

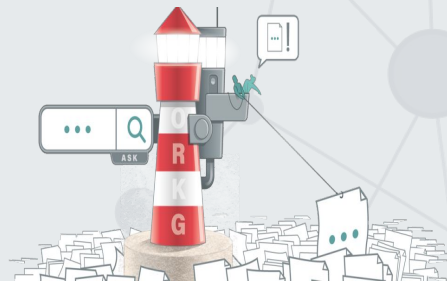
Neuro-Symbolic AI for Scholarly Research: Enhancing Discovery, Reasoning, and Assistance with LLMs and Knowledge Graphs

Introducing the TIB Alssistant

A platform for AI-supported research

Gollam Rabby

Slides partly created by Allard Oelen



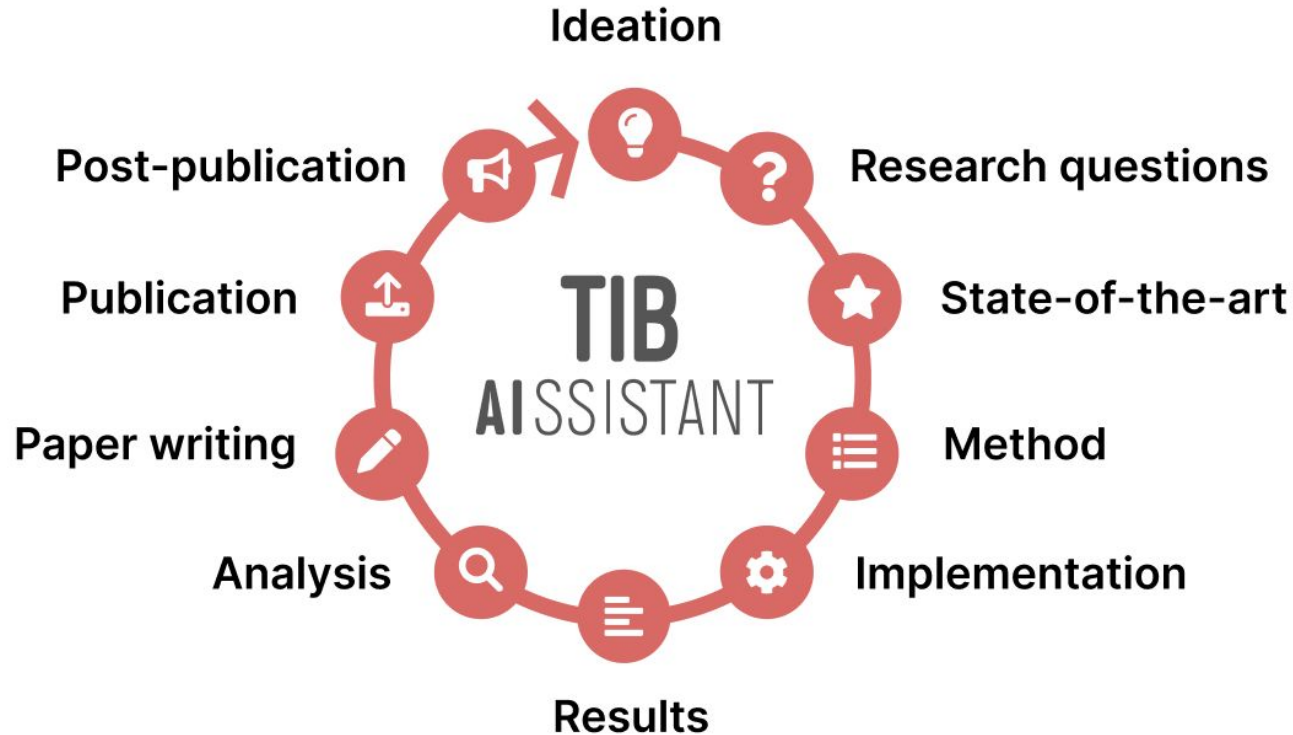
TIB
AISSISTANT

TIB Alssistant

- An AI-supported research assistant helping **throughout the research life cycle**
- Modular, flexible, domain-agnostic or domain-driven (where need)

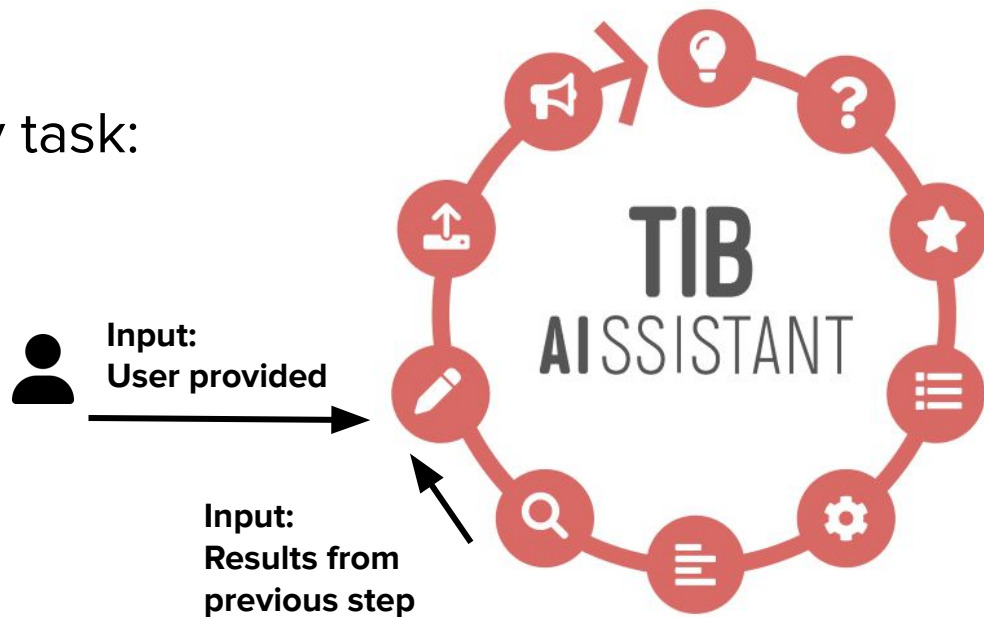


TIB AIssistant



TIB Aassistant

- General user interaction by task:
 - a. System prompts
 - b. Default set of tools
 - c. Assets
 - Input
 - Output
- Each phase can be used in isolation or in sequence



TIB AISSISTANT

Ideation

Research questions

Related literature

Method

Implementation

Results

Analysis

Paper writing

Review

Publication

Post-publication

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Ideation chat



The ideation phase helps you to explore possibly interesting research avenues. This can be based on your already existing work, or based on new topics you like to explore further. [Read more](#)

Task and system prompt

Please provide some of your existing papers (e.g., PDF, DOI, or your ORCID) to serve as inspiration for the rest of the ideation.

