in Neural Information Processing Systems*, 36:31466–31523, 2023.
- Dan Zhang, Sining Zhoubian, Min Cai, Fengzu Li, Lekang Yang, Wei Wang, Tianjiao Dong, Ziniu Hu, Jie Tang, and Yisong Yue. Datascibench: An llm agent benchmark for data science. *arXiv preprint arXiv:2502.13897*, 2025a.
- Kechi Zhang, Jia Li, Ge Li, Xianjie Shi, and Zhi Jin. Codeagent: Enhancing code generation with tool-integrated agent systems for real-world repo-level coding challenges. *arXiv preprint arXiv:2401.07339*, 2024a.
- Shujian Zhang, Chengyue Gong, Lemeng Wu, Xingchao Liu, and Mingyuan Zhou. Automl-gpt: Automatic machine learning with gpt. *arXiv preprint arXiv:2305.02499*, 2023a.
- Wenqi Zhang, Yongliang Shen, Weiming Lu, and Yueteng Zhuang. Data-copilot: Bridging billions of data and humans with autonomous workflow. *arXiv preprint arXiv:2306.07209*, 2023b.
- Xuanming Zhang, Yuxuan Chen, Yuan Yuan, and Minlie Huang. Seeker: Enhancing exception handling in code with llm-based multi-agent approach. *arXiv preprint arXiv:2410.06949*, 2024b.
- Xueqiao Zhang, Chao Zhang, Jianwen Sun, Jun Xiao, Yi Yang, and Yawei Luo. Eduplanner: Llm-based multi-agent systems for customized and intelligent instructional design. *IEEE Transactions on Learning Technologies*, 2025b.

- 
- Yaolun Zhang, Yinxu Pan, Yudong Wang, and Jie Cai. Pybench: Evaluating llm agent on various real-world coding tasks. *arXiv preprint arXiv:2407.16732*, 2024c.
- Yuge Zhang, Qiyang Jiang, Xingyu Han, Nan Chen, Yuqing Yang, and Kan Ren. Benchmarking data science agents. *arXiv preprint arXiv:2402.17168*, 2024d.
- Yuntong Zhang, Haifeng Ruan, Zhiyu Fan, and Abhik Roychoudhury. Autocoderover: Autonomous program improvement. In *Proceedings of the 33rd ACM SIGSOFT International Symposium on Software Testing and Analysis*, pp. 1592–1604, 2024e.
- Yuheng Zhao, Junjie Wang, Linbin Xiang, Xiaowen Zhang, Zifei Guo, Cagatay Turkay, Yu Zhang, and Siming Chen. Lightva: Lightweight visual analytics with llm agent-based task planning and execution. *IEEE Transactions on Visualization and Computer Graphics*, 2024a.
- Zixiao Zhao, Jing Sun, Zhiyuan Wei, Cheng-Hao Cai, Zhe Hou, and Jin Song Dong. Visioncoder: Empowering multi-agent auto-programming for image processing with hybrid llms. *arXiv preprint arXiv:2410.19245*, 2024b.
- Andy Zhou, Kai Yan, Michal Shlapentokh-Rothman, Haohan Wang, and Yu-Xiong Wang. Language agent tree search unifies reasoning acting and planning in language models. *arXiv preprint arXiv:2310.04406*, 2023.