

NOT SEARCH, BUT SCAN: BENCHMARKING MLLMS ON SCAN-ORIENTED ACADEMIC PAPER REASONING

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ABSTRACT

With the rapid progress of multimodal large language models (MLLMs), AI already performs well at literature retrieval and certain reasoning tasks, serving as a capable assistant to human researchers, yet it remains far from autonomous research. The fundamental reason is that current work on scholarly paper reasoning is largely confined to a search-oriented paradigm centered on pre-specified targets, with reasoning grounded in relevance retrieval, which struggles to support researcher-style full-document understanding, reasoning, and verification. To bridge this gap, we propose ScholScan, a new benchmark for scholarly paper reasoning. ScholScan introduces a scan-oriented task setting that asks models to read and cross-check entire papers like human researchers, scanning the document to identify consistency issues. The benchmark comprises 1,800 carefully annotated questions drawn from 9 error families across 13 natural-science domains and 715 papers, and provides detailed annotations for evidence localization and reasoning traces, together with a unified evaluation protocol. We assessed 15 models across 24 input configurations and conduct a fine-grained analysis of MLLM capabilities across error families. Across the board, retrieval-augmented generation (RAG) methods yield no significant improvements, revealing systematic deficiencies of current MLLMs on scan-oriented tasks and underscoring the challenge posed by ScholScan. We expect ScholScan to be the leading and representative work of the scan-oriented task paradigm.

1 INTRODUCTION

Scientific papers are crystallizations of human intelligence. Enabling multimodal large language models (MLLMs) (OpenAI, 2025; Anthropic, 2025; ByteDance Seed Team, 2025; Meta, 2025; xAI, 2025) to conduct comprehensive understanding and generation based on academic literature is the ultimate goal of Deep Research, and a critical milestone on the path toward artificial general intelligence (AGI) (Ge et al., 2023; Morris et al., 2024; et al., 2025c). With rapid advances, MLLMs are increasingly capable of supporting academic workflows through retrieval, reading, and writing. For example, PaSa (He et al., 2025) can invoke a series of tools to answer complex academic queries with high-quality results, while Google Deep Research (et al., 2025b) is capable of producing human-level research reports based on specific queries.

However, most of the existing work still follows *a search-oriented paradigm*, where models retrieve a few relevant passages and reason over local evidence based on prespecified targets (Gao et al., 2023; Lou et al., 2025). Such methods are effective for tasks with clearly predefined targets, but struggle with researcher-style full-document reasoning and verification (Zhou et al., 2024). ***To function as researchers, models must move beyond reactive question answering and toward proactive discovery of implicit problems.***

To fill this gap, as shown in Figure 1, we introduce *a scan-oriented paradigm*, where models address queries with targets absent and are required to actively **construct a document-level evidence view, perform exhaustive scanning over the full paper, and conduct evidence-based reasoning**. In contrast to search-oriented tasks that assess a model’s ability to identify and reason over *relevant* fragments, scan-oriented tasks emphasize *consistency*. ***Instead of relying on prespecified targets or hints, models must derive all necessary concepts and inferences solely from given documents.***

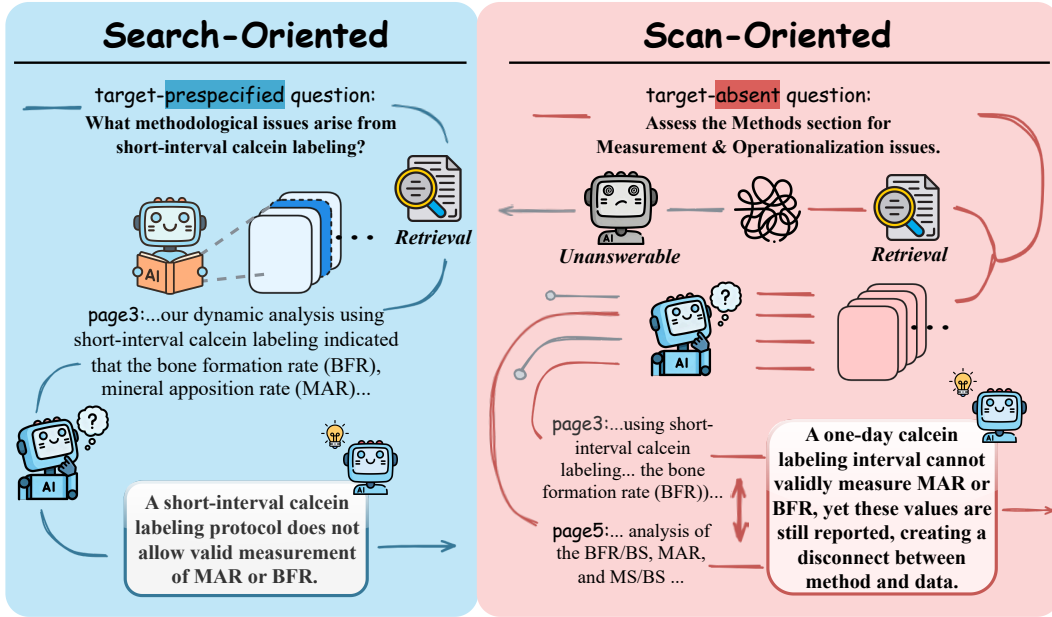


Figure 1: A comparison between search-oriented and scan-oriented task paradigms. Unlike the former, the scan-oriented paradigm provides no prespecified targets, requiring the model to actively scan the entire paper, construct a document-level evidence view.

We instantiate this setting via scientific error detection, as it naturally demands discovering non-obvious flaws without target cues, and present ScholScan, a new multimodal benchmark for scholarly reasoning. ScholScan features the following key highlights:

- **Scan-Oriented Task Paradigm.** ScholScan receive one or more complete academic papers together with target-absent queries, presenting a rigorous challenge to their evidence-based reasoning capabilities. The benchmark comprises 715 papers spanning 13 natural science disciplines.
- **Comprehensive Error Types.** ScholScan covers 9 categories of scientific errors across the entire research workflow. It also includes citation and referencing errors, providing a rigorous test of a model’s cross-source reasoning ability.
- **Process-Aware Evaluation Framework.** ScholScan provides fine-grained annotations for both evidence location and reasoning steps, enabling a comprehensive evaluation framework that assesses model performance in terms of both process and outcome.

We evaluate 15 models across 24 input configurations and 8 retrieval-augmented generation (RAG) frameworks. All models exhibit limited performance, and none of the RAG methods deliver significant improvements. These results highlight the inadequacy of search-oriented frameworks when applied to scan-oriented tasks, and underscore both the challenges and the potential of enabling MLLMs to perform reliable, document-level reasoning over full academic papers.

2 RELATED WORK

2.1 MULTIMODAL LARGE LANGUAGE MODELS

With the rapid progress of MLLMs, models have evolved beyond perception tasks (e.g., image recognition and explanation) (Liu et al., 2024) toward deep understanding of structured, multimodal long documents. Their strengths lie in the ability to integrate cross-modal information and perform multi-hop reasoning over extended contexts. These capabilities are not only valuable for specific question answering or instruction-following tasks (Yue et al., 2024) but are particularly well suited for simulating human thought processes and generating explainable reasoning trajectories (Zheng et al., 2023). Consequently, achieving comprehensive understanding of entire documents has emerged as a core challenge that MLLMs are inherently equipped to address.

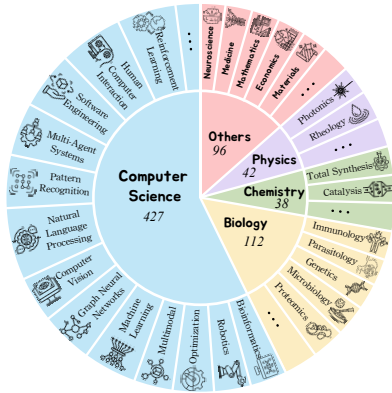
2.2 DOCUMENT UNDERSTANDING BENCHMARK

Document understanding tasks challenge models to identify relevant context and perform accurate reasoning grounded in that information. Progress in document understanding benchmarks has followed two main axes. Along the input dimension, it has evolved from short to long contents, from everyday to specialized domains, and from plain text to multimodal format (Chen et al., 2021; Yang et al., 2018; Tito et al., 2021; Deng et al., 2025). Along the scenario dimension, it has shifted from limited-output formats to more open-ended responses (Pramanick et al., 2024). DocMath-Eval (Zhao et al., 2024) evaluates numerical reasoning on long, specialized documents, revealing large performance gaps even for strong models in expert domains, while MMLongBench-Doc (Ma et al., 2024) builds a multimodal benchmark with layout-rich documents. However, a comprehensive benchmark that integrates all challenges above has yet to be introduced.

2.3 ACADEMIC PAPER UNDERSTANDING BENCHMARK

Compared with general documents, academic papers are distinguished by their rich domain knowledge and logical rigor. Reasoning over papers has emerged as a major challenge in recent research. Some studies ask for local elements like charts or snippets, leveraging their internal complexity, but neglect the need for cross-source integration and domain-specific interpretation within the full document (Wang et al., 2024; Li et al., 2024). Recent studies extend inputs to the document level and adopt image-based formats to better simulate real-world reading scenarios. (Auer et al., 2023; Yan et al., 2025) However, benchmarks based on the QA paradigm face inherent limitations, as they typically presuppose answer existence and embed explicit cues in the question itself, reducing the need for comprehensive understanding and information organization. Moreover, mainstream evaluation protocols focus on the final outcome, with limited assessment of whether intermediate reasoning is evidentially grounded and logically valid. More examples and analysis are shown in Appendix C.

3 THE SCHOLEVAL BENCHMARK



Benchmark	Mod.	Para.	Eval.	# Dom.
<i>Document Understanding</i>				
DocMath-EvalCompLong	T+TD	Search	A	N/A
MMLongbench-Doc	T+MD	Search	A	N/A
LongDocURL	T+MD	Search	A	N/A
SlideVQA	T+MD	Search	A	N/A
<i>Academic Paper Understanding</i>				
CharXiv	I	Search	A	8
ArXivQA	I	Search	A	10
MMCR	T+MD	Search	A	CS
AAAR-1.0	T+MD	Search	A	CS
ScholScan (ours)	T+MD	Scan	A+P	13

Figure 2: Left: Overview of ScholScan. Right: Comparison to related benchmarks. **Mod.:** Modalities; **Para.:** Task Paradigm; **Eval.:** Evaluation; **T:** Text; **I:** Image; **TD:** Text-Form Document; **MD:** Multimodal Document; **A:** Answer; **P:** Process; **Dom.:** Number of academic domains in the dataset.

3.1 OVERVIEW OF SCHOLSCAN

We introduce ScholScan, a benchmark designed to comprehensively evaluate MLLMs’ ability to detect scientific flaws in academic papers under scan-oriented task settings. As illustrated in Figure 2, ScholScan spans 13 disciplines across the natural sciences, including physics, chemistry, and computer science, and spans over 100 subfields such as immunology, total synthesis, and machine learning. The benchmark comprises 1,800 questions derived from 715 real academic papers, and covers 9 major error categories (Figure 3) that commonly observed in real-world research scenarios. These include issues in numerical and formulaic computation, experimental design, inference and conclusion, and citation misuse, among others. Figure 2 also provides a comparison ScholScan with existing benchmarks for multimodal paper understanding and long-document reasoning.







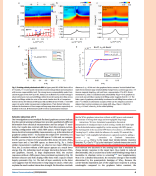





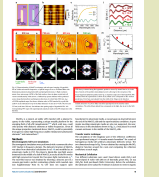








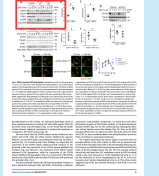




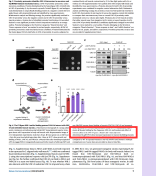
 Research Question & Definitions	 Design & Identifiability	 Sampling & Generalizability
  <p>Explanation: The definition of "actionable variants" shifts across sections (LOE 1–5 in Abstract, LOE 1–3 in Results), causing ambiguity.</p>	  <p>Explanation: The design is described as probing both short- and long-range interactions, yet the paper still claims unique large-q selectivity, creating a disconnect.</p>	  <p>Explanation: The experiments use a narrow diabetic mouse substrain, yet the paper generalizes findings to all patients, creating an invalid sample-to-population inference.</p>
 Measurement & Operationalization	 Data Handling & Preprocessing	 Computation & Formulae
  <p>Explanation: First-harmonic demodulation is dominated by far-field background and cannot produce the reported high-quality near-field images.</p>	  <p>Explanation: Feature selection for NSCLC and HCC models was done on the full dataset before splitting, causing data leakage, while the Discussion falsely claims unbiased validation.</p>	  <p>Explanation: The Methods claim a 200-fold concentration, but the 200 μL subsample is incorrectly said to represent \sim20 mL instead of 40 mL, creating a twofold calculation error.</p>
 Inference & Conclusions	 Referential & Citation Alignment	 Language & Expression
  <p>Explanation: The data show PGK1 promotes EGFR degradation, yet the Discussion claims inhibiting PGK1 as therapy, directly contradicting the results.</p>	  <p>Explanation: Figure 1 report an LPS dose of 1.5 mg/kg, but Figure 5 reports 15 mg/kg, creating a tenfold discrepancy that makes the actual experimental dose unclear.</p>	  <p>Explanation: The paper swaps <i>C. elegans</i> gene and protein nomenclature (e.g., 'unc-45' vs. 'UNC-45'), creating technically misleading references.</p>

Figure 3: Sampled ScholScan examples with 9 error types, covering the whole process of scientific research, each requiring the model to perform thorough cross-source evidence-based reasoning.

3.2 DATA COLLECTION & QUESTION GENERATION

We curated papers from ICLR 2024/2025 and Nature Communications, and collected public reviews for the former. Questions were constructed based on two dimensions, where the source is either generated or sampled, and the context is either within-paper or cross-paper.

Generation. On high-quality accepted papers, we prompt Gemini 2.5 Pro to perform coordinated sentence-level edits spanning multiple sections or pages. It then synthesizes composite errors and generates the corresponding question along with an explanation grounded in the edited context.

Sampling. From rejected ICLR submissions and their public reviews, we prompt Gemini 2.5 Pro to extract explicit, falsifiable scientific errors and convert them into questions with initial explanations. Subjective remarks about novelty or writing quality are excluded.

Within-paper. This setting focuses on verifiable facts and internal consistency within a single paper, and supports both Generation and Sampling.

Cross-paper. This setting examines citation consistency across papers. For each instance, Gemini 2.5 Pro receives an accepted paper and one of its cited sources, then edits the accepted paper to

introduce paraphrases or reasoning errors about the citation. As public reviews mainly address nonfalsifiable aspects such as appropriateness, all cross-paper instances are constructed exclusively using the generation method.

3.3 QUALITY CONTROL & ANNOTATION

Despite explicit instructions, initial outputs exhibited substantial hallucinations, logical inconsistencies, and low-quality questions. To ensure the quality, 10 domain experts conducted a rigorous annotation process. Each instance underwent independent dual review, and disagreements were resolved by a third expert. Among the 3,500 initially generated candidates, 1,700 were discarded, and 1,541 of the remaining were revised, including 535 question rewrites, 1,207 explanation edits, and 1,141 corrections to error categories or metadata. Further details are provided in Appendix D.

4 EXPERIMENTS

4.1 EXPERIMENTS SETTING

Models. We benchmark a total of 24 input configurations by feeding academic papers as either images or OCR text using the Tesseract (Smith, 2007) engine, covering 15 mainstream models (Yang et al., 2025; Bai et al., 2025; et al., 2025a; Guo et al., 2025; et al., 2025d).

Evaluation Protocol. Inspired by MMLongBench-Doc (Ma et al., 2024), we prompt models to generate necessary reasoning chains from evidence to detected anomalies without constraining the output format, which aims to assess the ability for evidence-grounded reasoning rather than mere instruction-following. For open-ended responses, we use GPT-4.1 (OpenAI, 2025) to extract cited evidence and reasoning steps, and quantify alignment with annotated explanations. Human evaluation confirms high agreement between our pipeline and expert annotations. Further implementation details are provided in Appendix F.

Metrics. We define a structured evaluation framework by parsing the model response a into a tuple:

$$\Psi(a) \Rightarrow (\mathbf{1}_{\text{exist}}, \mathbf{1}_{\text{contain}}, \hat{\mathcal{E}}, \hat{\mathcal{R}}, n). \quad (1)$$

Here, $\mathbf{1}_{\text{exist}}$ and $\mathbf{1}_{\text{contain}}$ are binary indicators for whether output contains any error and includes the annotated target error; $\hat{\mathcal{E}}, \hat{\mathcal{R}}$ and $\mathcal{E}^*, \mathcal{R}^*$ are the predicted and gold evidence sets and reasoning chains; $\hat{g} = \text{prefix_match}(\hat{\mathcal{R}}, \mathcal{R}^*)$ counts matched reasoning steps; $n \in \mathbb{N}$ is the number of unrelated errors. $\text{HasError}(a)$ is 1 if the output contains any predicted error, and 0 otherwise. Based on $\Psi(a)$, we define an end-to-end score $S(m) \in [0, 1]$ that combines all aspects of prediction quality:

(i) *Existence.* $S_{\text{exist}}(a) = 1$ if and only if the response includes the annotated target error.

$$S_{\text{exist}}(a) = \mathbf{1}\{\text{HasError}(a)\} \cdot \mathbf{1}\{\hat{\mathcal{E}} \cap \mathcal{E}^* \neq \emptyset\} \quad (2)$$

(ii) *Evidence location score.* Even when the target error is identified, the cited evidence may be incomplete or noisy. We compute a Dice score with a squared penalty for over-reporting:

$$S_{\text{location}} = \max\left\{0, \frac{2|\hat{\mathcal{E}} \cap \mathcal{E}^*| + \mathbf{1}\{|\hat{\mathcal{E}}| + |\mathcal{E}^*| = 0\}}{\max(|\hat{\mathcal{E}}| + |\mathcal{E}^*|, 1)} - 0.8 \left(\frac{|\hat{\mathcal{E}} \setminus \mathcal{E}^*|}{\max(|\hat{\mathcal{E}}|, 1)} \right)^2 \right\}. \quad (3)$$

(iii) *Reasoning process score.* Even if the target error is detected, the reasoning may diverge from the gold chain. We use prefix match to assess reasoning completeness:

$$S_{\text{reasoning}} = \mathbf{1}\{g_r = 0\} + \mathbf{1}\{g_r > 0\} \left(\frac{\hat{g}}{g_r} \right)^2. \quad (4)$$

(iv) *Unrelated-error penalty.* Models may list unrelated items to inflate recall at the cost of precision. We penalize this with a rapidly increasing function of unrelated error count:

$$P_{\text{unrelated.err}}(n) = 0.9^{\min(n, 2)} \exp(-0.6 [\max(n - 2, 0)]^{1.5}). \quad (5)$$

(v) *Overall outcome score.* The final score for a is defined as:

$$S(m) = S_{\text{exist}}(a) \sqrt{S_{\text{location}} \cdot S_{\text{reasoning}}} \cdot P_{\text{unrelated.err}}(n). \quad (6)$$

Table 1: Model performance (scaled by 100) across input configurations. **RQD**: Research Question & Definitions; **DI**: Design & Identifiability; **SG**: Sampling & Generalizability; **MO**: Measurement & Operationalization; **DHP**: Data Handling & Preprocessing; **CF**: Computation & Formulae; **IC**: Inference & Conclusions; **RCA**: Referential and Citation Alignment; **LE**: Language & Expression.