The DOI is 10.1145/3670419

Crossref ➕

ORCID ➕

Here are relevant topics, select the ones you are interested in:

- ☐ HCI with machine learning
- ☐ Impact of machine learning on modern HCI systems

Type your message here



DOI

ORCID

PDF

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Tools

Assets

Output

Ideation topics 4



≡ HCI for machine learning for a world x

≡ Lorem ipsum dolor sit amet x

≡ Attention is all you need x

≡ HCI for machine learning for a world x

Add a topic...

Assets, input/output

TIB AISSISTANT

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Assets

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Ideation topics 4



HCI for machine learning for a world x

Lorum ipsum dolor sit amet x

Attention is all you need x

HCI for machine learning for a world x

Add a topic...

Assets, input/output

TIB Alssistant

Ideation



Helps researchers with ideas of new topics, research directions, or gaps in the literature.

Input: papers, personal profiles

Output: list of ideas

TIB AISSISTANT

- Ideation
- Research questions
- Related literature
- Method
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Task and system prompt

Here are relevant topics, select the ones you are interested in:

☐

How can explainable AI improve user trust and decision-making in interactive ML systems?

☐

How can multimodal interaction (voice, gesture, gaze) combined with ML enhance accessibility for users with disabilities?

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Tools

Assets

Output

Research Question/s

Assets, input/output

TIB AISSISTANT

- Ideation
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Tools

Assets


Output

Research Question/s

Assets, input/output

TIB AISSISTANT

- Ideation
- Research questions
- **Related literature**
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- Implementation
- Results
- Analysis
- Paper writing
- Review
- Publication
- Post-publication

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Task and system prompt

User trust in AI is widely recognized as essential for real-world adoption. A systematic review by Bacha et al. (2022) identifies socio-ethical factors, technical/design elements, and individual characteristics as key influencers of trust [1]. They particularly highlight transparency—often achieved via explanations—as a critical determinant. Similarly, a meta-review in healthcare emphasizes that transparency is vital for clinicians to trust AI recommendations [2]. Explanations serve multiple roles: they help users assess model reliability, detect errors, and feel in control—countering algorithm aversion [3]. Although intuitively helpful, explanations don't always improve decision-making. Alufaisan et al. (2020) found that while AI predictions alone enhanced user accuracy, adding explanations showed *no significant improvement* [4]. This aligns with Papenmeier et al. (2019), who reported that model accuracy had more influence on users than explanation fidelity, and misleading explanations could actually erode trust [6]. In contrast, Kartikeya (2021) reported that transparency through explanations *did* significantly increase user trust in a Yelp star-rating task [6].

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Tools

Assets

Output

RQ1: How can explainable AI improve user trust and decision-making in interactive ML systems?

Assets, input/output

TIB Alssistant ❤️ ORKG Ask

Finds state of the art via various platforms, help to structure the state of the art

Input: topics, research questions

Output: bibliography

[77,368,538 Items with abstracts](#)




State-of-the-art

```
@article{schuhmann2025project,  
  title={Project alexandria: Towards freeing scientific  
    knowledge from copyright burdens via llms},  
  author={Schuhmann, Christoph and Rabby,  
    Gollam and Prabhu, Ameya and Ahmed, Tawsif  
    and Hochlehnert, Andreas and Nguyen, Huu and  
    Akinci, Nick and Schmidt, Ludwig and  
    Kaczmarczyk, Robert and Auer, Soren and  
    others},  
  journal={arXiv preprint arXiv:2502.19413},  
  year={2025}}
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- Ideation
- Research questions
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- **Method**
- Implementation
- Results
- Analysis
- Paper writing
- Review
- Publication
- Post-publication

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Ideation chat



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Task and system prompt

Hypothesis 1: *Providing context-adaptive explanations in interactive machine learning (IML) systems significantly increases user trust and decision-making accuracy compared to systems with no explanations or static, generic explanations.*

Hypothesis 2: *Users interacting with an IML system that offers personalized, fidelity-aware explanations will calibrate their trust more accurately—trusting correct predictions and questioning incorrect ones—compared to users receiving uniformly high-confidence outputs without explanation.*

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Tools

Assets

Output

RQ1: How can explainable AI improve user trust and decision-making in interactive ML systems?

Assets, input/output

Ideation

Research questions

Related literature

Method

Implementation

Results

Analysis

Paper writing

Review

Publication

Post-publication

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Reset all



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Assets, input/output

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- Related literature
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Task and system prompt

We will conduct a between-subjects user study with three conditions: (1) no explanations, (2) static/generic explanations, and (3) context-adaptive explanations. Participants will interact with a simulated IML system on a decision-making task (e.g., document classification or loan approval). Trust will be measured using a validated trust-in-AI scale and behavioral proxies (e.g., reliance, override rate).
Decision-making accuracy will be assessed based on task performance compared to ground truth. We will analyze results using ANOVA and post-hoc tests to compare the impact of explanation types on trust and accuracy.

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Tools


Assets

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Assets, input/output

 Deactivated items coming soon

Reset all



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Task and system prompt

We conducted experiments on synthetic and real-world datasets to evaluate the effectiveness of our compositional regularization.

