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Scientific Bespoke Artificial Intelligence Agents Optimized for Research Goals

SciBORG is an LLM-agnostic, modular agent framework with information retention capabilities, enabling robust, autonomous problem-solving for complex scientific discovery tasks like novel drug development.

Purdue researchers have developed an agentic framework titled, SciBORG, for use in complex scientific discovery tasks. SciBORG utilizes the Langchain software development kit (SDK), allowing for SciBORG to be LLM agnostic, thus supporting any LLM, including custom LLMs for powering these agents. The agents can also be linked together for creating an ensemble of domain specific agents that work together towards solving problems. Key characteristics of these agents is their modularity and ability to retain information. These characteristics allow for the removal of an agent from the workflow or addition of new LLMs without disrupting functionality. This characteristic coupled with the ability to retain information provides robustness for complex scientific discovery tasks, which is difficult in traditional LLMs or LLM-based agents such as ChatGPT or CRISPR-GPT respectively. The SciBORG agents can thus be utilized to perform autonomous or semi-autonomous problem-solving tasks in a stepwise and directed manner.

Technology Validation:

-Three categories of benchmarking were implemented for understanding the output, state and path for the agents

-Output-based benchmarking evaluated the agent its ability to produce desired results, disregarding both the actions taken and the final state of the interacting system.

-State benchmarking was used to evaluate the agent's ability to transition an interactive system from an initial state to desired final states, without considering the specific actions or their sequence

-Path-based benching was used to determine the specific actions taken, their sequence, and any inputs provided, rather than on the final output or state

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Category
Chemicals & Advanced Materials/Specialty & Performance Chemicals
Pharmaceuticals/Drug Discovery & Development
Chemicals & Advanced Materials/Materials Processing & Manufacturing Technologies
Pharmaceuticals/Computational & Software Tools
Pharmaceuticals/Research Tools & Assays

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-Synthetic benchmarking was performed on literature-know reactions to determine differences between human and AI run reactions

Advantages:

-Modularity of AI agents, allowing for addition or removal of agents without adversely affecting the framework

-Information retention for solving complex problems and improving functionality of AI agent

Applications:

-Pharmaceutical applications for novel dug discovery

TRL: 3

Intellectual Property:

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