Models	Avg.	RQD	DI	SG	MO	DHP	CF	IC	RCA	LE
MLLM (Image Input)										
<i>Proprietary MLLMs</i>										
Gemini 2.5 Pro	15.6	11.9	12.6	35.7	12.3	27.0	4.6	14.7	15.2	7.4
GPT-5	19.2	10.1	9.7	28.2	14.6	26.6	13.8	25.3	25.3	6.9
Grok 4	4.0	0.0	1.9	16.7	3.2	7.4	0.7	1.9	3.6	0.0
Doubao-Seed-1.6-thinking	10.2	3.4	3.5	22.3	7.5	15.1	10.2	12.2	10.9	3.3
Doubao-Seed-1.6	9.9	3.0	4.4	29.2	4.9	15.0	6.3	17.9	8.0	3.9
<i>Open-source LLMs</i>										
Llama 4 Maverick	7.0	7.0	7.3	9.4	4.5	4.0	6.5	6.7	8.8	3.0
Gemma 3 27B	1.7	0.5	2.7	2.3	1.7	1.0	1.0	1.3	2.6	0.0
Mistral Small 3.1	3.3	0.1	2.0	2.0	1.5	0.1	1.0	2.2	8.6	1.0
Qwen2.5 VL 72B	0.1	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.2	0.0
OCR + LLM (Text Input)										
<i>Proprietary LLMs</i>										
Gemini 2.5 Pro	30.3	21.5	34.2	44.3	27.6	56.6	10.3	28.8	35.6	8.1
GPT-5	22.5	16.1	21.4	26.0	20.3	36.7	4.7	29.8	30.0	2.6
Claude Sonnet 4	5.7	3.7	2.5	10.8	4.3	10.3	1.4	8.4	6.6	3.5
Grok 4	20.8	9.3	7.7	37.4	12.3	34.4	9.0	20.0	31.2	7.2
Doubao-Seed-1.6-thinking	15.3	8.2	10.1	24.3	10.1	24.2	6.4	19.2	21.0	4.2
Doubao-Seed-1.6	13.9	5.4	6.9	26.4	10.3	23.6	6.3	20.1	17.5	2.3
<i>Open-source LLMs</i>										
Qwen3 A22B (Thinking)	17.4	8.9	16.2	31.9	15.1	23.7	5.6	22.3	21.1	2.3
Qwen3 A22B	1.7	1.2	0.0	2.7	0.4	1.0	0.1	4.3	2.5	1.1
gpt-oss-120b	7.3	6.3	5.7	18.3	4.9	14.5	1.6	12.5	5.5	0.0
DeepSeek-R1	11.4	5.1	11.9	25.4	8.7	22.5	4.7	16.3	9.8	3.5
DeepSeek-V3.1	1.7	1.2	2.0	1.7	1.0	5.8	0.5	2.2	2.1	0.0
Llama 4 Maverick	2.3	1.5	2.0	4.8	3.0	3.6	0.0	5.8	1.6	0.2
Gemma 3 27B	2.0	2.1	1.6	3.0	2.7	0.2	0.7	7.7	1.0	0.0
Mistral Small 3.1	6.9	3.0	2.7	5.5	7.0	2.0	8.5	4.0	12.2	3.0
Qwen2.5 VL 72B	0.2	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.6	0.0

4.2 MAIN RESULT

Table 1 presents our evaluation results. Our main findings are summarized as follows:

Overall performance remains unsatisfactory. GPT-5 achieves the highest average score in the image input group (19.2), while Gemini 2.5 Pro, the best-performing model in the text input setting, still fails to surpass the 60-point threshold on any subtask. Even in the SG category, which yields the best performance overall, nearly half of the models receive single-digit scores. Most models perform poorly under the scan-oriented task formulation and fail to detect any issues in many papers. This challenge is particularly pronounced for open-source models.

Reasoning-enhanced models demonstrate clear advantages. Across both input configurations, reasoning-enhanced variants consistently achieve higher scores. Almost all top-performing models, measured by both subtask-specific and overall metrics, fall into this category. Notably, Qwen3-Thinking and Deepseek-R1 outperform their base versions by more than 10% in average scores, with substantial gains observed across all error types. These results indicate that reasoning-enhanced models are better able to simulate the iterative process of extraction followed by reasoning, which is essential for effectively handling scan-oriented tasks and producing higher-quality responses.

MLLMs face significant bottlenecks in handling long multimodal inputs. Across most evaluation metrics, text inputs outperform image inputs. Among the nine MLLMs tested, the average performance gap between text and image inputs reaches 4.81 points, highlighting visual processing as a key limitation in current MLLM capabilities.

In most evaluation metrics, text inputs consistently outperform image inputs. Among the nine MLLMs evaluated, the average performance gap between text and image inputs is 4.81 points, underscoring visual processing as a key limitation in current MLLM capabilities.

Although overall performance is generally weaker, multimodal input remains indispensable. In certain categories such as CF, where OCR-based text extraction leads to substantial loss of formulaic or tabular content, image inputs outperform their text counterparts. This highlights the essential role of multimodal reasoning and the irreplaceable value of visual information in addressing specific types of errors.

4.3 FINE-GRAINED ANALYSIS

Capability Dimensions. We compute pairwise Spearman correlations between error types across two input configurations (text and image) for the eight evaluated MLLMs excluding Qwen2.5-VL-72B, as shown in Figure 4. We derive the following insights:

(i) *With image input, CF exhibits consistently low correlations with other error categories, suggesting that the skills required for mathematical reasoning are relatively distinct.* In contrast, with text input, CF shows moderate correlation with LE, indicating that OCR-flattened formulas lose their structural specificity and are interpreted by models in a manner more akin to natural language. Combined with the overall poor performance on CF tasks, this underscores the unique challenges of this category and the need for targeted improvements.

(ii) *Although DI is also related to experimental settings, it does not exhibit strong correlations with SG, MO, or DHP.* This indicates that DI primarily emphasizes causal framing and variable identifiability, rather than the procedural understanding of experimental operations.

(iii) *OCR severely degrades structured content such as figures and formulas, making questions that depend on multimodal information unanswerable.* This diminishes the expression of multimodal reasoning capabilities and artificially inflates inter-category correlations under text input.

Based on the above analysis, we consolidate the original 9 error categories, each defined by its objective target, into 5 core latent skill dimensions evaluated by ScholScan under the image input setting. While each dimension highlights the primary competence emphasized by its corresponding error types, they are not mutually exclusive, as many questions involve overlapping reasoning abilities.

RQD and DI correspond to research concept comprehension, which requires models to *identify the scope and definition* of research objectives by integrating contextual cues and prior knowledge. SG, MO, and DHP fall under *experimental process modeling*, which tests a model’s ability to reconstruct procedural workflows such as sampling, measurement, and data handling. CF captures *formal reasoning and symbolic computation*, focusing on syntactic parsing and numerical logic. IC evaluates causal inference, where models must *synthesize dispersed causal evidence* to reach sound conclusions. RCA and LE reflect referential alignment and linguistic consistency, which assess the ability to *verify citations and maintain coherent expression* throughout the document.

Hidden Complexity in Scan-Oriented Tasks. We analyze the reasoning traces of GPT-5 and Gemini 2.5 Pro under both input configurations, focusing on the number of evidence pieces scanned and the reasoning steps performed. As illustrated in Figure 5, even the most advanced models often scan up to 8 times more evidence and execute 3.5 times more reasoning steps than the reference answers, merely to approximate a correct response, yet they still frequently fail. This highlights the substantial hidden complexity inherent in scan-oriented tasks, which significantly amplifies the challenge of successful task completion.

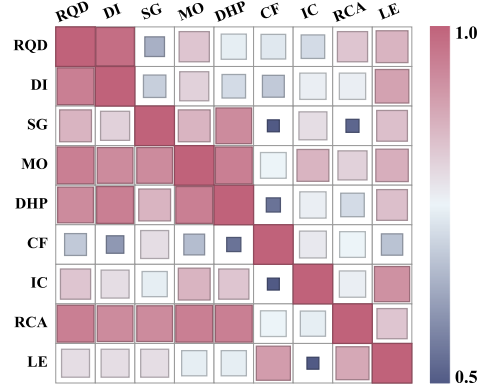


Figure 4: Spearman correlation matrix among the 9 error types.

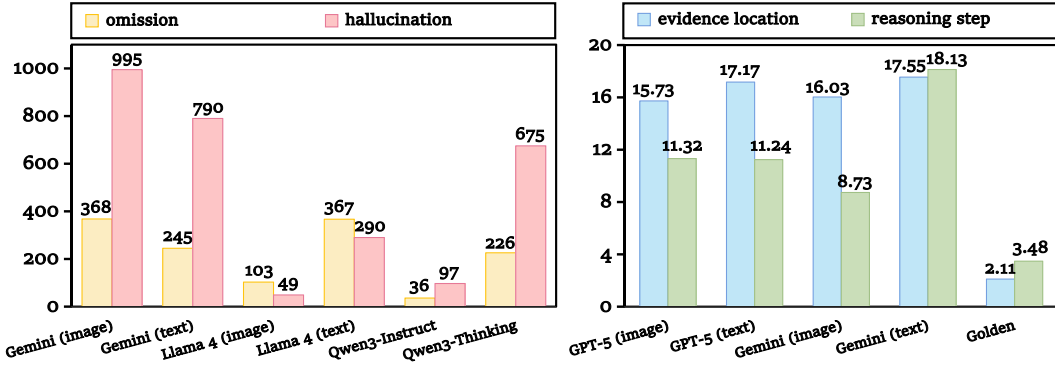


Figure 5: Left: Distribution of omission and hallucination errors. Right: Average reasoning steps and evidence locations involved in the answer generation, compared against the golden reference.

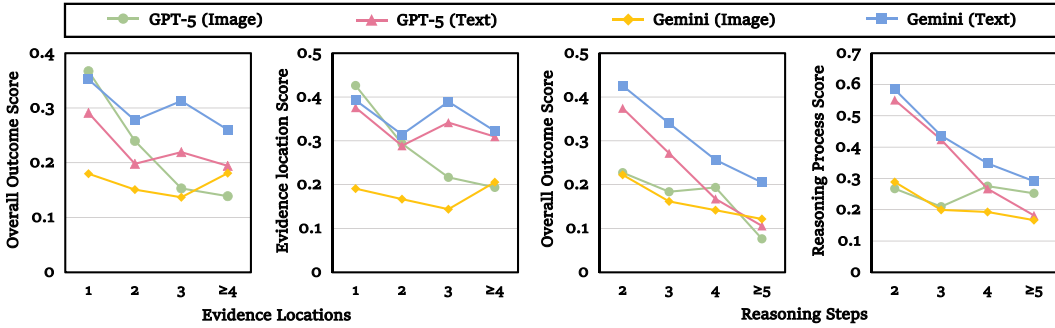


Figure 6: Performance trends across varying reasoning depths and evidence counts.

4.4 ERROR ANALYSIS

Omission and Hallucination. Most zero-score cases fall into two categories: either the model fails to detect any errors in the paper, or it becomes overwhelmed by hallucinations and entirely overlooks the actual errors present in the reference answer. We analyze the number of zero-score questions and the proportion of these two failure modes across models, as shown in Figure 5. Stronger models tend to have fewer zero-score cases overall, but are more prone to overconfident hallucinations.

Fragile Reasoning under Complex Evidence. Figure 6 shows how top-performing models behave under different numbers of reasoning steps and evidence locations. As reasoning steps increase, both reasoning and overall scores steadily decline, revealing a clear bottleneck in MLLMs’ ability to construct long causal chains. In contrast, variation in evidence count has a weaker and less consistent impact. However, this does not imply that multi-evidence questions pose only marginal difficulty. Since the evaluation metric allows partial evidence omissions, more evidence items do not necessarily incur large score penalties. Still, heavier evidence loads often require longer reasoning chains, which substantially affect the coherence and completeness of inferred logic. These results highlight the persistent challenge for MLLMs in integrating evidence and maintaining logical structure as task complexity grows.

4.5 RAG ANALYSIS

We evaluated 8 RAG methods under both input configurations (Robertson et al., 1994; Chen et al., 2024; Lee et al., 2025; Faysse et al., 2025; Yu et al., 2025; Wang et al., 2025; Izacard et al., 2022). Key findings are presented below, with detailed results shown in Tables 2 and 3.

Oracle Condition Yields Significant Accuracy Gains. Providing gold-standard images alleviates the scanning burden in long-context inputs, increasing the chances of generating correct answers. While overall performance improves, gains are limited for CF errors and minimal for LE errors. For

Table 2: Scores of RAG methods across the 9 error types (scaled by 100).

Models	Avg	RQD	DI	SG	MO	DHP	CF	IC	RCA	LE
<i>Text Input (Base Model: Qwen3 Thinking)</i>										
Baseline	17.4	8.9	16.2	31.9	15.1	23.7	5.6	22.3	21.1	2.3
Oracle	24.5	20.6	27.9	43.6	21.3	40.8	7.4	26.9	26.0	1.9
bm25	16.7	9.7	13.7	33.0	17.3	23.8	6.8	25.4	16.5	3.0
BGE-M3	11.3	8.6	7.5	24.8	9.1	15.4	5.3	15.6	11.4	1.0
Contriever-msmacro	16.6	9.7	18.2	33.7	10.7	20.8	6.4	18.5	19.8	1.8
nv-embed-v2	6.8	4.0	4.0	9.4	6.1	4.9	5.5	5.7	10.0	2.0
<i>Image Input (Base Model: Llama4 Maverick)</i>										
Baseline	7.0	7.0	7.3	9.4	4.5	4.0	6.5	6.7	8.8	3.0
Oracle	6.5	3.0	4.5	15.6	8.2	9.4	4.9	10.0	4.4	1.4
ColPali-v1.3	0.8	1.5	0.0	0.5	0.0	0.9	0.5	1.3	1.4	0.0
ColQwen2.5	1.2	2.1	0.7	0.5	0.0	1.2	0.2	2.7	2.0	0.0
VisRAG	1.0	2.0	0.0	1.0	0.0	1.0	1.6	1.3	1.2	0.0
VRAG-RL	10.9	9.8	11.6	17.8	8.2	11.0	6.8	13.1	10.8	8.1

CF, sparse formulaic content means gold images offer slight help. For LE, dense text distribution makes even direct access to target regions insufficient to reduce complexity for current models.

In consistency-centric scan-oriented tasks, most retrieval-based enhancement methods show minimal effectiveness. All embedding models exhibit poor retrieval accuracy. None achieves recall of 50% within the top-5 retrieved items. More critically, performance deteriorates after retrieval, especially for multimodal embedding models, where post-retrieval responses are almost entirely incorrect and scores approach 0.

Complex embedding model architectures do not yield better performance. Providing gold-standard images alleviates the scanning burden in long-context inputs, increasing the chances of retrieving correct answers. While overall performance improves, gains are limited for CF and minimal for LE errors. For CF, sparse formulaic content means gold images offer only slight localization help. For LE, dense error distribution makes even direct access to target regions insufficient to reduce task complexity for current models.

Reinforcement learning frameworks with a visual-centric focus have distinguished themselves as leading approaches. Despite being built on a compact 7B model, VRAG-RL consistently delivers improved performance and is the only method that achieves gains in the image-input setting following RL optimization. Its enhanced retrieval sharpens evidence selection, while strong reasoning provides effective guidance during document scanning. The retrieval and reasoning components are interleaved in design, with each stage informing the other in an iterative loop. This tightly coupled interaction contributes to the method’s superior performance potential.

5 CONCLUSION

In this paper, we introduce ScholScan, a benchmark designed to evaluate the performance of MLLMs on scan-oriented tasks that require detecting scientific errors across entire academic papers. We conduct a comprehensive evaluation and in-depth analysis of mainstream MLLMs and RAG methods. The results demonstrate that current MLLMs remain far from capable of reliably addressing such tasks, and that existing RAG approaches provide little to no improvement. This highlights the complexity, integrative demands, and originality of the ScholScan benchmark. Looking ahead, we aim to develop scan-oriented task paradigms suited to diverse academic scenarios and explore new techniques for enhancing model performance on target-suppressed inputs. These directions support the broader goal of advancing MLLMs from passive assistants to active participants in scientific research.

Table 3: Summary of retrieval performance for RAG methods.

Models	MRR@5	Recall@5
<i>Text Input (Base Model: Qwen3 Thinking)</i>		
bm25	0.41	0.48
BGE-M3	0.16	0.21
Contriever-msmacro	0.31	0.39
nv-embed-v2	0.30	0.38
<i>Image Input (Base Model: Llama4 Maverick)</i>		
ColPali-v1.3	0.26	0.31
ColQwen2.5	0.30	0.35
VisRAG	0.41	0.46

6 ETHICS STATEMENT

All data used in this paper were constructed by the authors and do not include any external public or proprietary datasets. The included academic papers and author names are publicly available through arXiv and OpenReview and can be freely accessed.

A team of 10 domain experts was assembled to comprehensively review all task instances initially generated by Gemini 2.5 Pro. All annotators gave informed consent to participate. To ensure the accuracy and neutrality of both model-generated and human-verified content, we employed a rigorous multi-stage validation process involving cross-review and third-party adjudication.

Evaluation across 15 mainstream models and 24 input configurations was conducted via legally authorized API access through the VolcEngine, Alibaba Cloud’s LLM services, and OpenRouter.

ScholScan is fully open-sourced and freely available for academic and non-commercial research purposes. We provide the complete download link and documentation through an anonymous GitHub repository. All personally identifiable information has been removed from the dataset, and its collection and release comply with the ethical and legal requirements in place at the time of data acquisition.

7 REPRODUCIBILITY STATEMENT

All results presented in this paper are fully reproducible. To facilitate verification and extension, we provide an anonymous repository (<https://anonymous.4open.science/r/ScholScan-6657/>) that contains the complete dataset, source code, and detailed documentation. The repository also includes step-by-step instructions and the exact hyperparameter configurations used in our experiments, ensuring that other researchers can replicate our findings with minimal effort.

The retrieval components in all retrieval-augmented generation (RAG) experiments were executed on a server equipped with 8 NVIDIA A40 GPUs.

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Not Search, But Scan: Benchmarking MLLMs on Scan-Oriented Academic Paper Reasoning

Supplementary Material

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A USE OF LLMs

Large language models (LLMs) were used solely to assist in language editing and stylistic refinement during manuscript preparation. All technical content, experiments, dataset construction, evaluation protocols, and analysis were conceived, implemented, and validated entirely by the authors. No LLMs were involved in the generation of benchmark data, research methodology design, or result interpretation. The use of LLMs did not influence the scientific conclusions of this paper.

B PROMPTS

B.1 WITHIN-GENERATE PROMPT

Within-Generate Prompt

You will receive a high-quality, already accepted scientific paper as a PDF. Working only with the PDF itself (and any appendix embedded in the same PDF), edit specific textual spans to inject one or more errors chosen only from the taxonomy below, such that the errors are hard yet clearly identifiable by a professional reviewer reading the PDF alone.

Error Type (fixed):

Research Question & Definitions

Definition: The core construct/hypothesis/variable is insufficiently or inconsistently defined (conceptual vs operational), leaving the estimand ambiguous.

Design & Identifiability

Definition: Given a clear estimand, the design violates structural identification conditions so the effect is not identifiable even with infinite data and perfect measurement.

Sampling & Generalizability

Definition: The sampling frame/process/composition or cluster/power setup does not support valid or stable sample→population claims.

Measurement & Operationalization

Definition: Measures/manipulations lack feasibility/reliability/validity/timing, so observed variables systematically diverge from the intended construct/treatment.

Data Handling & Preprocessing

Definition: Pipeline choices in missing handling, joins/keys, temporal splitting, feature construction, or partitioning introduce bias (incl. leakage or unit/scale conflicts).

Computation & Formulae

Definition: Arithmetic/algebra/notation errors (totals/ratios, unit conversion, CI vs point estimate, p-value vs label, symbol reuse, undefined variables, dimension mismatch).

Inference & Conclusions

Definition: Interpretations or causal statements exceed what methods/data support, or contradict the shown statistics/tables/captions.

Referential and Citation Alignment

Definition: Contradictions about the same quantity/term across text, tables, captions, or appendix within the paper.

Language & Expression

Definition: Terminology/capitalization/grammar ambiguities that affect meaning or domain-critical term consistency (not cosmetic typos).