```

1  # Import the necessary libraries
2  import pandas as pd
3  import numpy as np
4
5  # Create a sample dataset
6  n_rows = 1000
7  n_features = 10
8
9  # Generate random data
10 data = pd.DataFrame({
11     'feature_1': np.random.randn(n_rows),
12     'feature_2': np.random.randn(n_rows),
13     'feature_3': np.random.randn(n_rows),
14     'feature_4': np.random.randn(n_rows),
15     'feature_5': np.random.randn(n_rows),
16     'feature_6': np.random.randn(n_rows),
17     'feature_7': np.random.randn(n_rows),
18     'feature_8': np.random.randn(n_rows),
19     'feature_9': np.random.randn(n_rows),
20     'feature_10': np.random.randn(n_rows),
21 })
22
23 # Split the data into training and testing sets
24 train_data, test_data = train_test_split(data, test_size=0.2, random_state=42)
25
26 # Feature Engineering
27 # Create a new feature based on existing features
28 def create_new_feature(data):
29     # Example: Create a new feature 'feature_11' as the sum of 'feature_1' and 'feature_2'
30     data['feature_11'] = data['feature_1'] + data['feature_2']
31     return data
32
33 # Apply the function to the training data
34 train_data = create_new_feature(train_data)
35
36 # Feature Scaling
37 # Standardize the features (mean = 0, std = 1)
38 from sklearn.preprocessing import StandardScaler
39 scaler = StandardScaler()
40 train_data[['feature_1', 'feature_2', 'feature_3', 'feature_4', 'feature_5',
41            'feature_6', 'feature_7', 'feature_8', 'feature_9', 'feature_10', 'feature_11']] = scaler.fit_transform(
42     train_data[['feature_1', 'feature_2', 'feature_3', 'feature_4', 'feature_5',
43                'feature_6', 'feature_7', 'feature_8', 'feature_9', 'feature_10', 'feature_11']])
44
45 # Model Training
46 # Import a simple linear model
47 from sklearn.linear_model import LinearRegression
48 model = LinearRegression()
49
50 # Train the model on the training data
51 model.fit(train_data[['feature_1', 'feature_2', 'feature_3', 'feature_4', 'feature_5',
52                    'feature_6', 'feature_7', 'feature_8', 'feature_9', 'feature_10', 'feature_11']],
53         train_data['feature_11'])
54
55 # Model Evaluation
56 # Predict values for the test data
57 predictions = model.predict(test_data[['feature_1', 'feature_2', 'feature_3', 'feature_4', 'feature_5',
