R&D item

1. Experiment Automation AI Robot

Progress until the fiscal year 2023

1. Overview

We are developing an AI robot that, after conceiving experiments based on research hypotheses, estimates specific procedures in cyberspace and executes them in physical space.

Specifically, we are conducting R&D on (1) "AI for understanding experimental papers" to plan experiments from past cases, (2) "Exploration of AI robots performing organic synthesis" to conduct automated experiments, and (3) "XOR discovery AI for experimental predictions and results" to verify hypotheses from the outcomes.

2. Progress

This project sets the realization of AI that understands human research through scientific literature as its first milestone.

For the experiment automation AI robot, it is necessary to first plan experiments from related case studies in papers, as researchers would when replicating existing studies, and estimate and execute specific experimental parameters. However, since literature often only outlines experimental settings, this project attempted to infer by collecting knowledge from literature on different topics as well.

Additionally, it is necessary to examine results from experimental graphs to verify hypotheses. Thus, this project is developing AI models that can provide insights on experimental result figures in papers.

(1) AI for Understanding Experimental Papers

To understand and compare experimental content, we worked on "semantic analysis of tables" to extract and structure information such as tasks, data, and methods listed in paper tables. We input text-related information from tables into large language models (LLMs) to generate auxiliary explanatory text called synthetic context. Using this synthetic context as a feature for machine learning models improved entity linking accuracy by over 5 points compared to conventional methods. Moreover, utilizing text from cited literature complemented auxiliary knowledge not described in the paper itself, contributing to improved linking accuracy.

We also collected and annotated data on synthesis procedures targeting materials science literature, confirming that an initial BERT-based model could estimate synthesis procedures.

(2) AI Robots Performing Organic Synthesis

To represent compounds, we constructed a network-type database (Molecular Reaction Graph) with synthesis paths as edges and molecules as nodes, and fabricated a Kyoto University-style automated synthesis device, simplifying "Chemputor" (Fig. 1). Aiming for automatic input of experimental procedures, we approached the realization of an automatic generation program by converting experimental procedure text to Mermaid notation using ChatGPT. We successfully conducted 0.3 mol esterification, acetalization, and amidation experiments. Future work will address issues with post-processing and cleaning of experiments using deleterious and toxic substances.

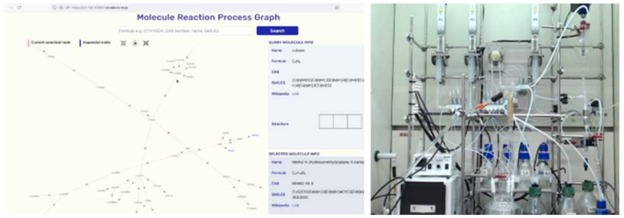

Fig. 1: Database (left) and automated synthesis device (right)

(3) XOR Discovery AI for Experiments

First, we built an AI that understands and explains figures in papers, developing a reliable AI incorporating researchers' insights. As existing models struggle with detailed explanations, we explored methods to input researcher-emphasized areas into the model. By manipulating Attention Weights in the Self-Attention mechanism, we generated captions detailing emphasized regions. Experiments confirmed the generation of captions containing words related to emphasized areas (Fig. 2).

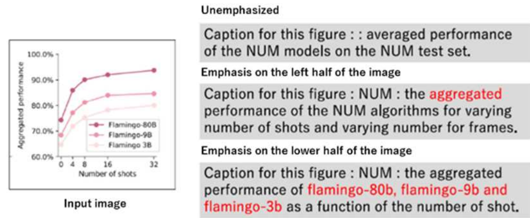

Fig. 2: Generated text given figures and emphasized areas

3. Future work

The milestone up to fiscal year 2025 includes not only continuing to understand research but also realizing hypothesis generation. Physical space experiments are crucial for this, and research acceleration is necessary to prevent this from becoming a bottleneck.

Specifically, we will first expand the exploration space of target substances by enhancing automated synthesis methods. We will simultaneously explore diverse synthesis methods such as flow synthesis and mechanochemical synthesis.

We also plan to incorporate synthesis execution while updating initial hypotheses for candidate substances to those easier to synthesize or more likely to react, considering hypothesis updates utilizing simulations.