Within-Generate Prompt (Continued)

Global constraints (must comply)

1. Each error must map to exactly one primary category in the taxonomy. Do not mix causes.
2. Each error must involve more than 2 micro-edits (each edit ≤ 20 English words) spread across distinct pages or paragraphs.
3. If an edit would create an immediate contradiction in the same sentence/paragraph/caption, you may add shadow patch(es) for the same error to keep the text natural (still counted as edit locations).
4. Independence across errors (per-copy generation)
Generate each error on a separate copy of the original PDF.
. Different errors must be logically and operationally independent:
No progression or variant relations: an error must not be a stricter/looser version, superset/subset, or minor wording variant of another error.
No anchor reuse: do not target the same sentence/caption/table cell or reuse the same old_str (or a near-duplicate paraphrase) across different errors.
Applying any single error in isolation to the original PDF must still yield a detectable, clearly categorizable error according to the taxonomy.
5. Every error must be supportable using text inside the PDF.
Do not rely on external supplementary files or prior knowledge.
6. Design as difficult as possible but clean errors. Prefer edits that force cross-checking between two spots (e.g., Methods vs Results). Avoid trivialities. Edits must remain locally plausible and not advertise themselves via obviously artificial phrases (e.g., avoid contrived tokens purely added to be detectable).
7. ``No cosmetic issues`` applies except for I (Language & Expression). For I, edits must affect meaning or domain-critical terminology (e.g., ambiguous phrasing, inconsistent technical terms). Pure typos, punctuation tweaks, or layout nits are not allowed.
8. Do not edit titles, author lists, bibliography entries, equation numbering, figure images, or add new figures/tables/references.
9. Frame each question as a neutral imperative that asks for a decision about a specific condition, using (but not limited to) Decide/Determine/Judge/Evaluate/Assess whether.... Do not presuppose an outcome or use suggestive intensifiers (e.g., clearly/obviously/likely/suspicious as examples).

Within-Generate Prompt (Continued)

```

10. Output English-only and strictly follow the JSON schema
   below. Do not include any additional text outside the
   JSON:
[
  {
    "id": "1-based integer as string",
    "modify": [
      {
        "location": "Page number + short unique nearby quote (
                     ≤15 tokens).",
        "old_str": "Exact original text from the PDF (verbatim)
                     .",
        "new_str": "Edited text after your change."
      }
      /* Add 1-2 more locations; each location ≤ 20 words
         changed.
         Shadow patches for local coherence count as locations.
         */
    ],
    "question": "One neutral audit-style task (1-25 words).",
    "explanation": "Explain in 2-4 sentences why a reviewer can
                  detect this error from the edited PDF alone.",
    "Type": "Name the primary category (e.g., Inference &
            Conclusions).",
  }
  /* More Errors */
]

```


B.2 WITHIN-SAMPLE PROMPT

Within-Sample Prompt

You will receive a paper PDF and the weaknesses mentioned in its peer-review comments. Your task is, based only on the content of that PDF, to sample from the review comments and verify possible errors related to the categories below, and for each confirmed or highly plausible error, generate one question and one explanation.

Error Type (fixed):

Research Question & Definitions

Definition: The core construct/hypothesis/variable is insufficiently or inconsistently defined (conceptual vs operational), leaving the estimand ambiguous.

Design & Identifiability

Definition: Given a clear estimand, the design violates structural identification conditions so the effect is not identifiable even with infinite data and perfect measurement.

Sampling & Generalizability

Definition: The sampling frame/process/composition or cluster/power setup does not support valid or stable sample→population claims.

Measurement & Operationalization

Definition: Measures/manipulations lack feasibility/reliability/validity/timing, so observed variables systematically diverge from the intended construct/treatment.

Data Handling & Preprocessing

Definition: Pipeline choices in missing handling, joins/keys, temporal splitting, feature construction, or partitioning introduce bias (incl. leakage or unit/scale conflicts).

Computation & Formulae

Definition: Arithmetic/algebra/notation errors (totals/ratios, unit conversion, CI vs point estimate, p-value vs label, symbol reuse, undefined variables, dimension mismatch).

Inference & Conclusions

Definition: Interpretations or causal statements exceed what methods/data support, or contradict the shown statistics/tables/captions.

Referential and Citation Alignment;

Definition: Contradictions about the same quantity/term across text, tables, captions, or appendix within the paper.

Language & Expression

Definition: Terminology/capitalization/grammar ambiguities that affect meaning or domain-critical term consistency (not cosmetic typos).

Within-Sample Prompt (Continued)

Global constraints (must comply)
 Output only the specified categories; even if other error types appear in the reviews, do not output them.
 Sample first, then verify: extract candidates from the review comments, then confirm them in the PDF. If you cannot locate supporting anchors in the PDF (page number plus phrase/label), do not output that candidate.
 Questions must be neutral and non-leading: use an "audit task + decision" style, avoiding yes/no bias.
 Independence: each question must target a different figure or different textual anchor; no minor variants of the same issue.
 Evidence first: the explanation must cite locatable anchors in the PDF (page number + original phrase/caption). You may mention a key short phrase from the review as a clue, but write the question and explanation in your own words
 Language & format: both question and explanation must be in English; output JSON only, with no extra text.
 Quantity: sort by evidence strength and output up to 5 items; if none qualify, output an empty array [].
 Example output

```
[
  {
    "id": "1",
    "question": "Audit y-axis baselines and possible axis breaks in Figure 2; decide presence/absence and cite evidence.",
    "explanation": "The review flags possible exaggeration in Fig.2. In the PDF (p.6, caption 'Performance vs baseline'), the y-axis starts at 0.85 with a break, magnifying small differences; panels use different ranges."
    "Type": "Visualization & Presentation Bias"
  }
]
```

B.3 EXTRACTOR PROMPT

Extractor Prompt

You will receive three inputs:

Q: the open-ended question;

E: the gold explanation (describes exactly one error; extra details still belong to the same single error);

A: the model's answer to be evaluated.

Your job is to extract counts only and output a single JSON object with the exact schema below. Do not compute any scores. Do not add fields.

Core selection rule (multiple errors in A)

1. Parse E into a single gold error (the "target error").

2. From A, identify how many distinct error claims are made. Cluster together mentions that support the same error (multiple locations for one error are still one error).

3. Existence decision (binary correctness only):

Let the gold existence be 1 if E asserts an error exists, else 0.

Let the predicted existence be 1 if A asserts any error, else 0 (e.g., states no error).

Set existence = 1 if predicted existence equals gold existence; otherwise set existence = 0.

4. If existence = 0: set contains_target_error = 0; set all location and reasoning counts to 0; and set unrelated_errors to the total number of distinct error claims in A. Then output the JSON.

5. If existence = 1:

If the gold existence is 1: determine whether A contains the target error (match by the main error idea in E: category/intent/scope; treat E's subpoints as the same error).

If yes, set contains_target_error = 1 and compute location and reasoning only for the target error. Count all other error claims in A as unrelated_errors.

If no, set contains_target_error = 0; set all location and reasoning counts to 0; set unrelated_errors to the total number of distinct error claims in A.

If the gold existence is 0: set contains_target_error = 0; set all location and reasoning counts to 0; set unrelated_errors to the total number of distinct error claims in A. (These negative items are for binary accuracy only; they are not used for detailed scoring.)

Matching guidance (A error \leftrightarrow target error): match by the main error idea in E (category/intent/scope), not by wording. Treat E's subpoints as part of the same single error. Prefer the best-matching cluster in A; if ties, choose the one with stronger alignment to E's core claim.

Extractor Prompt (Continued)

Counting rules
 Location (for the target error only when existence=1 and contains_target_error=1):
 gold_steps: number of unique error locations described in E (after normalization and deduplication).
 hit_steps: number of predicted locations in A that match any gold location for the target error.
 extra_steps: number of predicted locations in A for the target error that do not match any gold location.

Reasoning (for the target error only when existence=1 and contains_target_error=1):
 Convert E into a canonical set or ordered chain of reasoning steps for the target error.
 gold_steps: total number of such steps.
 reached_steps:
 single-chain tasks: length of the longest valid prefix of A along the gold chain;
 multi-path/parallel tasks: size of the intersection between A's steps and the gold step set (or the maximum across gold paths if multiple are defined).
 missing_steps: gold_steps - reached_steps (non-negative integer).

Unrelated errors:
 unrelated_errors: number of distinct error claims in A that are not the target error (0 if none).

Output schema (return exactly this JSON; integers only)

```
{
  "existence": 0,
  "contains_target_error": 0,
  "location": {
    "gold_steps": 0,
    "hit_steps": 0,
    "extra_steps": 0
  },
  "reasoning": {
    "gold_steps": 0,
    "reached_steps": 0,
    "missing_steps": 0
  },
  "unrelated_errors": 0
}
```

B.4 SYSTEM PROMPT

System Prompt

You are a neutral, careful academic reviewer. You will receive an open-ended question and the paper content. The paper may or may not have issues related to the question. Do not assume there are errors. If the question is about citations, you will be given a citing paper and a cited paper; evaluate only the citing paper for possible issues and use the cited paper only as the reference for comparison. Write in natural prose with no fixed template

Rules:

Speak only when sure. State an error only if you are confident it is a real error (not a mere weakness).

Stay on scope. Discuss only what the question asks about.

Evidence completeness. For every error you state, list all distinct evidence cues you are confident about from the PDF. Include plain identifiers (figure/table/section/equation/citation) or quotes. Avoid redundant repeats of the exact same instance; include all distinct locations needed to support the error.

Be clear and brief. Use short, direct sentences.

No metaphors. No fancy wording. No guesses or outside sources. Do not invent figures, tables, equations, citations, or results.

Report as many distinct, well-supported errors as you can within scope. If none are clear, write exactly: "No clear issue relevant to the question." and nothing else.

C EXAMPLES FROM EXISTING DATASETS

C.1 EXAMPLE FROM DocMATH-EVAL

One Example from DocMath-Eval

Question_ID: complong-testmini-30

Question: What is the percentage of total offering cost on the total amount raised in the IPO **if the total offering cost is \$14,528,328 and each unit sold is \$10?**

Context Modalities: Texts Documents

1. Offering costs consist of legal, accounting and other costs incurred through the balance sheet date that are directly related to the Initial Public Offering. Offering costs amounting to \$14,528,328 were charged to shareholders' equity upon the completion of the Initial Public Offering.

2. Pursuant to the Initial Public Offering on July 20, 2020, the Company sold 25,300,000 Units, which includes the full exercise by the underwriter of its option to purchase an additional 3,300,000 Units, at a purchase price of \$10.00 per Unit. Each Unit consists of one Class A ordinary share and one-half of one redeemable warrant ("Public Warrant"). Each whole Public Warrant entitles the holder to purchase one Class A ordinary share at an exercise price of \$11.50 per whole share (see Note 7).

NO Multi-Modal Documents Context

Covered areas:

Focus Only On the Field of Mathematics

Cross-evidence Reasoning:

Focusing on solving mathematical problems requires integrating evidence such as mathematical formulas, question stem conditions, and chart data from different positions in the document.

Task Paradigm: search

Search-oriented

C.2 EXAMPLE FROM SLIDEVQA

One Example from SlideVQA

Question ID: 1

Question: How much difference in INR is there between the average order value of CY2013 and that of CY2012?

Context Modalities: Multi-Modal Documents and Texts

Executive summary

Key findings

Increasing average order value

INR 1,080

CY2012

INR 1,860

CY2013

INR 3,600

CY2016P

67%

25% CAGR

Average order values climbing up rapidly

1. Last year there was a significant jump in average order value as there was a penetration of new categories like jewellery, home décor etc.

2. Also, users are becoming more comfortable buying higher priced items online.

Fashion + Footwear + Accessories GMV

\$278 M

CY2012

\$559 M

CY2013

\$2,811 M

CY2016P

100% Growth

71% CAGR

Fashion category doubled last year

1. Last year was the rise of the fashion category – fashion e-commerce GMV doubled since 2012.

2. Given the young demographic which is shopping for latest looks online and increasing choice online – we estimate that this category will see 400% growth in the next 3 years and rival electronics and mobile category in GMV.

Accel estimates and Industry sources

5

Covered areas:

The documents cover core technical research fields such as visual question answering and machine reading comprehension, as well as industry application fields including education and scientific research, finance and commerce, and healthcare (with derivative adaptation to pathological slice analysis), and also involves derivative technical fields like retrieval-augmented generation.

Cross-evidence Reasoning:

Simple question types only require a single piece of evidence

Not Cross-evidence Reasoning

Task Paradigm: search

Search-oriented

C.3 EXAMPLE FROM MMLONGBENCH-DOC

One Example from MMLongBench-Doc

Question ID:

Question: How much higher was the proposed dividend paid (Rupees in lacs) in 2002 compared to 2001?

Context Modalities: Multi-Modal Documents and Texts

ITC Limited

SHAREHOLDER REFERENCER

Unclaimed Dividend

Unclaimed dividend for the years prior to and including the financial year 1998-99 has been transferred to the General Revenue Account of the Central Government / the Investor Education and Protection Fund established by the Central Government (IEPF), as applicable.

Shareholders who have not encashed their dividend warrants relating to financial years) up to and including 1993-94 may claim such dividend (transferred to the General Revenue Account) from the Registrar of Companies, West Bengal, Government of India, Neam Palace, 8/MSO Building, 2nd Floor, 2344 A.J.C. Bose Road, Kolkata 700 020, in the prescribed form. This form can be furnished by the Investor Service Centre of the Company (ISC) on request or can be downloaded from the Company's corporate website www.itcportal.com under the section 'Investor Relations'.

The dividend for the undermentioned years, if unclaimed for 7 years, will be transferred by the Company to IEPF in accordance with the schedule given below. Attention is drawn that the unclaimed dividend for the financial year 1999-2000 will be due for transfer to IEPF later this year. Communication has been sent by the Company to the concerned Shareholders advising them to lodge their claims with respect to unclaimed dividend.

Once unclaimed dividend is transferred to IEPF, no claim shall lie in respect thereof.

Financial Year	Dividend Identification No.	Date of Declaration of Dividend	Total Dividend (Rs.)	Unclaimed Dividend as on 31/03/2007		Due for transfer to IEPF on
				(Rs.)	%	
1999-00	70th	28th July, 2000	1,84,06,11,780.00	1,26,32,087.00	0.69	18th September, 2007*
2000-01	71st	3rd August, 2001	2,45,41,49,040.00	2,09,42,133.00	0.84	9th September, 2008
2001-02	72nd	28th July, 2002	3,35,12,27,743.00	2,56,63,749.00	0.77	31st August, 2009
2002-03	73rd	28th July, 2003	3,71,26,78,200.00	2,38,48,718.00	0.64	30th August, 2010
2003-04	74th	30th July, 2004	4,95,35,77,000.00	3,35,88,520.00	0.68	4th September, 2011
2004-05	75th	28th July, 2005	7,73,34,48,386.00	5,07,55,301.00	0.66	3rd September, 2012
2005-06	76th	21st July, 2006	9,95,12,91,267.00	7,38,87,332.00	0.74	28th August, 2013

* It will not be possible to entertain claims received by ISC after 14th September, 2007.

Erstwhile ITC Hotels Limited

Financial Year	Date of Declaration of Dividend	Total Dividend (Rs.)	Unclaimed Dividend as on 31/03/2007		Due for transfer to IEPF on
			(Rs.)	%	
1999-00	28th August, 2000	3,02,16,492.00	3,19,648.00	1.06	18th October, 2007*
2000-01	17th August, 2001	3,02,16,492.00	3,04,652.00	1.01	21st September, 2008
2003-04	14th July, 2004	6,04,32,684.00	6,98,704.00	1.16	18th August, 2011

* It will not be possible to entertain claims received by ISC after 9th October, 2007.

Bank Details

Shareholders holding Shares in the physical form are requested to notify / send the following to ISC to facilitate better servicing:-

i) any change in their address / mandate / bank details, and

ii) particulars of the bank account in which they wish their dividend to be credited, in case the same have not been furnished earlier.

Shareholders are advised that respective bank details and addresses as furnished by them or by NSDL / CDSL to the Company, for Shares held in the physical form and in the dematerialised form respectively, will be printed on dividend warrants as a measure of protection against fraudulent encashment.

30

Covered areas:

The documents cover 7 diverse fields such as scientific research reports, business financial reports, and technical manuals.

Cross-evidence Reasoning:

33% of the questions are cross-page questions, which require integrating different types of evidence such as texts, tables, and charts from multi-page documents

Task Paradigm: search

Search-oriented

C.4 EXAMPLE FROM LONGDOCURL

One Example from LongDocURL

Question_ID: free_gemini15_pro_4061601_47_71_8
Question: What was the total fair value of options that vested in 2016, 2015, and 2014, in millions of Canadian dollars?

Context Modalities: Multi-Modal Documents and Texts

The following table summarizes additional stock option information:

year ended December 31 (millions of Canadian \$, unless otherwise noted)	2016	2015	2014
Total intrinsic value of options exercised	31	10	21
Fair value of options that have vested	126	91	95
Total options vested	2.1 million	2.0 million	1.7 million

As at December 31, 2016, the aggregate intrinsic value of the total options exercisable was \$86 million and the total intrinsic value of options outstanding was \$130 million.

21. PREFERRED SHARES

In March 2014, TCPL redeemed all of the 4 million outstanding Series Y preferred shares at a redemption price of \$50 per share for a gross payment of \$200 million.

22. OTHER COMPREHENSIVE (LOSS)/INCOME AND ACCUMULATED OTHER COMPREHENSIVE LOSS

Components of Other comprehensive (loss)/income, including the portion attributable to non-controlling interests and related tax effects, are as follows:

year ended December 31, 2016 (millions of Canadian \$)	Before Tax Amount	Income Tax Recovery/ (Expense)	Net of Tax Amount
Foreign currency translation gains on net investment in foreign operations	3	—	3
Change in fair value of net investment hedges	(14)	4	(10)
Change in fair value of cash flow hedges	44	(14)	30
Reclassification to net income of gains and losses on cash flow hedges	71	(30)	42
Unrealized actuarial gains and losses on pension and other post-retirement benefit plans	(30)	12	(18)
Reclassification to net income of actuarial loss on pension and other post-retirement benefit plans	22	(9)	14
Other comprehensive loss on equity investments	(127)	30	(97)
Other Comprehensive Loss	(29)	(9)	(38)

year ended December 31, 2015 (millions of Canadian \$)	Before Tax Amount	Income Tax Recovery/ (Expense)	Net of Tax Amount
Foreign currency translation gains on net investment in foreign operations	798	15	813
Change in fair value of net investment hedges	(505)	133	(372)
Change in fair value of cash flow hedges	(82)	35	(47)
Reclassification to net income of gains and losses on cash flow hedges	144	(56)	88
Unrealized actuarial gains and losses on pension and other post-retirement benefit plans	74	(23)	51
Reclassification to net income of actuarial loss and prior service costs on pension and other post-retirement benefit plans	41	(9)	32
Other comprehensive income on equity investments	62	(15)	47
Other Comprehensive Income	522	90	602

155 TCPL Consolidated financial statements 2016

Covered areas:
The document types of LongDocURL cover 8 major categories such as research reports, user manuals, and books.

Cross-evidence Reasoning:
Most questions require integrating evidence across chapters and elements

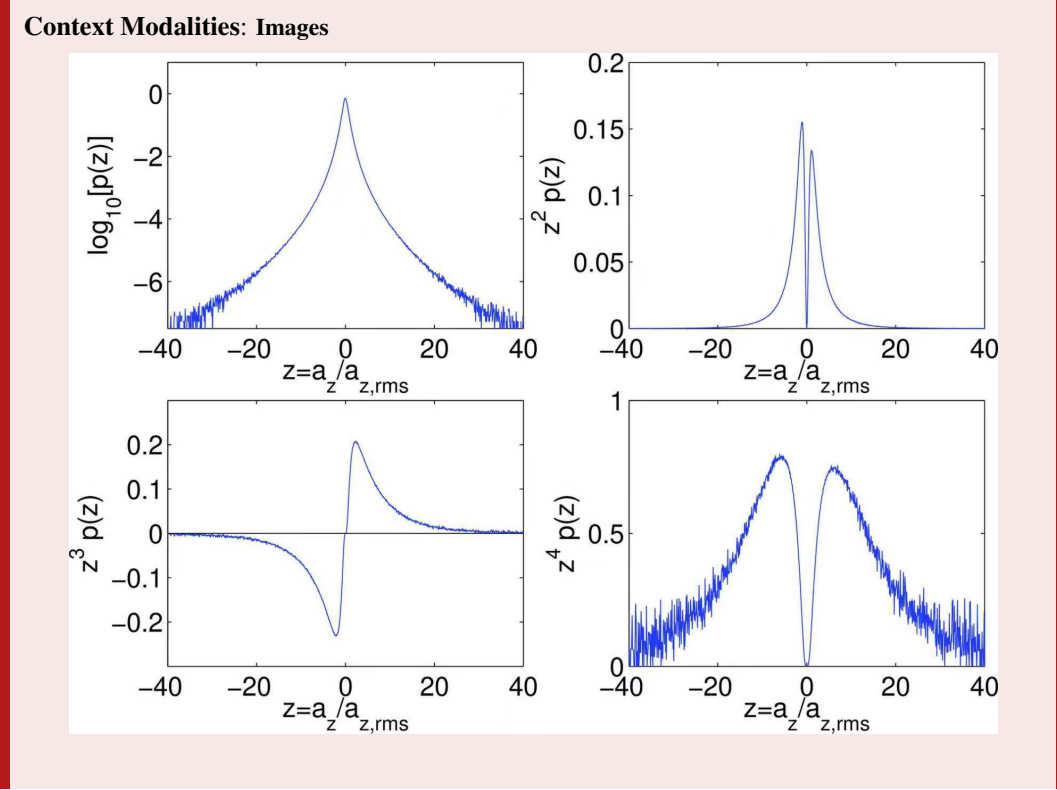
Task Paradigm: search
Search-oriented

C.5 EXAMPLE FROM ARXIVQA

One Example from ArXivQA

Question ID: physics-8049

Question: Based on the top-right graph, how would you describe the behavior of $P(z)$ as z approaches zero?