58                                       'feature_6', 'feature_7', 'feature_8', 'feature_9', 'feature_10', 'feature_11']])
59
60 # Calculate the Mean Squared Error (MSE)
61 from sklearn.metrics import mean_squared_error
62 mse = mean_squared_error(test_data['feature_11'], predictions)
63
64 # Print the MSE
65 print("Mean Squared Error (MSE):", mse)

```

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Assets

Output

RQ1: How can explainable AI improve user trust and decision-making in interactive ML systems?

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Assets, input/output

TIB AISSISTANT

- Ideation
- Research questions
- Related literature
- Method
- Implementation
- **Results**
- Analysis
- Paper writing
- Review
- Publication
- Post-publication

Deactivated items coming soon

Reset all



Ideation chat



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Task and system prompt

On the SCAN dataset, all models achieved similar validation and test accuracies, indicating that compositional regularization did not improve performance on this task.

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Tools

Assets

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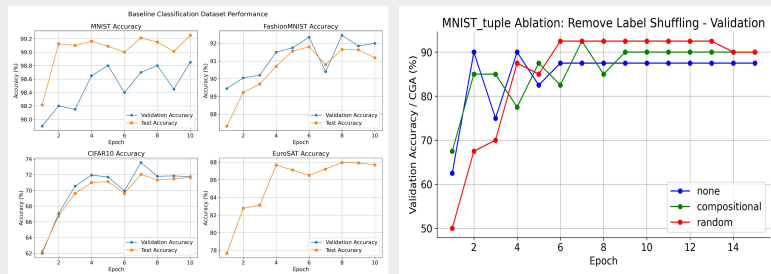


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Task and system prompt



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Tools

Assets

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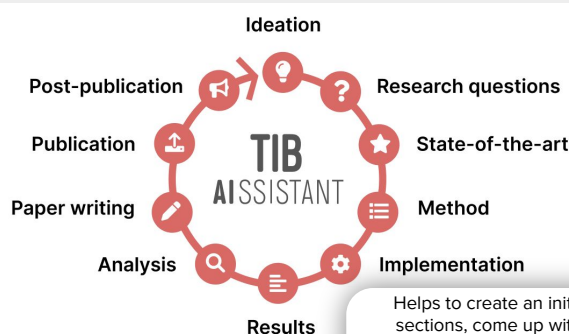


Ideation chat



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Task and system prompt



Helps to create an initial draft of sections, come up with suitable paper titles, etc.

Input: all output of previous steps
Output: article draft (LaTeX, Word, Docs etc.)

Type your message here



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Tools

Assets

Output

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- Ideation
- Research questions
- Related literature
- Method
- Implementation
- Results
- Analysis
- Paper writing
- Review
- Publication
- Post-publication

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Task and system prompt



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Tools