Lastly, synthesizing such candidate substances requires estimating synthesis routes and synthesis conditions.

Thus, this project aims to increase the throughput of the research loop by further advancing the experiment automation AI robot.

R&D item

2. Claim & Analysis AI

Progress until the fiscal year 2023

1. Overview

This research project models the research loop as: hypothesis, experiment, analysis, description & dialogue, and new hypothesis... Within this loop, the assertion and analysis steps, which include hypothesis generation and verification, require AI capable of understanding multimodal scientific data and responding with language-based evidence.

Therefore, we are working on a "Multimodal XAI Foundation Model" as the Argumentation & Analysis AI, developing an AI that can understand relationships between parts corresponding to assertions and analyses described in individual papers, as well as comprehend summaries and similarities across multiple papers.

2. Progress

As a starting point for the Multimodal XAI Foundation Model developed in this research project, we are advancing the initial development of a Multimodal XAI that mutually understands papers. Aiming for the project's 2023 milestone state of "AI robots capable of mutual understanding of research described in existing papers through knowledge exploration using literature," we constructed a pipeline to learn the foundational model from multimodal data combining figures, tables, and text in papers.

We conducted verifications on the project's overall 2023 milestones: "verification of internal consistency understanding in papers," "verification of mutual understanding between papers," "verification of survey generation including mutual understanding between papers," and "verification of similarity understanding between papers." These verifications were performed as downstream tasks of the foundation model, following fine-tuning.

Multimodal XAI Foundation Model

In this research, we worked on achieving technical goals based on milestone evaluation items. To reduce the cost of manually creating datasets related to paper comprehension, we built a framework utilizing general data and paper knowledge. We also conducted research on hypothesis generation and law discovery using generative AI.

For paper consistency understanding, as shown in Fig. 1, we constructed a model using BERT and GPT-4 to detect and explain consistency between paper claims and experimental results. This improved the accuracy of consistency detection using pre-training datasets of papers. In user studies, we received high satisfaction ratings from researchers.

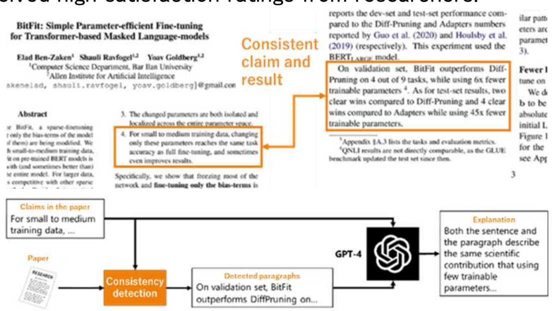

Fig. 1: Example of consistency (top) and pipeline (bottom)

For mutual understanding between papers, we developed a model that learns paper similarities and estimates similar parts between new papers. We obtained high-accuracy similarity evaluation results in both information and chemistry fields.

Furthermore, we automated survey generation including mutual understanding between papers. Based on the pipeline shown in Fig. 2, we selected relevant papers using a retrieval model based on specified topics and created surveys including figures and tables. In user studies, we received high evaluations from researchers.

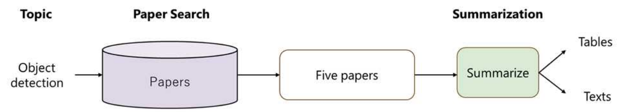

Fig. 2: Paper summary generation based on specified topics

Lastly, for similarity understanding between papers, we created similar paper pairs and automatically generated text explaining their similarity. This also received high evaluations in user studies.

3. Future work

We will continue to advance research understanding from literature while aiming to realize hypothesis generation. We will embed scientific and technological paper knowledge into a continuous space using large language models and multimodal foundation models, explore and reason within this space, and generate scientific hypotheses considering the balance between novelty and validity.

As scientific and technological knowledge is niche and prone to hallucination, retrieval expansion and stepwise reasoning that maintain creativity while suppressing misinformation are necessary. It is also important to realize XAI with explainability on multimodal paper understanding models.

Furthermore, our goal is to research and develop foundation models that allow AI to create new knowledge and hypotheses in scientific and technological fields, making them available to human researchers. We aim to realize mutual relationship understanding in research using AI with multimodal input/output and explainability and achieve multimodal hypothesis generation in collaboration with other research and development tasks.