Covered areas:
The document includes arXiv academic papers in various fields such as physics and mathematics.

Covers Few Areas

Cross-evidence Reasoning:
Only focus on a single element.

Not Cross-evidence Reasoning

Task Paradigm: search

Search-oriented

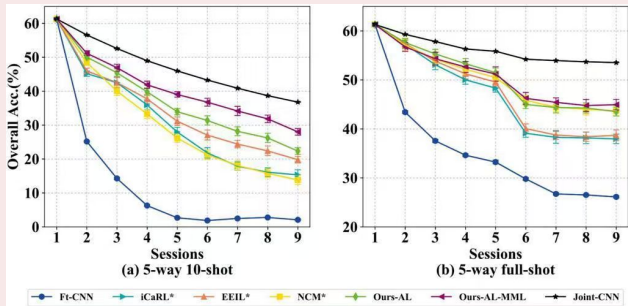
C.6 EXAMPLE FROM CHARXIV

One Example from Charxiv

Question_ID: 2004.10956

Question: Which model shows a greater decline in accuracy from Session 1 to Session 9 in the 5-way full-shot scenario?

Context Modalities: Images



Covered areas:

The document type consists of multi-type charts and graphs from 2323 papers in 8 disciplines, namely physics, computer science, mathematics, biology, chemistry, statistics, engineering, and economics, which are derived from the arXiv platform.

Cross-evidence Reasoning:

Only focus on a single element.

Not Cross-evidence Reasoning

Task Paradigm: search

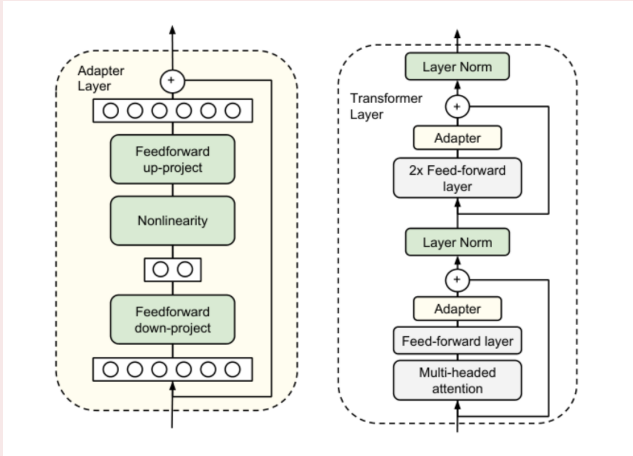
Search-oriented

C.7 EXAMPLE FROM AAAR

One Example from AAAR

Question_ID: 1902.00751
Question: What experiments do you suggest doing? Why do you suggest these experiments?

Context Modalities: Multi-Modal Documents



Covered areas:
The document types cover two core categories: one is the AAAR-1.0 benchmark dataset documents, which are used to evaluate the research capabilities of LLMs and contain annotated data for 4 types of research tasks such as equation inference; the other is the documents related to the academic organization operation of the American Association for Aerosol Research (AAAR).

Covers Few Areas

Cross-evidence Reasoning:
It is necessary to integrate textual evidence across paragraphs and chapters.

Task Paradigm: search

Search-oriented

C.8 EXAMPLE FROM MMCR

One Example from MMCR

Question ID: 1

Question: Which module's weights are frozen?

Context Modalities: Multi-Modal Documents and Texts



Covered areas:

Its document type focuses on multimodal information fusion and clinical semantic understanding in medical scenarios.

Focus Only On the Field of Medicine

Cross-evidence Reasoning:

It is necessary to forcibly integrate medical imaging evidence (such as abnormal areas in CT images) with clinical report text evidence

Task Paradigm: search

Search-oriented

C.9 EXAMPLE FROM DOCVQA

One Example from DocVQA

Question ID: 24581

Question: What is name of university?

Context Modalities: Multi-Modal Documents

UNIVERSITY OF CALIFORNIA, SAN DIEGO

To Paul

Date 11/30/82 Time 2:04 ^{AM}_{PM}

WHILE YOU WERE OUT

Dr. Wilson 455-8056

Ms. Sanjiv Clinic

From Sanjiv Clinic

☒ Telephoned ☐ Will phone again ☐ Please phone

☐ Came to see you ☐ Will come again ☐ Rush

MESSAGE

Re Program Committee

kidney Txn. It will

probably be 1st or 2nd

week in March (1983)

rather than latter half.

Phone party at (Home to call him)

Taken by Morgan

74475-136

Source: <https://www.industrydocuments.ucsf.edu/docs/nkbl0226>

Covered areas:

Including invoices, resumes, academic papers, financial reports, manuals, etc. in formats such as scanned copies, PDFs, and screenshots.

Cross-evidence Reasoning:

Simple question types (such as "invoice amount") only require evidence from a single location, while complex question types (such as "judging device compatibility based on parameter tables and explanatory texts across multiple pages of a manual") require integrating evidence across elements and locations.

Not All Cross-evidence Reasoning

Task Paradigm: search

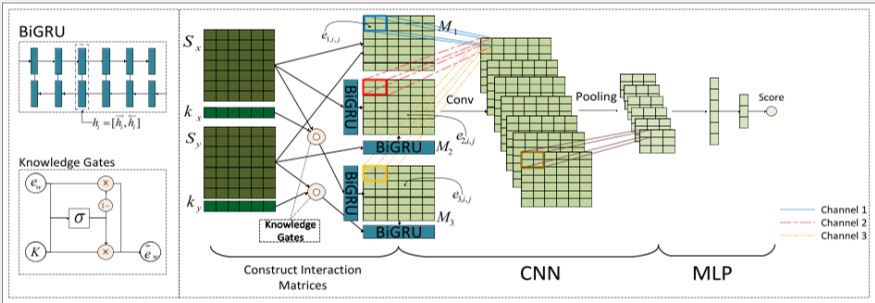
Search-oriented

C.10 EXAMPLE FROM SPIQA

One Example from SPIQA

Question ID: 1611.04684v1
Question: What is the role of the knowledge gates in the KEHNN architecture?

Context Modalities: Multi-Modal Figures and Charts



Covered areas:

The document type of SPIQA originates from academic papers in fields such as computer science and physics.

Covered Few Areas

Cross-evidence Reasoning:

Only focus on a single element.

Not Cross-evidence Reasoning

Task Paradigm: search

Search-oriented

D DATASET ANNOTATION AND CONSTRUCTION

D.1 HUMAN ANNOTATOR GUIDELINES

The defective academic papers in our dataset are curated from three primary sources: (1) We synthetically inject 9 types of errors into papers accepted at ICLR and Nature Communications. (2) For the papers rejected by ICLR, we identified the shortcomings in the papers based on the reviewers' comments and categorized them into 9 error types. (3) For accepted ICLR papers, we generate consistency-related errors by cross-referencing their content against cited literature. To ensure the quality of each error, all entries undergo a rigorous, multistage validation protocol executed by human annotators. For synthetically generated errors, annotators manually embed them into the source papers following this protocol:

- **Credibility Validation:** Each error must be logically sound and verifiable. For generated errors, annotators first confirm their logical coherence and unambiguity. Flawed error descriptions are revised whenever possible; only irreparable cases are discarded.
- **Evidence Verification:** All evidence substantiating an error must be either directly traceable to the source document or grounded in established domain-specific knowledge. Annotators are required to meticulously verify the origin and accuracy of all supporting data and background information.
- **Category Classification:** Each error must be accurately classified into one of the 9 predefined categories according to their formal definitions. Annotators verify the correctness of the assigned category and reclassify it if necessary.
- **Paper Revision:** Upon successful validation, annotators embed the generated error into the original manuscript by adding, deleting, or modifying relevant text segments as dictated by the error's specification.

This unified and standardized annotation protocol enables the creation of a high-quality dataset of academic papers with curated errors, providing a robust benchmark for evaluating the document scanning and error detection capabilities of Large Multimodal Models.

D.2 ANNOTATION STATISTICS

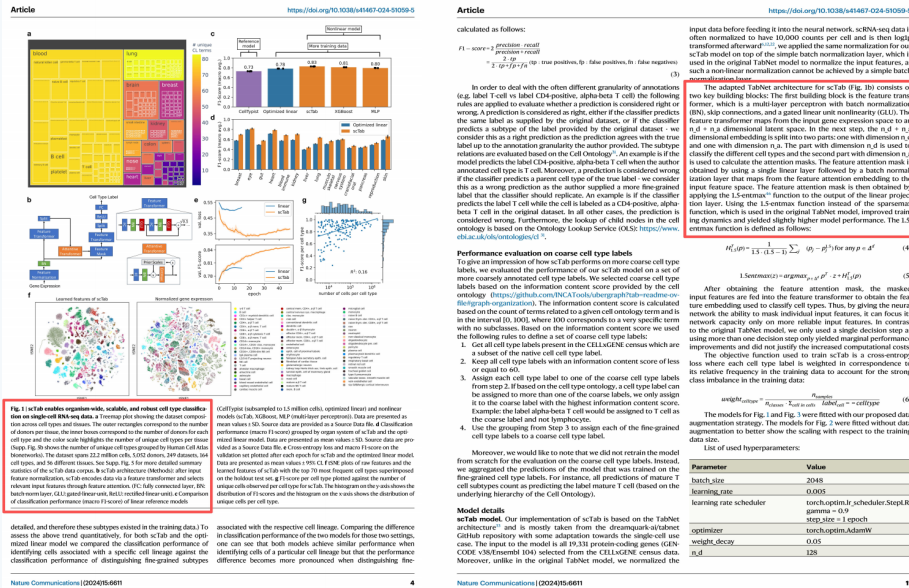
Initially, we generated or sampled a pool of 3,500 academic paper instances containing potential errors. During the manual annotation phase, following the protocol described above, we discarded 1,700 instances to ensure the logical rigor of the errors, the accuracy of the evidence, and a balanced distribution of categories.

Of the remaining 1,800 instances, 1,541 (85.6%) underwent manual revision. The distribution of these modifications is as follows:

- **535 questions** were rewritten to eliminate ambiguity or to increase their retrieval and reasoning difficulty.
- **1,207 explanations** were revised to correct erroneous evidence references and resolve logical flaws.
- **1,141 instances** underwent category reclassification or manual paper editing. This process served to fix classifications that were inconsistent with our definitions and, for errors generated, to manually inject them into the source papers to create the flawed documents.

D.3.2 CASE 2: MODIFY QUESTION

Example



Question: Judge whether the mathematical description of the scTab model architecture presents any dimensional mismatches.

Explanation: The Methods section on page 11 (and the Figure 1b caption) now states that the model’s feature transformer creates an embedding of dimension n_d . However, the same paragraph then describes splitting this embedding into two components of dimension n_d and n_a respectively. This is algebraically impossible for any non-zero n_a , and the hyperparameter table on page 12 confirms that n_a is set to 64, creating a fundamental dimensional mismatch in the model’s description.

Error Type: CF (Computation & Formulae)

Before:
question: Judge whether the mathematical description of the scTab model architecture presents any dimensional mismatches.

Decision: Modify

After:
question: Assess the Methods section for Computation & Formulae issues.

Analysis: Based on the error information and the text, the modified model description states that a vector of dimension n_d is split into two parts: one of dimension n_d and another of dimension n_a . This is algebraically impossible, as the total dimension (n_d) cannot equal the dimension of one of its parts (n_d) plus another non-zero part (n_a is set to 64). This constitutes a clear dimensional mismatch, rendering the model’s architectural description logically invalid. The original question was overly specific, as it explicitly prompted an assessment of whether the mathematical description of the scTab model architecture contained ‘any dimensional mismatches’. This hint was too detailed, reducing the analytical difficulty for the model. To increase the difficulty, we have revised the question’s phrasing to ask only whether the mathematical description of the scTab model architecture presents any problems.

D.3.3 CASE 3: MODIFY EXPLANATION

Example

Article

<https://doi.org/10.1038/s41467-024-55553-8>

Supplementary Fig. 4G; Supplementary Movie 2). In the PC, the nearby flexible RPA winged-helix domains 1 and 2 (WH1 and WH2) become stabilized, forming a ‘channel’ which stabilizes the DNA prior to entry into the active site (Supplementary Fig. 4H). Consistent with the role of the RPA winged-helix domain 1 in stabilizing the RPA, a folded solvent exposed on the periphery of the complex with a calculated solvent accessible surface area of 241 Å², ensuring this regulation in the PC context (Supplementary Fig. 4I). In each reconstruction, spontaneous DNA opening in the active site produces a disordered DNA bubble between L2 and L3 which is partially visible in the map (Supplementary Fig. 4J). Comparison of models for the OC, OC2 and MC states observed a highly similar structure for the THBSNAPC region, suggesting a rigid motion of the upstream transcription factors with respect to the polymerase (Supplementary Table 2). Despite PC assembly with the full-length protein, the density for the SNAPC^{mini} complex corresponded to a core assembly (termed miniSNAPC) of the SNAPC N terminus lacking the Myb DNA binding domain (residues 142–303). SNAPC1 and the N-terminal half of SNAPC2 (residues 1–141), with the SNAPC2 and SNAPC3 subunits not observed (Supplementary Fig. 4K), consistent with their dispensable role in DNA binding.

For a direct comparison, we imaged the class III PC assembled with SNAPC^{mini} consisting of SNAPC1 (555), SNAPC2 and SNAPC3 (1–265) using Cryo-EM. Three-dimensional classification was carried out as previously, yielding exclusively closed-clamp and open-clamp OCs (Supplementary Fig. 5). Only reconstructions for the closed OC, produced THBSNAPC^{mini} density of sufficient quality for THBSNAPC^{mini} mask classification and refinement, producing two OC structures (OC2^{mini} resolved at 3.7 Å resolution and OC2^{mini} resolved at 4.1 Å resolution which corresponded to SNAPC^{mini} fully and partially engaged THBSNAPC^{mini} OC structures, respectively (Supplementary Figs. 5a,b). In each instance, both SNAPC^{mini} and SNAPC^{mini} structures were very similar (Supplementary Table 1) and each displayed a similar fold to the miniSNAPC DNA complex resolved in isolation (Supplementary Table 1; Supplementary Fig. 4H–I). Together, these results suggest that the SNAPC core is unaffected by the presence of the mobile SNAPC2 and SNAPC3 subunits and is well defined, presenting PC assembly competent interfaces without any requirement for complex remodel. Fig. 5a,b all OC structures are highly similar and represent equivalent functional states, the OC2^{mini} structure, which displayed the highest quality reconstruction, was selected and will be henceforth referred to as OC^{mini}. All the following presented structural analysis was carried out with this model unless otherwise specified.

RPA uses a conserved interaction for transcription initiation
Structural comparison of the human H2A class III PC to the Saccharomyces cerevisiae (Sc) PC, formed on the 508S promoter (PDB:6ZU1) revealed that RPA shared a common mechanism of PC/II interaction with the Sc. RPA sequence and structural alignment of the N-terminal 25 ribonucleoprotein (RNP) region for both Sc RPA^{mini} and Hs RPA^{mini} displayed a high level of conservation and structural similarity (Fig. 2A). An alignment of both the human and Sc PC structures identified an equivalent docking position for RPA and RPA^{mini} on PC/II between the human and yeast structures, with the Pol II region involved presenting highly conserved interfaces (Fig. 2C; Supplementary Fig. 7A), demonstrating an equivalent mode of interaction irrespective of species and promoter sequence.

In contrast, the RPA and RPA^{mini}-associated factor RPA1 displays significant structural differences between the human and yeast PCs. Both Hs and Sc RPA1 from a conserved ‘SAND’ domain which facilitates interactions with THBSNAPC (Fig. 2D). However, in the yeast PC, RPA1 undergoes a significant conformational change from an extended to a largely ordered structure. The N-terminal ‘yester’ domain folds to engage the C3’ initiation/termination loop and stabilizes the WH1 and WH2 domains of the Sc RPA1 homologue C34^{mini}. C-terminal to this,

the vLpP domain (also previously identified as the RPA1 region, encompassing residues 203–312 in yeast)^{10,11} folds to form contacts with the Cyclic domain of RPA1. No such transition is observed for the human system, with both regions N and C-terminal to the SAND domain remaining disordered upon formation of PC/II. Alignment of human and yeast structures revealed a loss of the ordered initiation/termination loop in human RPA1 (Fig. 3). This suggests that the structure of the vLpP domain binding interface in RPA1, with significant changes also observed between the N-terminus of RPA1 and RPA2 and SNAPC4 in the human 16 PC structure (Fig. 3). Removal of the stabilizing interactions likely leads to the observed loss of RPA1 structure in the human system. Given the established role of these regions in transcription initiation¹⁰, this suggests a potential difference in the mechanism of transcription initiation at human and yeast origins. Despite the loss of RPA1 structure, the human RPA1 WH1 and C-terminal adopt a highly similar conformation to the yeast, which was unexpected in the absence of an ordered RPA1 loop and vLpP. Nevertheless, a comparison between both structures revealed a basic surface patch presented by RPA1 WH1 and C-terminal in both human and yeast structures (Fig. 3G), suggesting that the interaction with the upstream DNA is sufficient to stabilize RPA1 WH1 and C-terminal formation of PC.

The structural comparison also discerned differences within the polymerase active site. Whilst most functional regions including fork loops 1 and II, which II, the bridge helix and the trigger loop were conserved, as suggested by their sequence conservation (Supplementary Fig. 7B, c), differences were observed in the bridge helix and fork loops. Comparison of Hs and Sc, rDNA sequences revealed a difference between both regions which was also observed in the structure, with the human rDNA adopting a highly similar folded structure in apo, elongating and PC engaged states in contrast to the yeast polymerase, where this region is disordered in the PC (Fig. 3H) and folds upon transition to the elongating complex (EC)¹². The rDNA forms stabilizing interactions with the RNA-DNA hybrid in the active site, suggesting a difference in transcription initiation¹⁰. Differences were also observed in the switch II loop despite high sequence conservation. Importantly, Sc RPA1 N-terminal domain is critical for full expression of the initial transcription bubble around position +9 via an allosteric mechanism through direct contact with the Switch II loop¹³. Indeed, Sc RPA1 Zr16000 reconfigures the switch II loop, preventing the occlusion of the template strand from the active site and allowing for the substitution of the transcription bubble (PDB:6ZU1, see, ‘see’). However, RPA1 Zr16000 (Fig. 3H) suggests that human and yeast Pol II-mediated DNA opening, and therefore transcriptional initiation, may be differentially regulated.

In contrast, comparison of the human OC^{mini} structure with the closely related archaeal polymerase from Pyrococcus furiosus (PDB: 6ZU1), Thermococcus kodakarensis (PDB: 6ZU1), and Sulfolobus solfataricus (PDB: 7000)¹⁴ revealed a highly similar structure in the catalytic core (Supplementary Fig. 8A–C). Importantly, the switch II loop was consistently open in both apo and DNA bound states in all archaeal structures (Supplementary Fig. 8D–I), suggesting that the allosteric regulation of the switch II conformation in yeast may be a regulatory adaptation specific to eukaryotes.