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- Method
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- Review
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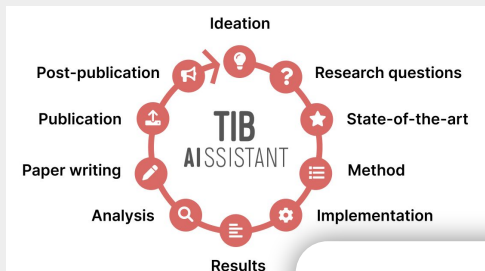


Ideation chat



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Task and system prompt



Determines suitable venues for publication

Input: paper text

Output: Updated version of the paper

Type your message here



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Tools

Assets

Output

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Assets, input/output

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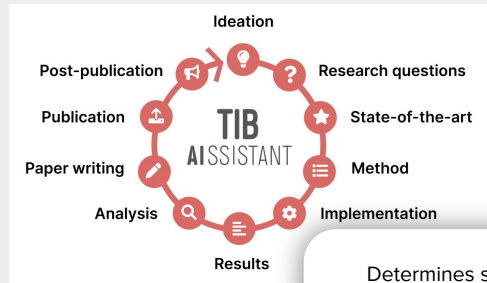


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Task and system prompt



Determines suitable venues for publication

Input: paper text

Output: list of suitable venues

Type your message here



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Assets, input/output

Ongoing research

1. Deep Hypothesis and Research Question/s
2. Deep Method and implementation
3. Deep Results and Analysis
4. Scientific Reasoning Models



Iterative Hypothesis Generation for Scientific Discovery with Monte Carlo Nash Equilibrium Self-Refining Trees

Gollam Rabby^{1†} (✉), Diyana Muhammed^{2†}, Prasenjit Mitra², and Sören Auer^{1,2}

¹ L3S Research Center, Leibniz University Hannover, Hannover, Germany
{gollam.rabby, mitra}@l3s.de


² TIB—Leibniz Information Centre for Science and Technology, Hannover, Germany
{diyana.muhammed, auer}@tib.eu

 [Dataset](#)  [Project Page](#)  [Codebase](#)

Abstract. Scientific hypothesis generation is a fundamentally challenging task in research, requiring the synthesis of novel and empirically grounded insights. Traditional approaches rely on human intuition and domain expertise, while purely large language model (LLM) based methods often struggle to produce hypotheses that are both innovative and reliable. To address these limitations, we propose the Monte Carlo Nash Equilibrium Self-Refine Tree (MC-NEST), a novel framework that integrates Monte Carlo Tree Search (MCTS) with Nash Equilibrium strategies to iteratively refine and validate hypotheses. MC-NEST dynamically balances exploration and exploitation through