R&D item

3. Description & Dialogue AI

Progress until the fiscal year 2023

1. Overview

Researchers typically summarize experimental results, discuss with other researchers, form further hypotheses, and proceed to the next experiment. An AI capable of describing results and updating hypotheses through interactive discussions is necessary.

This project advances R&D on (1) "Paper comprehension and experiment planning AI with Scientist-in-the-loop" for designing experiments as hypotheses, and (2) "Multimodal hypothesis generation using knowledge inference and dialogue" to interactively formulate hypotheses, realizing the Description & Dialogue AI.

2. Progress

Aiming to develop a Multimodal XAI that understands experimental content from figures, tables, and text in papers, we introduced technology reflecting researchers' experiences. Utilizing researcher feedback, we improved LLM performance without large datasets and developed techniques to enhance task allocation and prompt reliability based on expertise.

Furthermore, we worked on constructing paper comprehension and hypothesis generation models using large language models as a foundation for multimodal hypothesis generation.

(1) Paper and Experiment Understanding AI

First, to realize Multimodal XAI, we developed technology to reflect researchers' tacit knowledge in LLMs. Using specific output examples from researchers, we developed a technique for extracting relevant descriptions and outputting their rationale using In-context learning through prompts. This achieved LLM performance improvement without requiring large datasets.

Next, we developed a researcher knowledge understanding AI and techniques to estimate optimal allocation of feedback tasks and prompt reliability based on expertise.

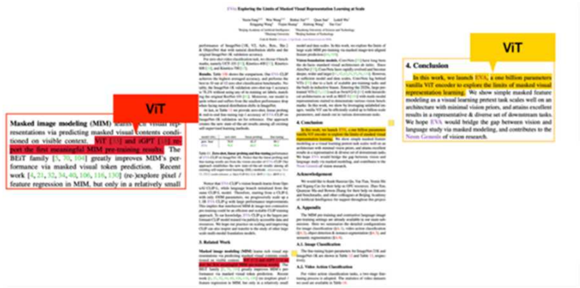

Fig. 1: Researcher knowledge understanding AI

This enabled high-quality output when multiple researchers collaboratively design LLM prompts (Fig. 1).

Furthermore, we worked on understanding experimental content using researcher knowledge acquisition AI and knowledge understanding AI. Targeting papers on object detection technology, we extracted and verified tags, improving accuracy compared to simple LLM usage. We confirmed that incorporating researchers' insights streamlined the understanding of experimental content (Fig. 2).

Lastly, we developed a web application for molecular editing as an interface to embed researchers' insights into molecular synthesis AI. Using RLHF technology, researchers can not only evaluate the foundation model's output but also propose improvements, enabling the reflection of researchers' thought processes in the model.

(2) Multimodal Hypothesis Generation

This research addressed multimodal hypothesis generation using knowledge inference and dialogue. We focused on constructing a paper comprehension framework using large language models, adjusting existing open-calm and T5 models using a paper database obtained from the Patent Office. We

Fig. 2: Tag extraction and related literature presentation based on experimental content understanding

used a general masked language model as the objective function. We generated hypotheses by providing prompts to the fine-tuned model. We created 100,000 hypothesis generation data related to causal relationships from patent data.
We also prepared necessary data for hypothesis generation, employing linguistically proficient annotators to construct annotation standards for 10,000 patent data and made over 300 annotations on selected patents.

In constructing the knowledge inference model, we focused on causal relationships and considered methods to select valid hypotheses using generated hypothesis data and external causal relationship dictionaries. Towards building an AI that dialogues with researchers about hypotheses, we explored an AI utterance modification method using reinforcement learning (RL-AIF). We plan to evaluate this method in the future.

3. Future work

We will continue to develop co-evolutionary artificial intelligence technology that improves AI performance through researcher dialogue and feedback, aiming to embed researchers' inspirations for hypothesis generation into AI. The hypothesis inspiration AI will acquire and reason knowledge, collaborating with humans through dialogue to trigger innovative discoveries and innovations.

Japan Science and Technology Agency