SNAPC structure within the Class III PC
Resolution of the SNAPC^{mini} core structure in the OC context observed a similar structure to the PC-bound miniSNAPC complex (PDB: 6ZU1) (Supplementary Table 1). SNAPC2 represents a central structural unit against which the entire SNAPC complex is assembled (Fig. 3A). First, a helices in the N-terminus of SNAPC2 the ‘base’ domain together with an anti-parallel β-sheet of the ubiquitin like domain (ULD) completely enclose the N-terminus of SNAPC1 (Fig. 3B). SNAPC4 assembles on the opposing face of SNAPC2, forming multiple contacts

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transcribed by Pol II despite their defined Pol II PSE-TATA box spacing^{15,16}. As a result, the small spacing difference observed between L2 and L6 promoters is unlikely to drive the flipping of the SNAPC. We propose that the flipped orientation in a specific adaptation of SNAPC to engage either with THBSNAPC complex at Pol I and Pol II promoters and is regulated by a mutually exclusive set of interactions and steric clashes that fix the SNAPC conformation in each complex. Thus, the only determinant of polymerase selectivity is the presence or absence of a TATA box, as previously demonstrated¹⁷. The presence of a canonical TATA box favours the recruitment of RPA1 THBSNAPC complex and subsequently RNA Pol II. In the absence of a TATA box, recruitment of THBSNAPC results, resulting in the subsequent recruitment of RNA Pol II. In both scenarios, SNAPC can interact in a similar manner with the cognate PSE box while adapting two distinct and mutually exclusive conformations to engage with either RPA1 THBSNAPC or THBSNAPC, resulting in the recruitment of RNA Pol II or Pol I, respectively.

Despite the increasing amount of structural data available for SNAPC and the class III PC^{18–20}, the arrangement of SNAPC2 and SNAPC3 subunits in the SNAPC complex remained elusive. Employing surface crosslinking mass spectrometry analysis, the location and arrangement of these subunits was investigated. Combining this with AlphaFold predictions, the SNAPC2 binding site was localized to a structural module in the C-terminus of SNAPC4, consistent with previous mutational analysis which identified the region spanning 1281–1393 of SNAPC4 as the interaction site²¹. We therefore confirm this as the binding site of SNAPC2 while defining contact sites in the N and C-termini (Fig. 4E). SNAPC3 was also identified as part of the wing 2 helical bundle despite the absence of a defined wing 2 structure in the Pol II PC and miniSNAPC^{mini} structures, consistent with the requirement for this region to produce a stable SNAPC complex²². Multiple consensuses were identified between both wing 2 and SNAPC2, suggesting that these subunits together form a large structural module which is highly mobile. MAP modelling placed this structure in proximity to the bound DNA, consistent with the role of these subunits in regulating DNA binding affinity²³. The observed localisation and flexibility of this module allows us to speculate that SNAPC2-SNAPC4 module may regulate DNA access to the binding site hence modulating the SNAPC-DNA binding affinity. Indeed, the identified mobile module encompassed the OC1 intersecting region (OC1) in SNAPC^{mini} which was close to several SNAPC2 crosslinking sites (Supplementary Fig. 10F) and has been implicated in alleviating the DNA-DNA binding repression and stabilising SNAPC at the promoter²⁴ a function which has also been suggested for SNAPC2²⁵ leading to the possibility that OC1 may interact with a SNAPC2 gate to regulate SNAPC-DNA binding. In the class III PC context, this SNAPC2-containing mobile module faces the upstream region, pointing towards the mechanism and bound OC1, potentially facilitating the interaction between SNAPC-containing PCs and upstream regulatory factors to give greater mechanistic insight into class III promoter transcription and a more complete structural description of the complex class III PC.

Methods
Cloning and Protein Expression

All THBSNAPC components were expressed recombinantly in Rosetta (DE3) *Escherichia coli* cells (Sigma Aldrich, 7400 M⁺). Briefly, N-terminally His-tagged THBSNAPC residues 130–310 (Hs-THBSNAPC) was expressed in a pET43b(+) vector. Following transformation, cells were grown in terrific broth (TB) at 37 °C in an optical density (A₆₀₀) of 0.6 and subsequently induced with 0.5 mM isopropyl β-D-1-thiogalactopyranoside (IPTG; Thermo Scientific, R0393) at 20 °C for 18 hours. Cells were harvested by centrifugation at 2000 × g for

30 mins at 4 °C and stored at -80 °C prior to purification. Full length, C-terminally tagged RPA2 was expressed in a pJPMR construct. Transformed cells were grown in TB at 37 °C to a final A₆₀₀ of 0.6 and induced for 4 hours at 30 °C with 1 mM IPTG. Cells were collected by centrifugation at 2000 × g for 20 mins at 4 °C and stored at -80 °C. C-terminally His-tagged RPA1 (1–484) was expressed in a pJPMR vector. Cells were grown in TB at 37 °C to a final A₆₀₀ of 0.6. The temperature was reduced to 16 °C and cultures subsequently induced with 0.5 mM IPTG. Cells were collected by centrifugation at 2000 × g for 20 mins at 4 °C and stored at -80 °C.

Full length SNAPC^{mini} and mini SNAPC (SNAPC^{mini}) were expressed using the baculovirus baculovirus expression system²⁶. Briefly, for SNAPC^{mini} expression, a double-tagged SNAPC^{mini} subunit, carrying a TEV-cleavable N-terminal stop and C-terminal His tag, SNAPC1, SNAPC2, SNAPC3 and SNAPC4 were each sub-cloned into a pRTR vector and subsequently combined into a pRTR2 expression construct by Multisite Gateway Assembly Cloning Kit (NEB, M2850A) using the baculovirus expression system. For SNAPC^{mini} expression, an N-terminal TEV-cleavable Stop and His tag were added to SNAPC1 (1–555) and SNAPC2 respectively. These constructs were sub-cloned into pRTR vectors alongside SNAPC1 (265aa), SNAPC2 and SNAPC3 and subsequently combined into a pRTR2 expression construct. Following cloning, both SNAPC^{mini} and SNAPC^{mini} pRTR2 constructs were used for baculovirus production via transfection into DH10Bac⁺ cells (Genesys Biotech). For baculovirus generation, baculovirus was isolated and transfected into 2 ml of adherent SP2 cells (Thermo Fisher Scientific, 1449603) at 0.5 × 10⁶ cell/ml density in Insect-XPRESS media (Lonza, 127302) in a 6-well plate. Cells were incubated at 27 °C for 72 hours and supernatant (total volume of 2 ml), containing the baculovirus, was collected following the P1 virus. Viral amplification was achieved by P1 infection of a 25 ml culture of SP2 cells growing in suspension at a cell density of 0.5 × 10⁶ cells/ml in Insect-XPRESS media (Lonza, 127302). Cells were incubated at 27 °C at 130 rpm for 5 days and supernatant collected following centrifugation of the cultures at 1000 × g for 15 mins at 4 °C. This produced the P2 virus which was stored at 4 °C. Large-scale protein expression was carried out through the addition of 2 ml of P2 virus stock to 500 ml of Five cells (ThermoFisher Scientific, B65502) grown to 0.5 × 10⁶ cells/ml in Insect-XPRESS media (Lonza, 127302) in a roller bottle flask (Greiner). Cells were grown at 27 °C for 3 days at 130 rpm, and harvested through centrifugation at 3000 × g for 20 mins at 4 °C. Cell pellets were resuspended in phosphate buffered saline (PBS), centrifuged as previously and the resulting washed pellet stored at -80 °C prior to purification.

Large endogenous human DNA polymerase β (Pol β) was purified from HEK293T cells (CRISPR-Cas9 modified to include a C-terminal Myc-tag) using His-tag-P4 tag on the RPA1 (POLR2B) subunit²⁷. To produce sufficient material for purification, large-scale cell cultivation was carried out in a 96L Autoclave Bioreactor (2x Control Bioreactor, Applikon) using a batch cultivation in Dynamic Qx Medium (Cytosol, A26520) supplemented with 10 μM penicillin-streptomycin, 0.1 mM stable glutamine (Gibco, EC690404), 0.3% Pluronic F68 non-ionic surfactant (Gibco, 24040102), and 90 μM silicone-based Antifoam C Emulsion (Sigma-Aldrich, AR01). Cultivation conditions included a temperature of 37 °C, pH 7.0 (controlled by CO₂) and dissolved oxygen at 40%. The latter was controlled by sparging gas with airflow ranging from 300 to 500 ml/min, along with a second cascade of O₂ sparging from 0 to 1000 ml/min. Agitation was maintained at 100 rpm using a three-bladed blade impeller. Initially, cells underwent subculture and expansion and reaching a density of 4 × 10⁶ viable cells/ml. Subsequently, the cells were used to inoculate the bioreactor at a concentration of 0.5 × 10⁶ viable cells/ml, depending on the desired cultivation time. Harvesting took place at 8 × 10⁶ viable cells/ml.

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Question: Evaluate if the composition of the SNAPmini construct is consistently defined throughout the paper.

Explanation: The results on page 4 state that the assembled SNAPmini construct includes the SNAPC2 subunit. However, the methods on page 12 describe the construction of SNAPmini using only SNAPC4, SNAPC3, and SNAPC1, with SNAPC2 explicitly removed from the cloning description. A third conflicting statement on page 6 implies SNAPC2 was expected to be part of the minimal core, creating conceptual and operational inconsistency regarding this key experimental complex.

Error Type: RQD (Research Question & Definitions)

Before:

Explanation: ...with SNAPC2 explicitly removed from the cloning description. A third conflicting statement on page 6...

Decision: Modify

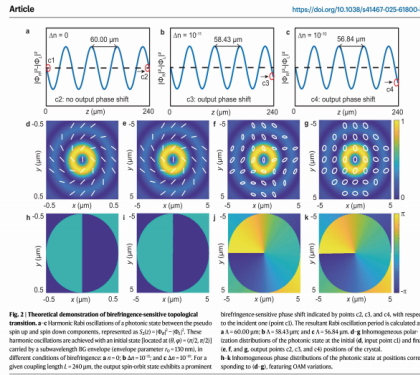
After:

Explanation: ...with SNAPC2 explicitly removed from the cloning description.

Analysis: Based on the modifications, the revised abstract and conclusion claim that the paper elucidates the protein’s ‘active-state’ structure and provides a roadmap for drug design. However, the original text repeatedly states (e.g., on pages 5 and 9) that it is the ‘apo’ (inactive) structure that was resolved, and critically notes on page 6 that the ‘activating ligand is still unknown’. This constitutes a clear RCA-type error, defined by the inconsistent description of a concept within the article. Yet, the large model misclassifies this as an IC-type (Inference & Conclusions) error, which is a significant mistake. Considering that the inconsistency regarding the ‘active-state’ description is overly superficial and obvious—a type of error almost never encountered in actual academic literature—it lacks practical value. Even reclassifying it as an H-type question would be of little significance. Therefore, we have decided to delete this instance.

D.3.4 CASE 4: MODIFY CATEGORY

Example



a result of circular symmetry of the disc that allows to fully recover the initial state. (b) Harmonic Rabi oscillation of photonic state between the pseudo spin-up and spin-down components, represented as $\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = \langle \hat{S}_z \rangle$. These harmonic oscillations are achieved with an initial state located at $(0, \pi/2, \pi/2)$ (corresponding to a subwavelength Rabi envelope parameter $\mu = 0.01$). In different conditions of birefringence $\Delta n = 0$ to 10^{-3} and $\Delta n = 10^{-3}$ for a coupling length $L = 200 \mu\text{m}$, the output spin-orbit state exhibits a prominent result of circular symmetry of the disc that allows to fully recover the initial state. (c) Harmonic Rabi oscillation of photonic state between the pseudo spin-up and spin-down components, represented as $\langle \hat{S}_x \rangle = \langle \hat{S}_y \rangle = \langle \hat{S}_z \rangle$. These harmonic oscillations are achieved with an initial state located at $(0, \pi/2, \pi/2)$ (corresponding to a subwavelength Rabi envelope parameter $\mu = 0.01$). In different conditions of birefringence $\Delta n = 0$ to 10^{-3} and $\Delta n = 10^{-3}$ for a coupling length $L = 200 \mu\text{m}$, the output spin-orbit state exhibits a prominent result of circular symmetry of the disc that allows to fully recover the initial state. (d) Homogeneous polarization distribution of the photonic state at the initial, input plane and first and second output planes. (e) Homogeneous polarization distribution of the photonic state at position corresponding to all g. (f) Homogeneous polarization distribution of the photonic state at position corresponding to all g. (g) Homogeneous polarization distribution of the photonic state at position corresponding to all g. (h) Homogeneous polarization distribution of the photonic state at position corresponding to all g. (i) Homogeneous polarization distribution of the photonic state at position corresponding to all g. (j) Homogeneous polarization distribution of the photonic state at position corresponding to all g.

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Article <https://doi.org/10.1038/s41467-025-61800-3>

conditions, we simplify the above coupled-wave equation as

$$\begin{aligned} \left(\nabla_{\perp}^2 + \frac{\partial^2}{\partial z^2} \right) \exp(i\mathbf{k}_{\perp} \cdot \mathbf{r}_{\perp}) &= \frac{1}{2} \left(\nabla_{\perp}^2 + \frac{\partial^2}{\partial z^2} \right) \Psi \\ \left(\nabla_{\perp}^2 + \frac{\partial^2}{\partial z^2} \right) \exp(i\mathbf{k}_{\perp} \cdot \mathbf{r}_{\perp}) &= \frac{1}{2} \left(\nabla_{\perp}^2 + \frac{\partial^2}{\partial z^2} \right) \Psi \end{aligned} \quad (8)$$

where $\nabla_{\perp}^2 = \nabla_{\perp}^2 + \frac{\partial^2}{\partial z^2}$ denotes a Laplace operator. We expand the term Ψ in the Cartesian coordinate system, and consider using the constant condition

$$\frac{\partial \Psi}{\partial z} = \frac{\partial \Psi}{\partial z} + \frac{\partial \Psi}{\partial z} + \frac{\partial \Psi}{\partial z} = 0 \quad (9)$$

As a consequence, we obtain a general Schrödinger-like equation governing the evolution dynamics of photonic state in the crystal. It is expressed as

$$\frac{\partial}{\partial z} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \begin{pmatrix} -\nabla_{\perp}^2 + \epsilon_0 & \epsilon_0 \\ \epsilon_0 & -\nabla_{\perp}^2 + \epsilon_0 \end{pmatrix} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \quad (10)$$

where $\epsilon_0 = (\epsilon_0 + \epsilon_0)/2$ for a shallow birefringence. We introduce another parameter $\epsilon_0 = \epsilon_0 - \epsilon_0$ to describe photonic anisotropy. The value of ϵ_0 can be either negative or positive, relying on crystal polarity. Given shallow birefringence, we reasonably assume $\epsilon_0 = (\epsilon_0 + \epsilon_0)/2$. Δn is a phase mismatch, defined as $\Delta n = \epsilon_0 - \epsilon_0$. It arises from birefringence of the crystal which leads to a mutual coupling between A_+ and A_- .

Since the Schrödinger-like equation contains rapid oscillatory terms $\exp(\pm i\Delta n z)$, it is relevant to demonstrate photonic spin-orbit dynamics in a rotating frame³⁰. We achieve this by using the following transformation

$$\begin{aligned} A_+(x, y, z) &= \exp(i\Delta n z/2) \tilde{A}_+(x, y, z) \\ A_-(x, y, z) &= \exp(-i\Delta n z/2) \tilde{A}_-(x, y, z) \end{aligned} \quad (11)$$

In this rotating frame, the Schrödinger-like equation is modified as

$$\frac{\partial}{\partial z} \begin{pmatrix} \tilde{A}_+ \\ \tilde{A}_- \end{pmatrix} = \begin{pmatrix} -\nabla_{\perp}^2 + \epsilon_0 + \beta \Delta n & \epsilon_0 \\ \epsilon_0 & -\nabla_{\perp}^2 + \epsilon_0 - \beta \Delta n \end{pmatrix} \begin{pmatrix} \tilde{A}_+ \\ \tilde{A}_- \end{pmatrix} \quad (12)$$

To obtain an equivalent of the Pauli equation, which describes spin dynamics of a quantum particle in a driven magnetic field³¹, we further transform the present setting from the Cartesian basis (x, y) into the circular basis $(\hat{r}, \hat{\phi})$ via a transformation matrix $T = (1, -i, i, 1)$. This transformation yields a magnetic-like Hamiltonian

$$\hat{H} = \begin{pmatrix} 0 & \Delta n/2 - \beta \Delta n \\ \Delta n/2 + \beta \Delta n & 0 \end{pmatrix} \quad (13)$$

In the circular basis, the complex light field can be expressed as a superposition of \hat{r} and $\hat{\phi}$ with different weights Φ_0 and Φ_1 , i.e., it can be written as

$$A(x, y, z) = A_+(x, y, z) \Phi_0 + A_-(x, y, z) \Phi_1 \quad (14)$$

These weight coefficients become propagation-variant during state evolution and can be expressed in a normalized form as $\Phi_0(z) = \sin(kz/2) \exp(i\phi(z)/2)$ and $\Phi_1(z) = \cos(kz/2) \exp(i\phi(z)/2)$, respectively³². Thus, a pseudo spin defined in this setting can be denoted as $\hat{\sigma} = \Phi_0^\dagger \hat{\sigma} \Phi_0$, which can be geometrically

represented as a point on the normalized higher-order Poincaré sphere³³. Substituting the expression of $A(x, y, z)$ into the Schrödinger-like equation, we obtain the Pauli equation equivalent represented in the spin-orbit framework as

$$\frac{\partial}{\partial z} \begin{pmatrix} \Phi_0 \\ \Phi_1 \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) + \frac{1}{2} \left(\frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) + \frac{1}{2} \left(\frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) \right) \right) \end{pmatrix} \begin{pmatrix} \Phi_0 \\ \Phi_1 \end{pmatrix} \quad (15)$$

where $\hat{\sigma} = \begin{pmatrix} \sigma_x & \sigma_y \\ \sigma_y & \sigma_x \end{pmatrix}$ and $M = 2\Delta n(2 - \beta)$ is the equivalent mass of the spin. Here $\hat{\sigma}$ is the Pauli matrix vector $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. In the circular basis having the following form

$$\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \sigma_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (16)$$

$\hat{\sigma}$ represents a magnetic field equivalent presented in the rotating frame. It is a three-component vector field $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, where $\hat{\sigma} = \hat{\sigma}_x \hat{r} + \hat{\sigma}_y \hat{\phi} + \hat{\sigma}_z \hat{z}$, and $\hat{\sigma}_x = \hat{\sigma}_y = \hat{\sigma}_z = 1$. In the presence of the synthetic magnetic field $\hat{\sigma}$, the left and right circular polarization components become mutually coupling in the course of spin evolution, manifested as a conversion between the spin and orbital angular momenta. Particularly, the Pauli equation admits harmonic oscillatory solutions, when $\hat{\sigma}$ is propagation-invariant. With an initial state denoted as $\hat{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, we demonstrate such harmonic solutions in terms of $\Phi_0 = \exp(i\phi(z)/2) \exp(i\phi(z)/2) \exp(i\phi(z)/2)$, where the oscillation frequency is expressed as

$$\Omega = \left[\frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) + \frac{1}{2} \left(\frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) + \frac{1}{2} \left(\frac{\partial}{\partial z} \left(\frac{\Phi_0}{\Phi_1} \right) \right) \right) \right]^2 \quad (17)$$

This formula reveals a close relationship between the spin-orbit oscillation and the birefringence Δn , allowing us to reveal birefringence value by measuring the topological wavefunction variation.

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Question: Assess whether the conclusions drawn about the protein's functional state and therapeutic applicability are supported by the presented methods and results.

Explanation: Edits in the abstract and discussion claim the paper presents an active-state structure that reveals the activation mechanism and provides a roadmap for drug design. This overstates the findings, as the paper repeatedly describes solving the 'apo' (unbound) structure and explicitly states the activating ligand is unknown (p.6). To make the error subtle, a contradictory sentence was added to the methods (p.9) claiming a stabilizing agonist was used, but this is falsified by the numerous, unmodified mentions of the 'apo GPR179' structure throughout the results and methods.