adaptive sampling strategies, which prioritize high-potential hypotheses while maintaining diversity in the search space. We demonstrate the effectiveness of MC-NEST through comprehensive experiments across multiple domains, including biomedicine, social science, and computer science. MC-NEST achieves average scores of 2.65, 2.74, and 2.80 (on a 1-3 scale) for novelty, clarity, significance, and verifiability metrics on the social science, computer science, and biomedicine datasets, respectively, outperforming state-of-the-art prompt-based methods, which achieve 2.36, 2.51, and 2.52 on the same datasets. These results underscore MC-NEST's ability to generate high-quality, empirically grounded hypotheses across diverse domains. Furthermore, MC-NEST facilitates structured human-AI collaboration, ensuring that LLMs augment human creativity rather than replace it. By addressing key challenges such as iterative refinement and the exploration-exploitation balance, MC-NEST sets a new benchmark in automated hypothesis generation. The framework provides a robust and adaptable approach that advances the boundaries of scientific discovery. Additionally, MC-NEST's ethical design enables responsible AI use, emphasizing transparency and human supervision in hypothesis generation.

Keywords: Scientific Hypothesis Generation · Monte Carlo Tree Search · Adaptive Sampling Strategies · Hypothesis Refinement.

Ongoing research

1. Deep Hypothesis and Research Question/s
2. Deep Method and implementation  LLM write code
3. Deep Results and Analysis
4. Scientific Reasoning Models

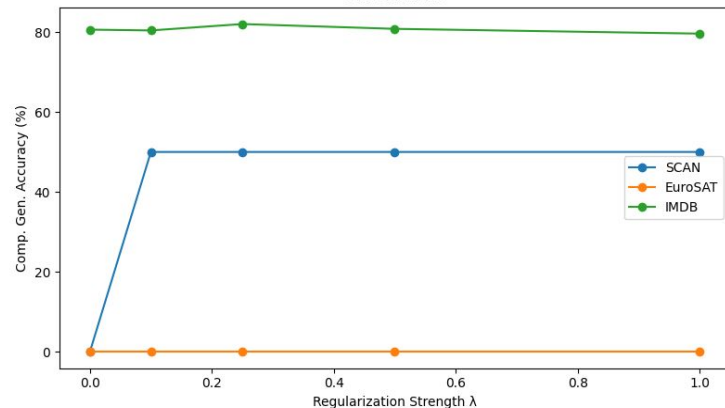
```
experiments - 2025-06-04 12:10:55_compositional_regularization_on_attention_0 > logs > D:\run > experiment_results > experiment_2ab07f726ed4ec409c51e020f0405_proc_1569088 > experiment_code.py
1 # Set random seed
2 import random
3 import numpy as np
4 import torch
5
6 seed = 2
7 random.seed(seed)
8 np.random.seed(seed)
9 torch.manual_seed(seed)
10 if torch.cuda.is_available():
11     torch.cuda.manual_seed(seed)
12
13 import os
14
15 working_dir = os.path.join(os.getcwd(), "working")
16 os.makedirs(working_dir, exist_ok=True)
17
18 import numpy as np
19 import torch
20 import torch.nn as nn
21 import torch.optim as optim