Error Type: MO (Measurement & Operationalization)

Before:

Error Type: MO (Measurement & Operationalization)

Decision: Modify

After:

Error Type: RCA (Referential and Citation Alignment)

Analysis: The introduced error systematically changes the laser wavelength used in the experiment to 532.0 nm. However, the calculation of a key physical quantity (birefringence) continues to use material constants (the electro-optic coefficient) that are only valid at the old wavelength of 632.8 nm. Because the optical properties of materials are wavelength-dependent, this systematic mismatch between experimental conditions and calculation parameters creates a significant contradiction in a core part of the paper. Compared to a Measurement & Operationalization (MO) error, this error is more accurately described as an internal inconsistency. Therefore, we are reclassifying this question from MO to RCA.

Example2: 816

Under review as a conference paper at ICLR 2025

In addition (Equation 3), it holds:

$$\mathbb{E} \left[L, \Phi \frac{1}{\sqrt{p}} \right] = \mathbb{E}[H(\text{vec}(\theta))].$$

Following Lemma Theorem 3.1, we further estimate a hessian-gradient product using GFM, corresponding to the $(H(\theta)^{-1})^T \nabla_{\theta} f_k$ term in Equation 1. Given an invertible matrix A , we have $(I, A)^T \sim L, A^T$. Therefore, denote the GFM matrix as $G(\theta) \triangleq (gg^T) \in \mathbb{R}^{d \times d}$ for any matrix $g \in \mathbb{R}^{d \times 1}$, it holds that:

$$H(\text{vec}(\theta))^{-1} \text{vec}(v) \approx \left[L, A \left(\frac{1}{p} gg^T \right)^{-1} \right] \text{vec}(v) = \text{vec}(G(\theta)^{-1} v). \quad (4)$$

Consider a LoRA-tuned model with LoRA dimension r and rank r . We assume that each column in our LoRA block $\Delta W \in \mathbb{R}^{d \times r}$, corresponding to each rank, is i.i.d. distributed with zero mean. In the ideal case that the model is trained to converge with $\mathbb{E}[-\nabla_{\theta} \log p(y|x, \theta)] = 0$, the zero-mean assumption on the columns of gradient matrices could stand. Then, we apply Equation 4 to approximate the original Hessian-gradient product. To further guarantee that $G(\theta)$ is invertible, we add a damping factor λI to the GFM matrix following Martins (2018).

We eliminate the constant in Equation 4 then derive the final formula of HYPERINF influence score. On a specific datapoint $\{x_k, y_k\} \in \mathcal{D}^{\text{val}}$, denote the inflated gradient on a parameter block θ as g_k, θ , we compute:

$$\mathcal{I}_{\text{inflated}}(x_k, y_k) = -g_k^T (G(\theta) + \lambda I_k)^{-1} g_k(\theta), \quad (5)$$

where $g_k = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} f_k(x_i^{(n)}, y_i(x_i^{(n)}))|_{\theta=\theta}$, $\theta_{\text{val}} \in \mathbb{R}^{d \times r}$, representing the average inflated gradient on θ on the validation set.

3.2. MATRIX INVERSE APPROXIMATION WITH SCHULZ'S METHOD

Schulz's method (Petrović, 1995). To compute the inverse of one matrix A , the hyperpower iterative family of matrix iteration methods has attracted the attention of many researchers due to its rigorous convergence guarantee (Altman, 1985; Garret III et al., 1971; Rutin & Boos, 2018):

$$X_{k+1} = X_k(I + T_1 + T_1^2 + \dots + T_1^{p-1}), \quad T_1 = I - AX_k. \quad (6)$$

The iterative approach requires p matrix-matrix multiplications per iteration and has an order of convergence p (Rutin & Boos, 2018). When choosing $p = 2$, it yields the Schulz iteration, which can also regarded as a by-product of the Newton method applied to the non-linear equation $f(X) = A - X^{-1}$:

$$X_{k+1} = X_k + X_k T_1, \quad T_1 = I - AX_k. \quad (7)$$

It is proved by Ben-Israel & Cohen (1966) and Petrović (1995) that with a proper initialization, Schulz's method would converge to A^{-1} in the order of convergence at least $p = 2$. We provide the complete proof of convergence in Appendix C. Compared to other conventional matrix inverse algorithms (e.g. gaussian elimination, conjugate gradient, GMRES), Schulz's method demonstrates superior accuracy in terms of error rate and significant efficiency gains from the GPU acceleration on matrix multiplications. We include more details in Appendix E. With the convergence test on matrix inversion (section E), we show that starting from a small identity matrix or random gaussian initialization, Equation 7 could converge to a desirable error rate in finite steps (≤ 20). We provide the pseudo-code in Algorithm 1.

Summary. We hereby provide the holistic view of the HYPERINF algorithm for influence function estimation. Firstly, we compute the generalized Fisher information $G(\theta)$ on all tunable parameter blocks (LoRA blocks on LoRA-tuned models). Secondly, we compute the inverse of the damped GFM $(G(\theta) + \lambda I_k)$ with Schulz's iterations (Equation 7). Last, we compute the influence score with cached validation gradient g and the inflated gradient on each training sample, i.e. $\mathcal{I}_{\text{inflated}}(x_k, y_k)$ (Equation 5). We provide the detailed pseudo-code in the Appendix (Algo. 2).

5

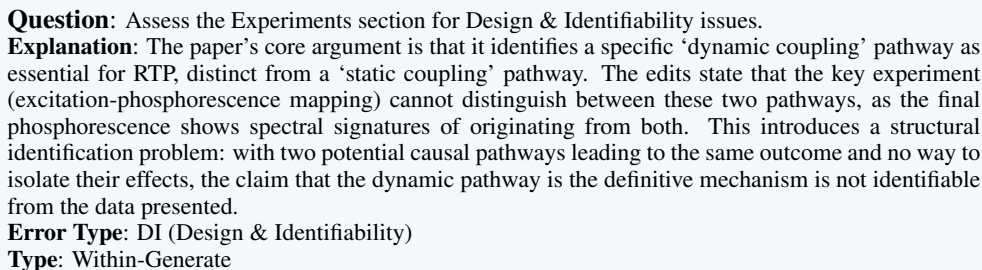
Question: Scrutinize the Methods section for Research Question & Definitions issues.

Explanation: Lemma 3.1, which is a cornerstone of the paper's theoretical contribution for low-rank Hessian approximation, relies on a strong and insufficiently justified assumption. The lemma states: "Assume that each column of the sample gradient ... is independent and identically distributed random vector with zero mean under the distribution $p(y|x, \theta)$ ". The paper provides only a brief, hand-wavy justification (p.5, lines 230-232), suggesting it "could stand" in an "ideal case" of model convergence. These critical i.i.d. and zero-mean conditions are not rigorously established or empirically validated for the contexts in which the method is applied. This leaves a core hypothesis of the paper ambiguously defined and justified, which is an error of type Research Question & Definitions.

Error Type: RQD (Research Question & Definitions)

Type: Within-Sample

Example1: 1006



Explanation: The paper's core argument is that it identifies a specific 'dynamic coupling' pathway as essential for RTP, distinct from a 'static coupling' pathway. The edits state that the key experiment (excitation-phosphorescence mapping) cannot distinguish between these two pathways, as the final phosphorescence shows spectral signatures of originating from both. This introduces a structural identification problem: with two potential causal pathways leading to the same outcome and no way to isolate their effects, the claim that the dynamic pathway is the definitive mechanism is not identifiable from the data presented.

Type: Within-Generate

Example2: 724

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by setting it to zero in S and reconstructing the weight using the original singular vectors

$$W = USV^T, \rightarrow \tilde{S}_i = \begin{cases} s_i & \text{for } i \neq r \\ 0 & \text{else} \end{cases} \rightarrow \tilde{W} = U\tilde{S}V^T. \quad (9)$$

Because removing a single singular value in a full transformer model has negligible effect, we grouped the singular values of each matrix into ten equally sized sets and removed these sets individually from the transformer. To assess the effect of removing singular values, we fine-tuned a pretrained BERT transformer using five different random seeds for initializing the model heads on the BoolQ dataset, achieving an average validation accuracy of 73.6%. We then removed one of the singular value deciles from a specific matrix type in all layers; for example, we set the largest 10% of singular values in each query matrix to zero and measured how the validation accuracy dropped compared to the full model.

We present the results in Fig. 3, which shows good agreement between the regions that deviate from RMT and the regions that are crucial for the transformer’s test performance. As expected, for all matrix types, the removal of the largest singular values leads to the greatest accuracy drops. This is corroborated by the p -values of the right singular vectors; in five out of the six cases, we observe significant drops in p -values for vectors corresponding to the largest singular values. As a reference for the p -value drops, we consider the plateau value, indicated by the dashed black line as a visual guide. In the case of the intermediate dense matrices, the singular vectors corresponding to small singular values have the largest deviations from RMT. This is reflected as a large accuracy drop when removing these small singular values. Although less pronounced than in the intermediate dense matrices, the key matrices also exhibit significant RMT deviation for singular vectors corresponding to small singular values. However, when we tested the impact of removing these small singular values from the key matrices on the BoolQ dataset, we did not observe a significant effect on the generalization performance. Such behavior is expected when the information learned during pretraining is not utilized by the downstream task (see Appendix E for an example on the SuperGLUE-WC dataset, where removing these small singular values impacts performance).

Although one might consider using this scheme to reduce the network size, we find that removing large portions of the “random” parts of the spectrum significantly degrades the network’s performance. To understand this behavior, we consider the case where weight matrices in the network architecture is completely random and is kept frozen during training. In this scenario, the network is still able to learn, but the removal of small and intermediate singular values from the random weights significantly impacts the overall performance, as the subsequent layers are sensitive to small changes in the random matrix. In Appendix E we demonstrate that matrices which have learned robust features are highly resilient to such removal, whereas removing singular values from a random matrix destroys the subtle details that subsequent layers depend upon.

7 FINE-TUNING

Recent studies have debated the relevance of small singular values in transformer networks. Some argue that these values are crucial for network performance (He et al. 2020), while others have observed performance improvements when they are removed (Sharma et al. 2022). Our RMT analysis reveals significant deviations only for some of the smaller singular values and their corresponding vectors, providing a diagnostic tool to assess their importance. This finding supports the notion that small singular values can play a significant role.

In Figure 3 we investigate the relevance of singular values before and after fine-tuning by removing deciles of singular values from all weight matrices simultaneously. We observe a clear difference between the two scenarios: when singular values are removed before fine-tuning and the model is fine-tuned afterward, the performance is not significantly affected by the removal. However, when the model is fine-tuned first and singular values are removed afterward, the performance drops significantly, indicating that these singular values are crucial to the model’s performance after fine-tuning. This observation explains the differences found in the literature: He et al. (2020) fine-tuned BERT and found that the small singular values are important to the network, while Sharma et al. (2022) found it beneficial to remove them from a model that is directly evaluated on a benchmark without fine-tuning. We interpret this behavior as evidence that fine-tuning, and potentially alignment, are encoded in the smaller singular values and their corresponding vectors. Notably, singular 11.8k

Question: Assess the Methods section for Design & Identifiability issues.

Explanation: A reviewer points out a flaw in the experimental design for the pruning experiments. The paper states on page 9, “We then removed one of the singular value deciles from a specific matrix type in all layers”. The reviewer argues this “coarse intervention” constitutes a design flaw because by modifying all layers simultaneously, it becomes impossible to attribute performance changes to specific layers. This confounds the effects, making it difficult to identify where in the model the removed information was critical. This directly undermines the paper’s stated goal of “locating information.” The design choice violates the conditions for identifying layer-specific contributions, which is an error of type Design & Identifiability.

Error Type: DI (Design & Identifiability)

Type: Within-Sample

E.3 SG (SAMPLING & GENERALIZABILITY)

Example1: 1014



Question: Assess the Methods section for Sampling & Generalizability issues.
Explanation: The Methods section is edited to state that the experiments used a “specific substrain of diabetic” mice, a highly specialized sample. However, the Abstract and Discussion make broad, unsupported claims of generalizability to “all patients” and the “general patient population.” This constitutes an invalid sample-to-population inference.
Error Type: SG (Sampling & Generalizability)
Type: Within-Generate

Example2: 935

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Corollary 3. (Regret bound under stationary preferences) Let $\mathcal{F}_T = \{f \in \mathcal{F} \mid \forall x \in \mathcal{X}, f(x) \in \mathcal{F}_T\}$. Let $\beta_T \in \Theta$ denote the minimum of the NS-DPO loss (Equation (3)). Then, for $\lambda \geq C_1 \sqrt{\log(4T/\beta_T)/n}$, some constant $C_1 > 0$, $\gamma = 1 - (\frac{\beta_T}{C_1})^2$ and $0 < \alpha < 2/3$, we have with probability at least $1 - 2\delta$:

$$\lim_{T \rightarrow \infty} \frac{\mathbb{E}[\text{Reg}_T]}{T} \leq 4\alpha\beta_T \sqrt{\frac{C_1}{T\alpha\gamma}} \sqrt{\frac{d + \log(1/\delta)}{n}}$$

and recover the complexity of $\mathbb{E}[\text{Reg}_T] = O(n^{-1})$ under stationary preferences.

5 EXPERIMENTS

In this section, we empirically evaluate NS-DPO’s ability to learn under preference drift. We first show that NS-DPO outperforms DPO in the log-linear policy setting, supporting our theoretical results introduced in Section 2. We then analyze how NS-DPO performs under different types of preference drift and under different strengths of preference change using the Llama LLM (Jain et al. 2023) and the Llama LLM (Jain et al. 2023). We provide the code used for the experiments.

5.1 EXPERIMENTAL SETUP

5.1.1 SYNTHETIC EXPERIMENTS

To analyze the performance of NS-DPO in the log-linear policy class, we construct a synthetic environment with a known feature space and preference drift. We use the feature space from [23] where $x \in \mathcal{X} = [0, 1]^d$, $a \in \mathcal{A} = [0, 1]$. The dimensions of the feature space and the policy parameter are both $d = 4$. We use $d_a = 4, d_\pi = 4, \beta = 16$ for synthetic experiments.

Non-stationary Dataset. To construct a dataset $\mathcal{D} = \{(x, a, r, \pi')\}_{x \in \mathcal{X}, a \in \mathcal{A}, r \in \mathcal{R}, \pi' \in \Pi}$, we randomly sample $x \sim \mathcal{X}$ and $a, \pi' \sim \mathcal{A}$. We assign 20 datapoints per time step $t \in [100]$. We sample 100 datapoints for evaluation at $T = 101$. To introduce preference drift, we follow an approach similar to [23] where we sample the preferences over a_1 and a_2 from the class of log-linear policies given in Equation (2), parameterized by θ . We denote preferred response as a and the rejected response as a' . When $t < 33$, we set the optimal parameter $\theta^* = (1, 0, 1, 0, 1, 0)^T$. For $t > 66$, we set $\theta^* = (0, 1, 0, 1, 1, 0)^T$. For $33 \leq t \leq 66$, we rotate θ^* smoothly between the two. For full details on the feature space and rotation see Appendix D.5.

Algorithm for Synthetic Experiments. We compare NS-DPO with DPO and SW-DPO in synthetic experiments. SW-DPO uses a “sliding” window to only consider points close to the current timestep T , which is commonly used in the non-stationary bandit literature (Gittis & Mehta 2009). We test the performance of NS-DPO and SW-DPO over several values of $\tau \in [0.7, 0.9]$ and window size $w \in [23, 50]$. The regularization coefficient is $\lambda = 1.0$ for all algorithms. We normalize the scale of the gradient for each method to address the differences caused by the application of exponential weighting and sliding window. For the reference policies, we use a uniform policy, whose parameter $\theta_{\text{unif}} \in \mathbb{R}^6$ is a zero vector.

Evaluation Metrics. To analyze the performance of the algorithms, we use the reward accuracy of the trained policies. The reward accuracy is computed by the portion of test response pairs with correctly estimated preferences, using the implicit rewards defined in Equation (9). For each tested algorithm, we report averaged results of the experiments across 10 different random seeds.

5.1.2 LARGE LANGUAGE MODEL EXPERIMENTS

To test the performance of NS-DPO in an LLM setting, we create three preference datasets with known and controlled preference drift.

Creating Non-Stationary Preference Datasets. To create datasets with varying preference drift, we select two reward models r_1, r_2 that result in different preferences for the responses a and a' . We assign each datapoint an arbitrary time across 100 timesteps $t \in [100]$ and adjust the response

<https://huggingface.co/datasets/Anthropic/ultrafeedback>

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D.2 NON-STATIONARY PREFERENCE DATASET CREATION

1) NS-DPO Dataset. We modify the GlobalOptimQA dataset (Gao et al. 2023) to create a time varying dataset. GlobalOptimQA consists of questions regarding global issues, different responses, and preferences from several countries represented as a probability vector. We split the questions and responses to create multiple time steps $t \in [100]$. We then vary the preferences with time by linearly interpolating between the preferences of two different countries. This simulates gradual preference drifts that can be caused by demographic shift or a series of external events. We generate preference drift using three pairs of countries. In each pair the starting country is the US, and the ending country is either Brazil, Japan or Germany. The preferences at the first and last time step correspond to either country in the pair. The last time step is held out as a test dataset and located as the current time $T = 101$. We divide the prompt-response pairs so that training and test data do not share any prompts.

2) UltraFeedback-RLM Datasets. Using the prompt and response candidates of UltraFeedback (Lin et al. 2023), we obtain preferences from two different reward models, PAIRRM (Jiang et al. 2023) and ARMORM (Wang et al. 2023). The datapoints in the training set are randomly assigned to one of $t \in [100]$ time steps, and assigned preferences of PAIRRM at the time step t is earlier than the change point $t_{cp} \in [33, 66, 81]$. We assign the preferences of ARMORM for the datapoints with time steps $t \geq t_{cp}$ and datapoints in the test set with $T = 101$. To test the effect of varied degrees of preference drift, we also vary the portions of datapoints whose preferences flip as reward model changes. We denote this portion as p_{flip} and use $p_{flip} \in \{(0.7, 0.3, 0.05, 1, 0)\}$ to create both training and test data. We use 10k datapoints for training and 50k datapoints for testing.

3) UltraFeedback-LLM Datasets. Using the same UltraFeedback dataset as above, we construct another dataset with the information of language models used for generations. The datapoints in the training set are randomly assigned to one of $t \in [100]$ time steps. Among the datapoints whose time step is earlier than the change point $t_{cp} \in [21, 51, 81]$, $p_{flip} \in \{(0.7, 1, 0)\}$ of the datapoints have responses that are generated by smaller language models as preferred responses. The other datapoints have responses generated by gpt-4 as preferred. We use 23.5k datapoints for training. We use the generations of `gpt-4o-mini`, `llama-2-70b-chat`, `vicuna-70b`, `pythia-7.12b`, `alpaca-70b`, `llama-2-130b-chat`, `vicuna-130b`, `ultra-130b` for smaller language models in the dataset.

4) Time Varying Helpful Harmless Datasets. Using the *helpfulness* subset of the Helpful Harmless dataset (Bai et al. 2022a), we create a time varying preference dataset. To do so, we use two reward models, the *helpfulness* and *harmfulness* outputs from the ARMORM model (Wang et al. 2023). Figure 8 shows that these rewards result in different preferences on the *helpfulness* dataset. We then assign each datapoint in the dataset a random time value from $t \in [100]$. We construct two methods to assign preferences using the time step information: change point preference shift and gradual variation. Under the change point preference shift, datapoints are assigned preferences according to *helpfulness* before the change point t_{cp} and *harmfulness* after the change point. Under gradual variation, we use the following reward model

$$r(x, y, t) = \begin{cases} r_1(x, y) & t < 33 \\ r_1(x, y) \cos(\frac{t-33}{66}\pi) + r_2(x, y)(1 - \cos(\frac{t-33}{66}\pi)) & 33 \leq t < 66 \\ r_2(x, y) & t \geq 66 \end{cases}$$

<https://huggingface.co/datasets/Anthropic/ultrafeedback>
We modify the financial version of UltraFeedback
<https://huggingface.co/datasets/Anthropic/ultrafeedback-finance>
<https://huggingface.co/datasets/Anthropic/ultrafeedback-rlm>
<https://huggingface.co/datasets/Anthropic/ultrafeedback-llm>

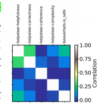


Figure 8: The correlation of different preference models generated by rewards from the ARMORM reward model on the Helpful Harmless dataset (Bai et al. 2022a). We observed that concepts such as safety and helpfulness were more correlated preferences, while the *helpfulness*-*harmfulness* reward model is uncorrelated with the preferences of preference drift, we also vary the portions of preference drift.

E.4 RCA (REFERENTIAL AND CITATION ALIGNMENT)

Example1: 0

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Second, they assume the sensors form a fixed spatial grid and record data simultaneously, which is not the case in our setup where the data could come from a single sensor at each time point (Fig. 1). For example, some earlier methods assume the observations are made on a fixed and regular spatiotemporal grid (Gong et al., 2018; Peters & Zahner, 2020), other methods work with irregular but still fixed observation locations (Jakovlev et al., 2021; Lerner & Glimm, 2022), and other works go further and allow the observation locations to change over time (Graf et al., 2021; Yin et al., 2022) but fix the observation times and assume dense observations. Whereas, another line of research has proposed methods that model only the spatiotemporal observation process without modeling the system dynamics (Chen et al., 2021; Zhu et al., 2021; Zhou et al., 2022; Zhou & Yu, 2023; Du et al., 2024).

Our work fills this gap and proposes a model for randomly observed spatiotemporal dynamical systems. Our model incorporates techniques from amortized variational inference (Kong et al., 2013), neural differential equations (Chen et al., 2019; Rackačius et al., 2020), neural point processes (Mey & Forster, 2017; Chen et al., 2021), and implicit neural representations (Chen et al., 2022; Yin et al., 2022) to efficiently learn both the underlying system dynamics and the random observation process. Our model uses initial observations to obtain the variational estimate of the latent initial state via a transformer encoder (Vaswani et al., 2017), simulates the latent trajectory with neural ODEs (Chen et al., 2018), and uses implicit neural representations to parameterize the point process and observation distribution. Furthermore, we identify a computational bottleneck in the latent state evaluation and propose a technique to alleviate it, resulting in up to 4x faster training. Our model shows strong empirical results outperforming other models from the literature on challenging spatiotemporal datasets.

2 BACKGROUND

2.1 SPATIOTEMPORAL POINT PROCESSES

Spatiotemporal point processes (STPP) model sequences of events occurring in space and time. Each event has an associated event time $t_i \in \mathbb{R}_{>0}$ and event location $\mathbf{x}_i \in \mathbb{R}^d$. Given an event history $H_t \triangleq \{(t_i, \mathbf{x}_i) | t_i < t\}$ with all events up to time t , we can characterize an STPP by its conditional intensity function

$$\lambda^*(t, \mathbf{x}) \triangleq \lim_{\delta t \rightarrow 0} \frac{P(t_i \in [t, t + \delta t], \mathbf{x}_i \in B_{\delta t}(\mathbf{x}) | H_t)}{\delta t | B_{\delta t}(\mathbf{x})} \quad (1)$$

where δt denotes an infinitesimal time interval, and $B_{\delta t}(\mathbf{x})$ denotes a δt -ball centered at \mathbf{x} . Given a history H_t with $t-1$ events, $\lambda^*(t, \mathbf{x})$ describes the instantaneous probability of the next, t th, event occurring at time t and location \mathbf{x} . Given a sequence of N events $\{(t_i, \mathbf{x}_i)\}_{i=1}^N$ on a bounded domain $A \subset [0, T] \times \mathbb{R}^d$, the log-likelihood for the STPP is evaluated as (Shibata et al., 2007)

$$\log p(\{(t_i, \mathbf{x}_i)\}_{i=1}^N) = \sum_{i=1}^N \log \lambda^*(t_i, \mathbf{x}_i) - \int_A \lambda^*(t, \mathbf{x}) dtd\mathbf{x}. \quad (2)$$

Marked STPP extends the above simple STPP by a mark $\mathbf{y}_i \in \mathbb{R}^k$ that is associated to each event (t_i, \mathbf{x}_i) .

2.2 ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

Given a deterministic continuous-time dynamic system with state $\mathbf{x}(t) \in \mathbb{R}^k$, we can describe the evolution of its state in terms of an ordinary differential equation (ODE)

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(t, \mathbf{x}(t)). \quad (3)$$

For an initial state \mathbf{x}_1 at time t_1 , we can solve the ODE to obtain the system state $\mathbf{x}(t)$ at later times $t > t_1$. The solution exists and is unique if \mathbf{f} is continuous in time and Lipschitz continuous in state (Coddington et al., 1980), and can be obtained either analytically or using numerical ODE solvers (Heun et al., 1997). In this work we solve ODEs numerically using ODE solvers from

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Model	Poisson		Epidemiology JP		COVID-19 NJ		BOLD5000	
	Temporal	Spatial	Temporal	Spatial	Temporal	Spatial	Temporal	Spatial
Baseline Process	-875.000	-	-811.100	-	-6.670e+00	-	-8.000e+00	-
Self-exciting Process	-2.170e+00	-	-1.010e+00	-	-1.607e+00	-	-6.070e+00	-
Markov Process	-8.750e+00	-	-0.110e+00	-	-1.000e+00	-	-1.000e+00	-
Neural Hawkes Process	-6.000e+00	-	0.000e+00	-	0.000e+00	-	0.000e+00	-
Conditional KDE	-	-2.950e+00	-	-2.370e+00	-	-2.300e+00	-	-3.807e+00
Time-varying CNF	-	-2.100e+00	-	-1.090e+00	-	-2.000e+00	-	-1.880e+00
Neural Jump SDE (GDE)	-4.000e+00	-2.077e+00	0.100e+00	-1.032e+00	2.250e+00	-2.200e+00	5.670e+00	8.750e+00
Jump CNF	6.077e+00	-1.500e+00	0.100e+00	-1.007e+00	2.250e+00	-1.900e+00	5.700e+00	1.200e+00
Attentive CNF	8.000e+00	-1.575e+00	0.280e+00	-1.227e+00	2.250e+00	-1.800e+00	5.800e+00	1.250e+00

Table 1: Log-likelihood per event on held-out test data (higher is better). Standard dev. estimated over 7 runs.

Results & Analyses

The results of our evaluation are shown in table 1. We highlight all results where the intervals containing one standard deviation away from the mean overlap. Across all data sets, the Time-varying CNF outperforms the conditional KDE baseline despite not being conditional on history. This suggests that the overall spatial distribution is rather complex. We also see from Figure 7 that Gaussian clusters tend to compensate for far-reaching events by learning a larger band-width whereas a flexible CNF can easily model multi-modal event propagation.

The Jump and Attentive CNF models achieve better log-likelihoods than the Time-varying CNF, suggesting prediction in these data sets benefit from modeling dependence on event history.

For COVID-19, the self-exciting Hawkes process is a strong baseline which aligns with similar results for other infectious diseases (Fort et al., 2013), but Neural STPPs can achieve substantially better spatial likelihoods. Overall, STPP is competitive with the Neural Jump SDEs; however, it tends to fall short of the Attentive CNF which jointly models spatial and temporal variables.

In a closer comparison to the temporal likelihood of Neural Jump SDEs (Yu & Brown, 2019), we find that overly-regularized spatial models can negatively affect the temporal model since both domains are highly coupled. Since our realization of Neural Jump SDEs and our STPP use the same underlying architecture to model the temporal domain, the temporal likelihood values are often close. However, there is still a statistically significant difference between our Neural STPP models and Neural Jump SDEs even for the temporal log-likelihood on all data sets.

Finally, we note that the results of the Jump and Attentive CNFs are typically close. The Attentive model generally achieves better temporal log-likelihoods while maintaining competitive spatial log-likelihoods. This difference is likely due to the Attentive CNF’s ability to attend to all previous events, while the Jump CNF has to compress all history information inside the hidden state at the time of event. The Attentive CNF also enjoys substantially faster computation (see Appendix A).

6 CONCLUSION

To learn high-fidelity models of stochastic events occurring in continuous space and time, we have proposed a new class of parameterizations for spatio-temporal point processes. Our approach combines ideas of Neural Jump SDEs with Continuous Normalizing Flows and allows us to retain the flexibility of neural temporal point processes while enabling highly expressive models of continuous marks. We leverage Neural ODEs as a computational method that allows computing, up to negligible numerical error, the likelihood of the joint model, and we show that our approach achieves state-of-the-art performance on spatio-temporal datasets collected from a wide range of domains.

A promising area for future work are applications of our method in earth and climate science which often are concerned with modeling highly complex spatio-temporal data. In this context, the use of Riemannian CNFs (Vlastakis & Nikolov, 2020; Liu et al., 2020; Fisher & Frenk, 2020) is especially interesting as it allows us to model Neural STPPs on manifolds (e.g. the earth’s surface) by simply replacing the CNF in our models with a Riemannian counterpart.

Question: Scan the errors in cited reference Chen et al.(2021)

Explanation: The edited P contains a Type H error by misrepresenting the performance of the cited model. P (p. 8) claims that the NSTPP model from Chen et al. (2021) ‘reported performance comparable to a standard Hawkes process baseline’. This contradicts the results in S, where the proposed models (i.e., NSTPP) consistently outperform the Hawkes process baseline, often by a large margin. For example, S (p. 9, Table 1) shows on the BOLD5000 dataset that the ‘Attentive CNF’ model achieves a temporal log-likelihood of 5.842 ± 0.005 , which is substantially better than the Hawkes Process at 2.860 ± 0.050 .

Error Type: RCA (Referential and Citation Alignment)

Type: Cross-Generate

Example2: 570

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Table 1: Knowledge graph completion results for the WN18RR and FB15k-237 datasets.

Method	WN18RR				FB15k-237			
	MRR	Hit@1	Hit@3	Hit@10	MRR	Hit@1	Hit@3	Hit@10
<i>Rule-based Methods</i>								
TransE	36.1	36.8	38.8	40.8	22.7	17.3	25.9	36.1
DistMult	38.2	36.9	38.8	41.0	23.8	17.4	26.1	36.8
RotatE	62.2	59.3	63.4	68.2	-	-	-	-
<i>Embedding-based Methods</i>								
TuckER	24.3	4.3	44.1	53.2	27.9	18.8	37.6	44.1
TransH	48.4	41.2	47.6	50.4	26.1	19.9	30.1	44.6
RotatE	12.3	8.0	13.7	20.7	16.4	10.0	18.1	30.0
TransD	47.8	42.8	46.2	57.1	33.8	24.1	37.5	51.1
TransR	47.0	43.1	48.2	53.6	31.8	26.6	36.4	54.1
RotatE	30.3	46.2	51.6	58.4	37.3	27.9	40.9	49.4
NeuralE	46.4	44.3	50.1	57.8	37.2	27.7	40.2	55.6
KRACL	25.2	48.2	54.2	61.3	36.0	26.6	39.5	54.8
<i>Hybrid Methods</i>								
KG-BERT	21.4	4.1	36.2	52.4	-	-	-	42.0
MTL-KGC	33.1	26.3	38.3	50.7	26.7	17.2	29.8	45.4
StAR	48.1	24.3	49.1	70.9	26.6	20.7	32.2	48.2
StAR2	46.6	51.7	71.0	80.0	33.6	24.9	37.1	51.1
KG-SSL	57.4	53.1	59.5	66.1	33.6	25.7	37.2	49.4
GRN	67.6	58.0	71.0	82.1	33.0	25.7	37.4	51.1
DSLM-KGC	76.4	63.1	74.8	84.2	35.5	26.4	38.8	53.2

Table 2: KGC results for the WikidataM datasets.

Method	MRR	Hit@1	Hit@3	Hit@10
DSLM	23.1	5.9	32.0	54.6
DSLM+KG	40.1	22.2	51.4	71.0
DSLM+KG+KG	48.9	26.2	66.4	87.7
DSLM+KG+KG+KG	44.1	26.9	64.9	86.4
DSLM+KG+KG+KG+KG	73.1	60.7	78.7	91.5

The most substantial improvement is seen on the WikidataM dataset, where our model shows a 5.0% increase in MRR (from 71.3% to 76.3%) and a 6.5% increase in Hit@1 (from 60.7% to 67.2%) compared to StAR2. Similar improvements are observed on the WN18RR dataset, where DSLM-KGC surpasses the second-best model (GRN) across all metrics, with enhance-
 ment, demonstrating a strong predictive ca-
 pability. On the FB15k-237 dataset, while our model falls short of embedding-based models, it still outperforms rule-based and text-based methods, narrowing the gap between text-based and embedding-based approaches by approximately 2-3 percentage points.

To clarify the results obtained from the WN18RR and FB15k-237 datasets, we perform a detailed analysis of the underlying KGs. First, we assess the topological structure of each KG by calculating the average degree M/N , where M and N represent the number of edges and nodes, respectively. The FB15k-237 dataset exhibits a denser structure, with an average degree of 27.3, compared to 2.27 for WN18RR. Second, we examine the topological structures of both datasets. In FB15k-237, relationships show a high degree of correlation (e.g., "went to" and "went to school"), resulting in a densely interconnected structure with a less pronounced clustering pattern. Finally, we carry out in-depth ablation studies to further examine the challenges our model experiences when capturing latent community structures from the FB15k-237 dataset, as discussed in the following section.

4.3 ABLATION RESULTS

We conduct diverse ablation experiments to investigate into how key components of our model impact KGC performance.

Stitch-breaking prior. We conduct KGC experiments with α_{sp} and α_{sm} chosen from the grid $\{0.0, 0.0, 1.0\} \times \{0.0, 20, \dots, 100\}$, while keeping all other hyperparameters fixed. Table 3 reports the mean and standard deviation of these 30 results for each dataset. The minimal variation in performance with different α_{sp} and α_{sm} values, as seen in Table 3 highlights the robustness of our model under diverse prior settings.

7

Question: Evaluate the Results section for Internal Consistency problems.

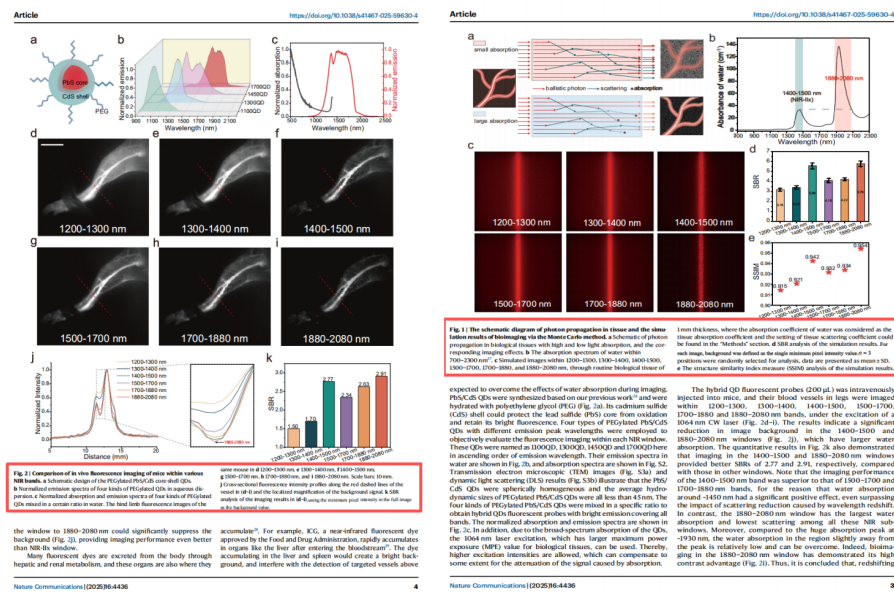
Explanation: A reviewer points out that the paper’s reported performance on FB15k-237 is lower than a state-of-the-art method. The paper’s main text makes a claim that is directly contradicted by its own table. Specifically, the text states that on the FB15k-237 dataset, their model “still outperforms rule-based and text-based methods” (page 7, ‘On the FB15k-237 dataset...methods’). However, Table 1 on the same page presents results for KRACL, a method listed under the “Text-based Methods” category, which achieves higher scores than the proposed model on both MRR (36.0 vs. 35.5) and Hit@1 (26.6 vs. 26.4). This discrepancy between the narrative claim and the tabular data constitutes a clear internal consistency error.

Error Type: RCA (Referential and Citation Alignment)

Type: Within-Sample

E.5 MO (MEASUREMENT & OPERATIONALIZATION)

Example1: 1015



Question: Assess the Figures/Tables section for Measurement & Operationalization issues.

Explanation: The figure captions on pages 3 and 4 have been edited to specify that the background for Signal-to-Background Ratio (SBR) calculations was defined as the single minimum pixel intensity in the image. This is not a valid or reliable operationalization of the “background” construct, as it’s highly susceptible to single-point noise or detector artifacts. This flawed measurement procedure systematically undermines all conclusions based on the SBR metric.

Error Type: MO (Measurement & Operationalization)

Type: Within-Generate

Example2: 1090

Article

https://doi.org/10.1038/s41467-024-5060-8

(August 2002–July 2022) monthly time series of surface chlorophyll-a concentration (Chl) derived from Moderate-resolution Imaging Spectroradiometer (MODIS) data (MODIS-Aqua). The potential forcing underlying Chl changes were discussed based on wind and ocean currents data of the same period.

Results

Westward extension of the chlorophyll-rich tongue in the equatorial Pacific

Here, we define the boundary of the CRT as the Chl index of 0.15 mg/m³ within the climatology boundary (indicated in Fig. 1a, see the black curve). Clearly, within the boundary of the CRT are the poleward equatorial upwelling and the westward EEZ (Fig. 1b).

Not obtained from Chl measurements by MODIS-Aqua (Fig. 1a), a linear trend fitting was first applied to this time series of CRT area, which suggests an statistically significant trend ($P < 0.05$, see the red line in Fig. 1a). The EM, which is powerful in detecting trend³⁸, was then used and to decompose the CRT area time series into seasonal and interannual components, as well as a residual trend component, as the focus of this analysis is on distinguishing between these variables and the residual trend (see “Methods” and Supplementary Fig. 1). Following the approach of Seta et al.³⁹, we obtained an estimate of the weight of the amplitude of the trend, which contributes 9% to the variability of the trend signal, while the interannual and seasonal components explain 39% and 52%, respectively.

The seasonal variation of the CRT area highlights peaks of the CRT area in January and May/June and a minimum in October/November (see the inset figure in Fig. 1b). This pattern is in general in phase with the known seasonal cycle of the equatorial current system⁴⁰.

The interannual variability of the CRT area, the deviation component, is negatively correlated with the Multivariate ENSO Index

(MEI) ($R^2 = 0.45$, $P < 0.05$) (Fig. 1c), which is consistent with prior findings that the CRT interannual variability is primarily influenced by ENSO^{38,39,41}. For example, the notable reduction in size of the CRT in 2016 coincided with an intense El Niño event, characterized by a positive MEI (Fig. 1c). During strong El Niño events, the 2006, anomalous westerly winds in the tropical western Pacific suppress the westward advection and lead to weakened equatorial upwelling⁴², which hampers the extension of the CRT.

Interestingly, the residual component demonstrates a notable increasing trend of the CRT area from 2002 to 2022 (Fig. 1d). The rate of CRT expansion is $1.17 \times 10^3 \text{ km}^2 \times 10^{-3} \text{ yr}^{-1}$, equivalent to an increase of 0.8% per year. Notably, a similar increasing trend is also observed when applying the same EM to a longer record of CRT area from 1997–2023, calculated from a merged Chl dataset derived from multiple ocean color satelites (see Supplementary Fig. 2). Furthermore, the application of the ensemble empirical mode decomposition (EMD) method³⁸ to the CRT area time series in 2002–2022 results in a similar expanding rate ($1.31 \pm 0.46 \times 10^3 \text{ km}^2 \text{ yr}^{-1}$) (see Supplementary Fig. 3). The confidence interval appears wider near the end of the study period due to a higher standard deviation, which results from random white noise added in the EMD analysis and is not related to the direction of the residual trend.