22 import random
23 from torch.utils.data import Dataset, DataLoader
24 import matplotlib.pyplot as plt
25
26 device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
27 print(f"Using device: {device}")
28
29 lambda settings = {0.0, 0.1, 0.25, 0.5, 1.0}
30 experiment_data = {}
31
32 ##### SCAN-like (Synthetic) #####
33 PRIMITIVES = ["jump", "walk", "look"]
34 MODIFIERS = ["twice", "around right", "opposite left"]
35 ACTIONS = {"jump": "JUMP", "walk": "WALK", "look": "LOOK"}
36 MOD_ACTIONS = {"twice": 2, "around_right": 1, "opposite_left": 1}
37 random.seed(1111)
38 all_pairs = [(p, m) for p in PRIMITIVES for m in MODIFIERS]
39 random.shuffle(all_pairs)
40 num_pairs = len(all_pairs)
41 num_comp_gen = max(1, int(num_pairs * 0.3))
42 comp_gen_pairs = all_pairs[num_comp_gen:]
43 train_pairs = all_pairs[num_comp_gen:]
44 primitive_only = [(p, None) for p in PRIMITIVES]
45
46
47 def build_examples(pairs):
48     examples = []
49     for p, m in pairs:
50         if m is None:
51             inp = [p]
52             tgt = [ACTIONS[p]]
53         else:
54             inp = [p, m]
55             tgt = [ACTIONS[p]] * MOD_ACTIONS[m]
56         examples.append((" ".join(inp), " ".join(tgt)))
57     return examples
58
59
60 train_data = build_examples(train_pairs) + build_examples(primitive_only)
61 comp_gen_data = build_examples(comp_gen_pairs)
62 val_data = train_data[-4:]
63 train_data = train_data[:-4]
64
65
66 def build_vocab(examples):
67     vocab = set()
68     for src, tgt in examples:
```

Ongoing research

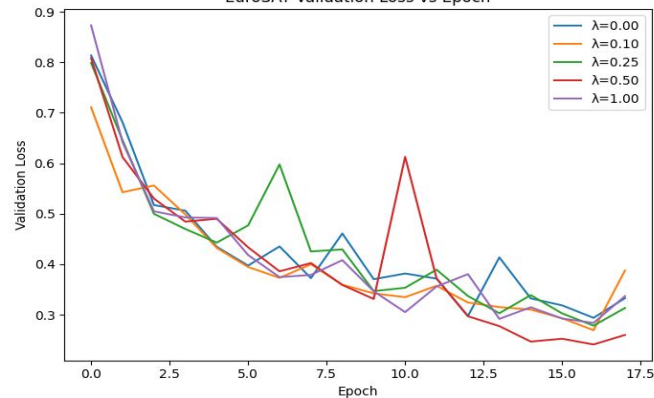
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LLM write code and compiles

Compositional Generalization Accuracy at Last Epoch
All Datasets



EuroSAT Validation Loss vs Epoch



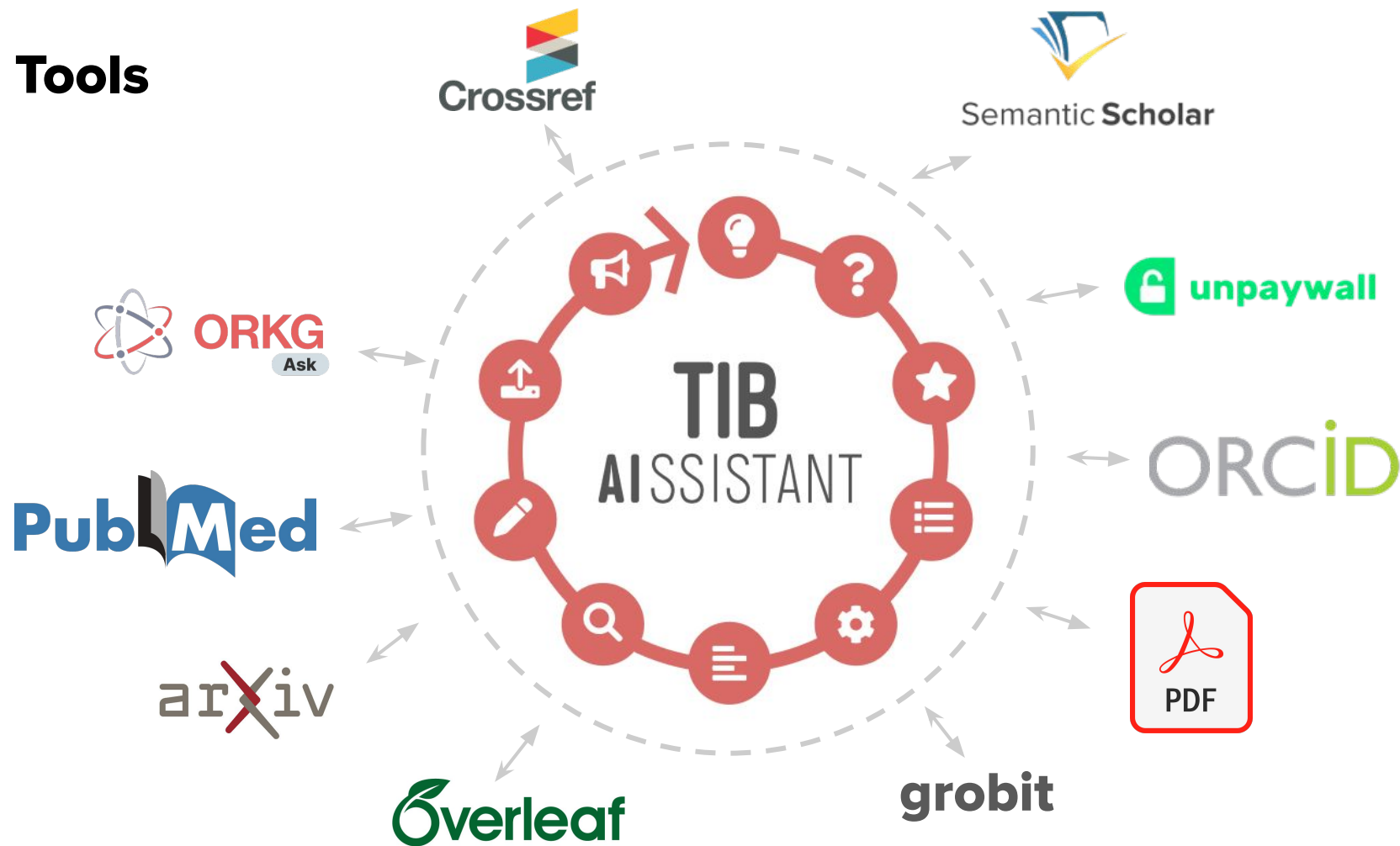
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3. Deep Results and Analysis
4. Scientific Reasoning Models →

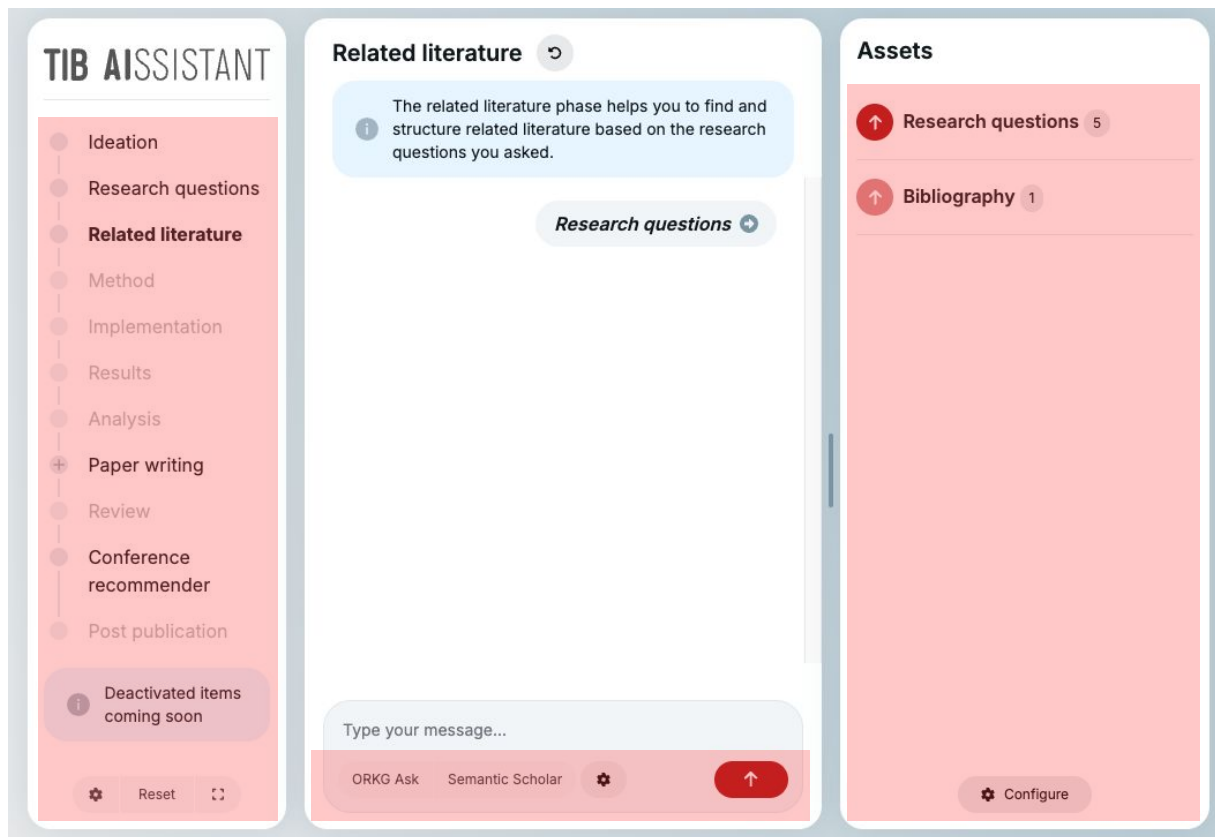


COMING SOON

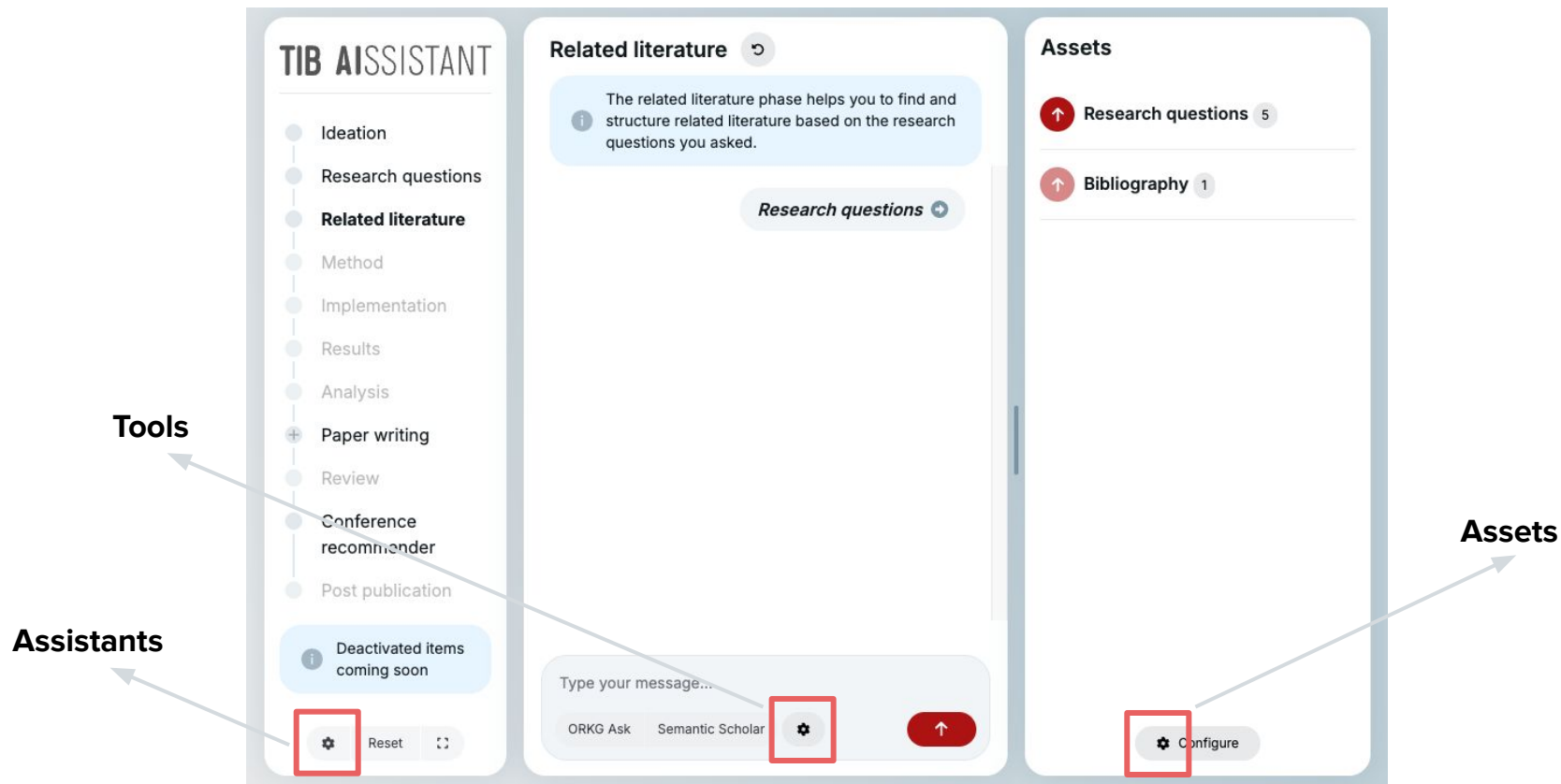
Tools



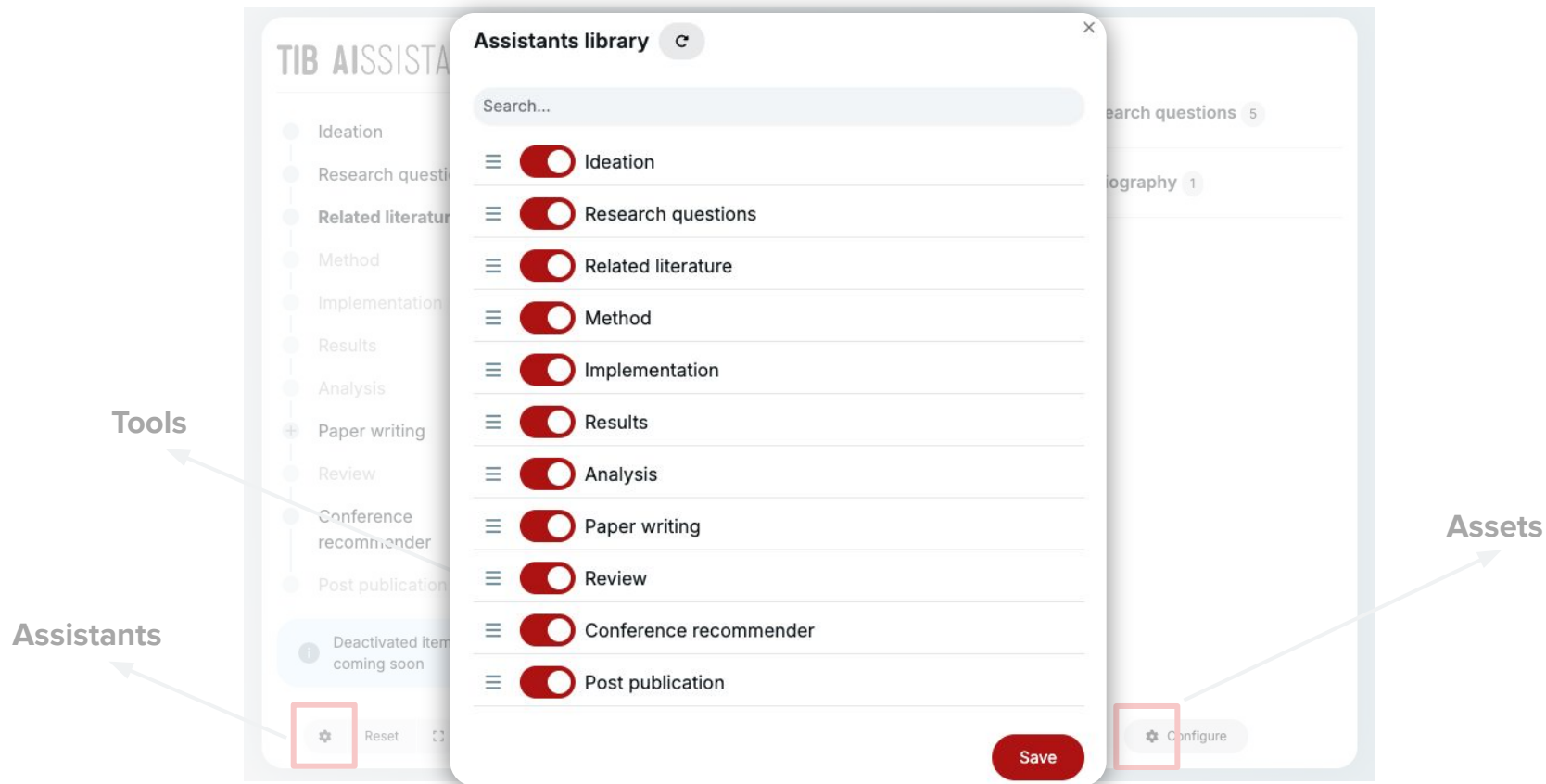
Configurability



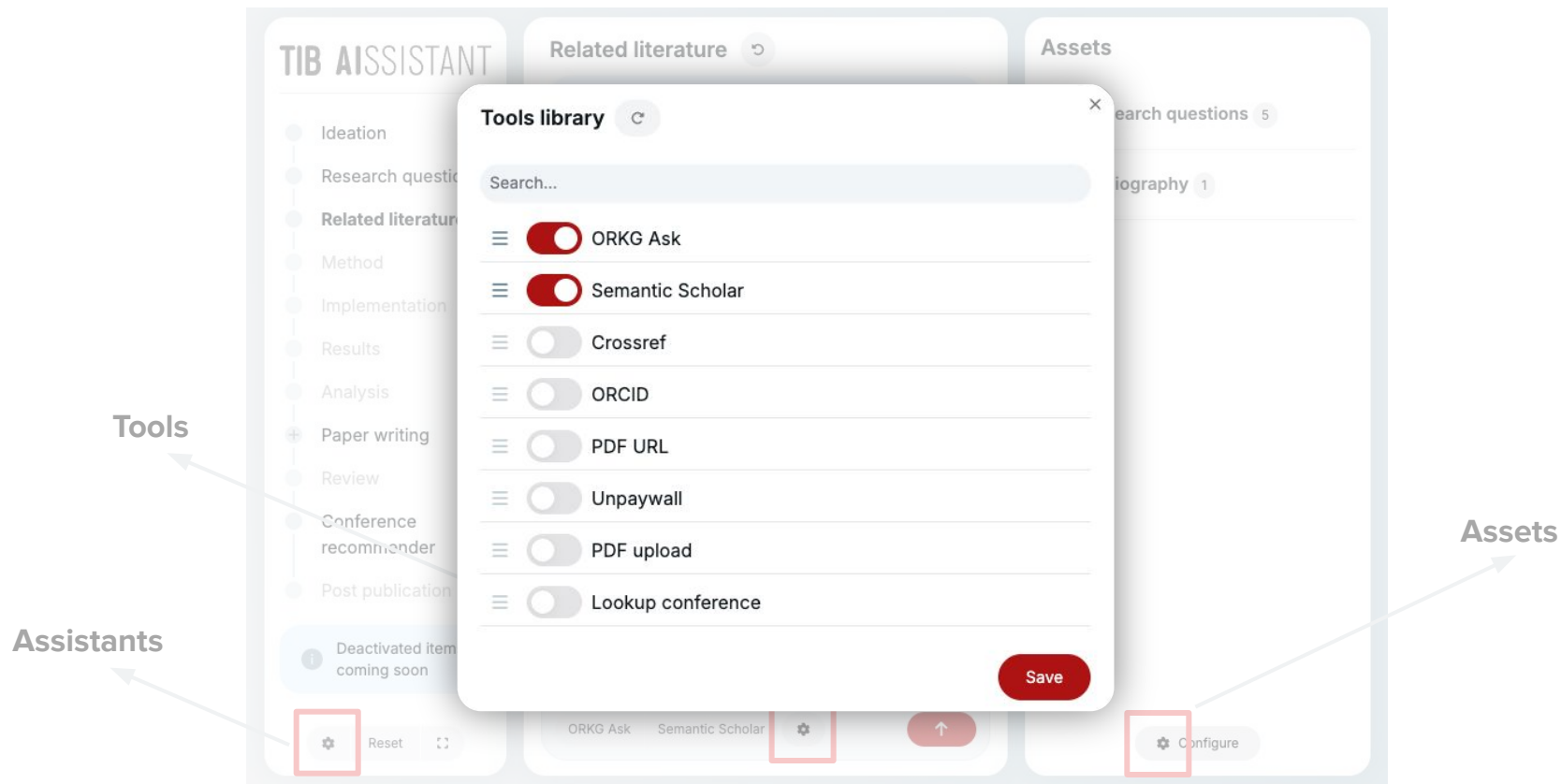
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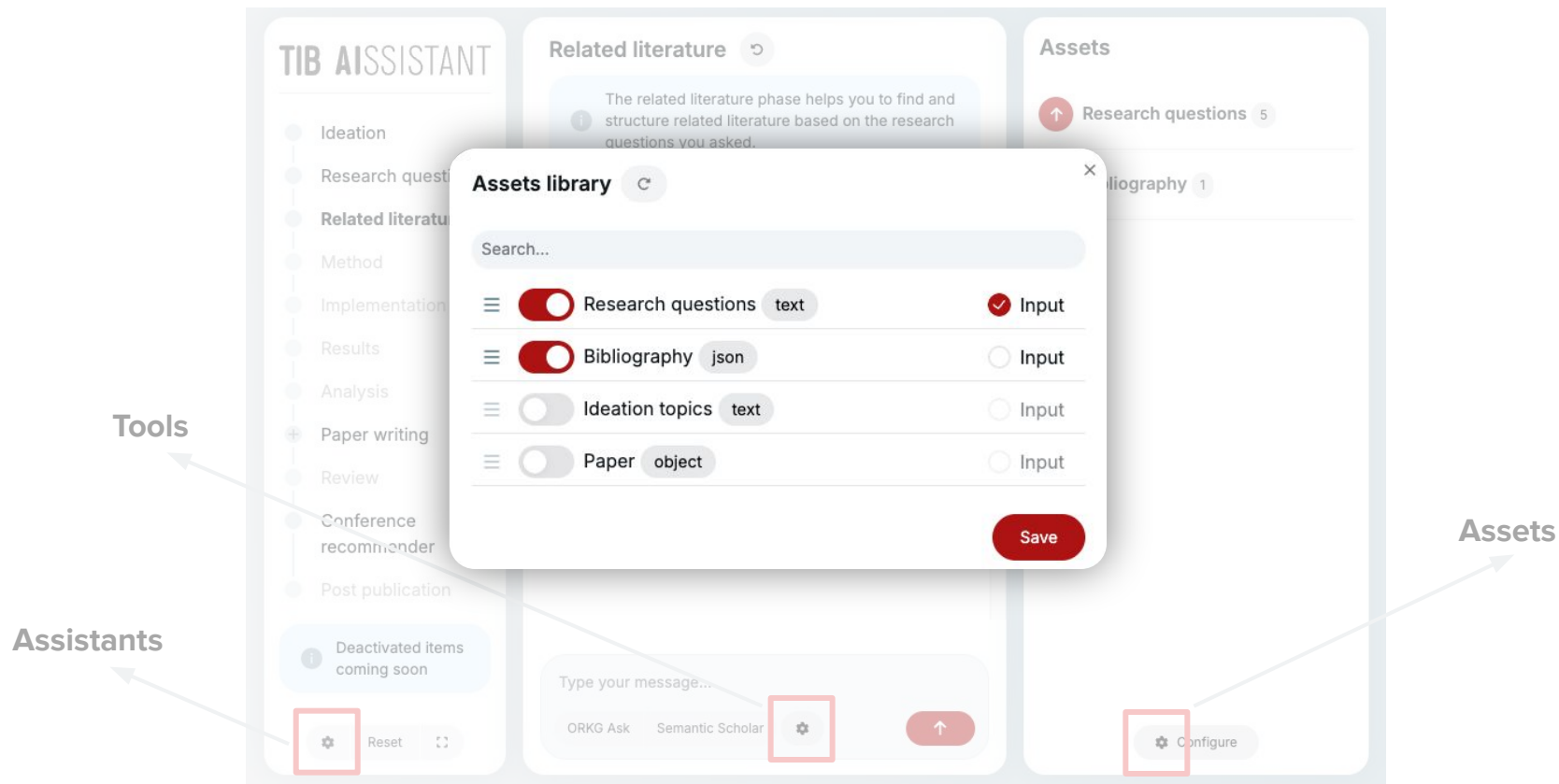
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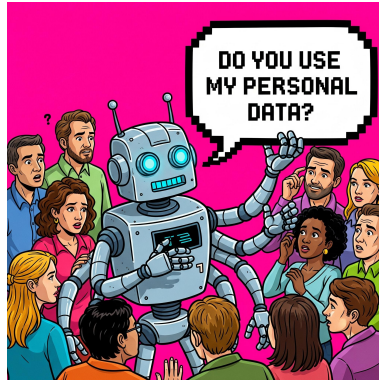


Configurability



Ethical Considerations

1. **Transparency:** Clearly disclose when and how AI contributes to scientific research to maintain trust and accountability.
2. **Peer Review Integrity:** Prevent misuse of AI to manipulate publication metrics or game the peer-review process.
3. **Ethical Oversight:** Ensure research involving AI-generated work is conducted with proper approvals and institutional cooperation.
4. **Community Standards:** Collaborate with the scientific community to develop norms and guidelines for responsible AI use in research.
5. **Avoiding Bias:** Balance transparency with fair evaluation by addressing concerns about bias in reviewing AI-assisted research.



Publications

1. Farhana Keya, Gollam Rabby, Prasenjit Mitra, Sahar Vahdati, Sören Auer, and Yaser Jaradeh. "**SCI-IDEA: Context-Aware Scientific Ideation Using Token and Sentence Embeddings.**" *arXiv preprint arXiv:2503.19257* (2025).
2. Gollam Rabby, Diyana Muhammed, Prasenjit Mitra, and Sören Auer. "**Iterative hypothesis generation for scientific discovery with monte carlo self-refining trees.**" *arXiv preprint arXiv:2503.19309* (2025).
3. Christoph Schuhmann, Gollam Rabby, Ameya Prabhu, Tawsif Ahmed, Andreas Hochlehnert, Huu Nguyen, Nick Akinici et al. "**Project alexandria: Towards freeing scientific knowledge from copyright burdens via llms.**" *arXiv preprint arXiv:2502.19413* (2025).
4. Diyana Muhammed, Gollam Rabby, and Sören Auer. "**SelfCheckAgent: Zero-Resource Hallucination Detection in Generative Large Language Models.**" *arXiv preprint arXiv:2502.01812* (2025).
5. Gollam Rabby, Farhana Keya and Sören Auer. "**MC-NEST--Enhancing Mathematical Reasoning in Large Language Models with a Monte Carlo Self-Refine Tree.**" *arXiv preprint arXiv:2411.15645* (2024).

Resources

Repository:

<https://gitlab.com/TIBHannover/orkg/tib-aissant/web-app>



Developer documentation:

<https://tibhannover.gitlab.io/orkg/tib-aissant/web-app/storybook/?path=/docs/introduction--docs>

Thank you!

Any Questions?

Gollam Rabby

gollam.rabby@tib.eu

[linkedin.com/in/gollam-rabby-28203095/](https://www.linkedin.com/in/gollam-rabby-28203095/)

Meet the team:

<https://orkg.org/about/9/Team>