To determine the direction of the CRT extension, we applied EMD analysis to the time series of the CRT western, northern, and southern boundaries (see the definition of boundaries in “Methods”). The western boundary exhibits a significant westward movement trend from 2002 to 2022, with a rate of $0.41 \pm 0.25 \text{ km yr}^{-1}$ (Fig. 1d). In contrast, both the northern and southern boundaries move northward slightly at almost the same rate, which is an order of magnitude lower than that of westward extending (Fig. 1d, c). Thus, their contributions to the expansion of CRT could be largely neglected. Therefore, the expansion of CRT is predominantly attributed to the westward extension. With

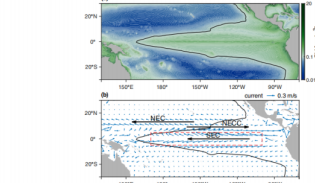


Fig. 1 | Distribution of the chlorophyll-rich tongue (CRT) and spatial distribution of ocean current fields in the equatorial Pacific. (a) Climatological mean surface chlorophyll concentration (Chl, mg/m³) and the current fields (m/s) between August 2002 and July 2022. The CRT climatology boundary is indicated with the black curve, representing the Chl index of 0.15 mg/m³. The right surface

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Article

https://doi.org/10.1038/s41467-024-5060-8

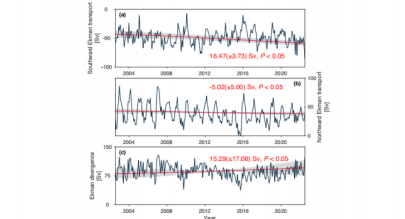


Fig. 2 | Monthly variation of the total western Chl transport calculated at 5°S. (a) The total western Chl transport (mg/m²) calculated at 5°S. (b) The total western Chl transport (mg/m²) calculated at 5°S. (c) The total western Chl transport (mg/m²) calculated at 5°S. (d) The total western Chl transport (mg/m²) calculated at 5°S. (e) The total western Chl transport (mg/m²) calculated at 5°S. (f) The total western Chl transport (mg/m²) calculated at 5°S. (g) The total western Chl transport (mg/m²) calculated at 5°S. (h) The total western Chl transport (mg/m²) calculated at 5°S. (i) The total western Chl transport (mg/m²) calculated at 5°S. (j) The total western Chl transport (mg/m²) calculated at 5°S. (k) The total western Chl transport (mg/m²) calculated at 5°S. (l) The total western Chl transport (mg/m²) calculated at 5°S. (m) The total western Chl transport (mg/m²) calculated at 5°S. (n) The total western Chl transport (mg/m²) calculated at 5°S. (o) The total western Chl transport (mg/m²) calculated at 5°S. (p) The total western Chl transport (mg/m²) calculated at 5°S. (q) The total western Chl transport (mg/m²) calculated at 5°S. (r) The total western Chl transport (mg/m²) calculated at 5°S. (s) The total western Chl transport (mg/m²) calculated at 5°S. (t) The total western Chl transport (mg/m²) calculated at 5°S. (u) The total western Chl transport (mg/m²) calculated at 5°S. (v) The total western Chl transport (mg/m²) calculated at 5°S. (w) The total western Chl transport (mg/m²) calculated at 5°S. (x) The total western Chl transport (mg/m²) calculated at 5°S. (y) The total western Chl transport (mg/m²) calculated at 5°S. (z) The total western Chl transport (mg/m²) calculated at 5°S.

In addition, the ENSO-CRT area correlation observed in this effort and prior studies^{38,39} suggests that if the occurrences of consecutive La Niña events increase under global warming as projected⁴³, the CRT will probably further extend to the west. Of course, the observed long-term trend of the CRT area highly depends on the data span used for trend analysis³⁸. Thus, it is necessary to stress that the reported westward extending trend of the CRT is observed within a temporal period of 2002–2022. Nevertheless, our finding of the CRT westward expansion, never reported in previous observational and modeling efforts, highlights the importance of lower frequency variations hidden under major interannual variability of ENSO in the equatorial Pacific. Continued long-term observations spanning over 30 years or more would be essential for a more comprehensive and definitive understanding of the trend of CRT and its impact³⁸.

Methods

Calculation of the area of the high chlorophyll tongue

The standard Level 3 monthly Chl products (version R2022.06, at a spatial resolution of 1/4°), of Moderate Resolution Imaging Spectroradiometer (MODIS-Aqua) from August 2002 to July 2022 were acquired from NASA Ocean Color Web (<https://ocecolor.gsfc.nasa.gov/>). The computation of the chlorophyll-rich tongue (CRT) area was confined to the open-ocean tropical Pacific region (20°N to 20°S). The eastern boundary was set 1000 km from the shore, and a similar constraint was applied to the western boundary. Pixels with Chl greater than 0.1 mg/m³ within this region were identified as part of the CRT. The area of each pixel was computed based on its latitude, longitude, Earth radius, and the intervals of latitude and longitude between two adjacent pixels. Subsequently, the CRT area was determined by summing up the area of all pixels within the CRT.

An extended Chl monthly series from September 1997 to August 2023, distributed by the USA Ocean Color project under the Climate

Change Initiative (CCI-CCI), was also acquired to supplement our analysis. The CCI-CCI provides merged Chl products at a 4 km spatial resolution from several ocean color missions, including MODIS-Aqua, the SeaWiFS Wide Field-of-view Sensor, the Medium Resolution Imaging Spectrometer, and the Ocean and Land Color Instrument⁴⁴. The CCI-CCI monthly Chl products can be directly accessed via <https://www.cci-cci.org/>.

Definition of the boundaries of the CRT

The western boundary of the CRT for each month was identified as the longitude of the pixel where the meridional mean Chl between 1°N and 1°S from 10°W to westward first declined to 0.1 mg/m³. Note that the western boundary could be absent in some months when Chl in the entire Equatorial Pacific month is 0.1 mg/m³ or less. Blank longitude values for these months. Most blank values were filled using cubic spline interpolation. However, those from May to September 2020, at the end of the time series, remain blank (see Fig. 1d) because it is unreasonable to do extrapolation. For the northern and southern boundaries of CRT in each month, we first computed the meridional mean Chl between 10°W and 10°E and established a latitudinal profile of mean Chl from 20°N to 20°S. We then scanned the latitudinal profile and extracted the two latitudes with mean Chl of 0.1 mg/m³ as the northern and southern boundaries.

Empirical mode decomposition for trend analysis

The Empirical Mode Decomposition (EMD) has demonstrated its efficacy in extracting intrinsic trends and natural variability from diverse data in geophysical research^{38,39}. Briefly, the original data is decomposed into a finite number of intrinsic Mode Functions (IMFs), which correspond to the scale in the data ranging from the smallest to the largest, and the trend of the original data is defined as the average of the residual components from the decomposed IMFs. There is an upgraded version of the EMD called the Ensemble Empirical Mode Decomposition

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Question: Assess the Methods section for Measurement & Operationalization issues.

Explanation: The Results section and the Figure 1 caption define the CRT boundary using a chlorophyll-a (Chl) concentration of 0.15 mg/m³. The Methods section also uses this 0.15 mg/m³ threshold for the western boundary. However, the same Methods section then defines the northern and southern boundaries using a different threshold of 0.1 mg/m³, creating an inconsistent operational definition for the paper’s primary construct.

Error Type: MO (Measurement & Operationalization)

Type: Within-Generate

E.6 DHP (DATA HANDLING & PREPROCESSING)

Example1: 528

Under review as a conference paper at ICLR 2025

the likelihood that the output configuration will satisfy the desired constraints. In our case, the constraint is energy, the output of the energy network, must decrease. We specifically employed GBI to directly update the task-net’s predictions using gradient signals derived from the energy network.

The implementation of GBI involves three main steps. The task-net, serving as our baseline model, is trained in a supervised manner to predict 3D poses. Next, a structured energy network is trained using the predictions from the task-net as negative samples. Lastly, the trained energy network is employed to iteratively update the task-net’s predictions through gradient-based optimization.

Algorithm 2 Gradient-Based Inference

Require: (x, y) : training data (3D inputs and 3D ground-truth outputs)

Require: F_T : task-net, F_E : energy network

Require: optimizer : torch -optimizer for F_T

Require: T : training iterations, K : GBI steps

- Phase 1: train Task-Net**
- for** $t = 1$ to T **do**
- Sample batch $B_t = \{(x_i, y_i)\}_{i=1}^{B_t}$
- Update $\phi: \phi \leftarrow \phi - \eta_t \nabla_{\phi} \frac{1}{|B_t|} \sum_{(x_i, y_i) \in B_t} \text{MSE}(F_T(x_i) - y_i)$
- end for**
- Phase 2: train energy network**
- for** $s = 1$ to T **do**
- Sample batch $B_s = \{(x_i, y_i)\}_{i=1}^{B_s}$
- Generate $z = F_T(x_i)$ for $x_i \in B_s$
- Update $\theta: \theta \leftarrow \theta - \eta_s \nabla_{\theta} \frac{1}{|B_s|} \sum_{(x_i, y_i) \in B_s} [F_E(x_i, y_i) - F_E(x_i, z)]$
- end for**
- Phase 3: gradient-based inference**
- Initialize $\hat{y}^{(0)} = F_T(x_i)$ for $x_i \in B_t$
- for** $k = 1$ to K **do**
- Refine $\hat{y}_i^{(k)}: \hat{y}_i^{(k)} \leftarrow \hat{y}_i^{(k-1)} - \eta \nabla_{\hat{y}} F_E(x_i, \hat{y}_i^{(k-1)})$
- end for**

3.3 SETTING

Datasets. We conduct our experiments on Human3.6M 3D WholeBody dataset (H3WB) [22], [23] and Human3.6M dataset (H36M) [Kneiss et al. 2012]. H36M is one of the most widely used datasets for 3D human pose estimation [Zhang et al. 2025], [Zou et al. 2025]. H3WB extends H36M by providing whole-body annotations using the VICON Wholebody system, which includes 133 whole-body keypoint annotations, capturing detailed information about hands, face, and feet, making it suitable for tasks that require fine-grained pose estimation. We utilize the ground truth 3D joint locations provided in the dataset to align the 3D and 2D poses. For the H36M dataset, we zero-center the 3D poses around the pelvis joint, following standard protocols and prior work. For the H3WB dataset, we zero-center the 3D poses around the midpoint of the two hip joints.

Implementation Details. We employ the SimpleBaseline [Martinez et al. 2017], SfmGCN [Zou et al. 2025] and single frame version of VideoPose [Zou et al. 2025] as task-nets. For the H3WB dataset, we modify the input and output layers of these task-nets to align with data. For the loss-net, we adjusted the SimpleBaseline by modifying the dimension and depth of the hidden layers. We set the hidden size to 2048 with 2 residual block stages without batch normalization and dropout layers for H3WB and SimpleBaseline task-net for H36M. For the other task-net for H36M, we set the hidden size to 256 with 2 residual block stages with dropout layers. We use separate Adam optimizers [Kingma & Ba 2017] without learning rate decay for the loss-net and the task-net. All models are trained with a batch size of 64 for 50 epochs on H36M and a batch size of 64 for 200 epochs on H3WB. For hyperparameter tuning, we employed Bayesian optimization with the wandb sweep tool [Bender 2025], aiming to minimize MPJPE for the S9 and S11 in the H36M dataset and PA-MPJPE for the S8 in the H3WB dataset, following the convention of prior works. To avoid overfitting to a specific random seed, we reported the average results from experiments with different random seeds using the optimized hyperparameters.

Question: Assess the Methods section for Data Handling & Preprocessing issues.

Explanation: The reviewer correctly identifies that the authors tuned hyperparameters on the test set. The paper’s “Implementation Details” section on page 5 states: “For hyperparameter tuning, we employed Bayesian optimization with the wandb sweep tool (Biewald, 2020), aiming to minimize MPJPE for the S9 and S11 in the H36M dataset and PA-MPJPE for the S8 in the H3WB dataset, following the convention of prior works.” According to standard protocols for the H36M dataset, subjects S9 and S11 constitute the test set. Tuning hyperparameters directly on the test set introduces data leakage, leading to an optimistic bias in the reported results and invalidating claims of generalization. This is a critical violation of machine learning best practices and fits the Data Handling & Preprocessing (E) category, as a pipeline choice introduces bias.

Error Type: DHP (Data Handling & Preprocessing)

Type: Within-Sample

Explanation: The modified text on page 3 states that data for the COVID-19 lockdown period were imputed using pre-pandemic averages. This data handling choice is highly problematic, as it smooths over a major, non-random structural break in the time series rather than modeling or excluding it. The imputation method introduces significant bias and data leakage, as a simple average does not accurately reflect the known, drastic reduction in elective surgeries during that specific period, compromising the validity of the causal model.

Type: Within-Generate

Under review as a conference paper at ICLR 2025

Figure 2: Comparison of applying different core-set pairs for training a Single-Network model as in Fig. 14. We can see these six augmentations integratably based on other best mAP results or direct convergence curves.

Figure 3: Illustrations of two novel super-set combinations T_{C5C8} and T_{C5A6} . Either of them is a novel operation using ready-made collaborative augmentation. And T_{C5} and T_{C8} introduce extra patches cropped from other images which are not developed.



Figure 3: Illustrations of two novel superior combinations T_{JOCO} and T_{JCCM} . Either of them is a sequential operations using ready-made collaborative augmentation. And T_{JO} and T_{CM} introduce extra patches cropped from other images which are not displayed.

$\mathbf{H} \in \mathbb{R}^{b \times p \times s}$ downsampled s times. For inference, each keypoint is located by finding the pixel with the highest value in its predicted heatmap. We denote the labeled and unlabeled training sets as $\mathcal{D}^L = \{(\mathbf{I}_i^L, \mathbf{H}_i^L)\}_{i=1}^N$ and $\mathcal{D}^U = \{(\mathbf{I}_i^U)\}_{i=1}^M$, respectively. Here, the \mathbf{I}_i^L or \mathbf{I}_i^U means a labeled or unlabeled image sample, respectively. And N or M is the total number of image samples. The \mathbf{H}_i^L are ground-truth heatmaps generated using 2D keypoints. For supervised training of the network \mathcal{F} , we calculate

$$\mathcal{L}_s = \mathbb{E}_{\mathbf{I} \in \mathcal{D}^s} \|f(T_s(\mathbf{I})) - T_s(\mathbf{H})\|^2, \quad (1)$$

where T_x represents an easy affine augmentation including a random rotation angle from $[-30^\circ, 30^\circ]$ and scale factor from $[0.75, 1.25]$ (denoted as $T_{(30)}$). For unlabeled images, we calculate the unsupervised consistency loss:

$$\mathcal{L}_g = \mathbb{E}_{\mathbf{I} \in \mathcal{D}^*} \|T_{c+h}(f(T_c(\mathbf{I}))) - f(T_h(\mathbf{I}))\|^2, \quad (2)$$

where T_h is a harder augmentation with stronger perturbations than affine-based T_r . The T_r -sb, which is a known affine transformation on heatmaps if T_h contains additional rotation and scaling operations. In this way, we can obtain a paired easy-hard augmentations $(L_r, h_r) = (T_r(I_r), T_h(I_r))$ for generating corresponding teacher signals and student signals. During training, we should stop gradients propagation of teacher signals to avoid collapsing. Next, we answer two questions Q1 and Q2 by extensive empirical studies in Sec. [A7](#) and Sec. [A8](#), respectively. After that, we provide a theoretical perspective for understanding the pursuit of designing stronger augmentations in Sec. [A9](#).

3.1 PARADIGMS OF GENERATING SUPERIOR AUGMENTATIONS

Ranking of Basic Augmentations The core of the easy-hard pair paradigm (I_n, I_{n+1}) is a more advanced augmentation. For this reason, Dual Network (Xie et al., 2017) and SSPCM (Huang et al., 2019) propose pseudo-keypoint-based augmentations Joint Cutsout (T_{JC}) and Joint Cut Occlude (T_{JCO}), respectively. They also reach a similar yet crude conclusion about difficulty levels of existing augmentations: $\{T_{JC}, T_{JCO}\} \ll \{T_{TC}, T_{TCO}, T_{MC}, T_{MCO}, T_{MCU}, T_{MCUC}, T_{TCU}, T_{TCUC}\} \ll \{T_{MCU}, T_{MCUC}\}$. In this paper, we propose a new RandomAugment (Gulak et al., 2019), Cutout (DeVries and Selman, 2017) and Mixup (Zhang et al., 2018), where T_{MC} consists of two T_{JC} . We give them a new ranking by conducting more rigorous trainings one-by-one. The T_{MC} is removed for it contains repetitions with T_{JC} and T_{JCO} . As shown in Fig. 15 we divide the rest by their distinguishable gaps into four levels: $T_{JC}, T_{JCO} \ll \{T_{CO}, T_{TC}, T_{MCU}\} \ll T_{MCUC} \ll T_{TCU}$.

Synergy between Augmentations Then, instead of laboriously designing stronger augmentations, we consider to conduct two or more augmentations in sequence to obtain super combinations conveniently. This idea is feasible because it essentially belongs to the AutoAug families [Cubuk et al., 2018, 2019, Tan et al., 2019, Huaya et al., 2020, Zheng et al., 2020]. Instead of auto-searching, we expect to find some heuristic strategies for the HPE task. In fact, after performing joint-related T_{JO} and T_{JC} on one image, we can continue to perform some joint-unrelated augmentations (such as T_{CO} , T_{CC} and T_{MC}) on random areas. As shown in Fig. 3, applying T_{JO} (a T_{CO} after T_{JO}) or

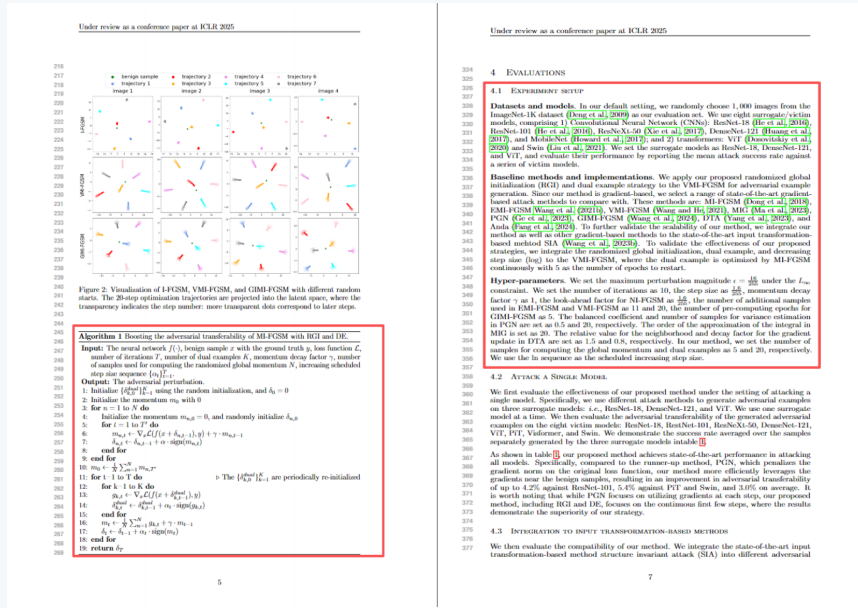
Question: Check the Methods section for Computation & Formulae errors.

Explanation: The Problem Definition section introduces core variables for the mathematical setup, including N and M for the sizes of the labeled and unlabeled datasets. On page 4, line 183, these are defined with the sentence: “And N or M is the total number of image samples.” This statement is ambiguous and fails to clearly define N and M individually. A reader cannot determine from this phrase that N is the number of labeled samples and M is the number of unlabeled samples. This notational ambiguity in the definition of variables that are fundamental to the subsequent equations and problem formulation constitutes a Computation & Formulae error, as key variables are left undefined or poorly defined.

Error Type: CF (Computation & Formulae)

Type: Within-Sample

Example2: 1909



Question: Scan the Methods section for Computation & Formulae errors.

Explanation: Algorithm 1 on page 5 uses the parameter T' in the loop definition on line 5: for $t = 1$ to T' do. This parameter determines the number of iterations for the Randomized Global Initialization phase. However, the value of T' is never specified anywhere in the paper, including the “Hyper-parameters” section (Section 4.1 on page 7). An algorithm cannot be implemented or reproduced with an undefined critical parameter. This fits the Computation & Formulae category as an “undefined variable”.

Error Type: CF (Computation & Formulae)

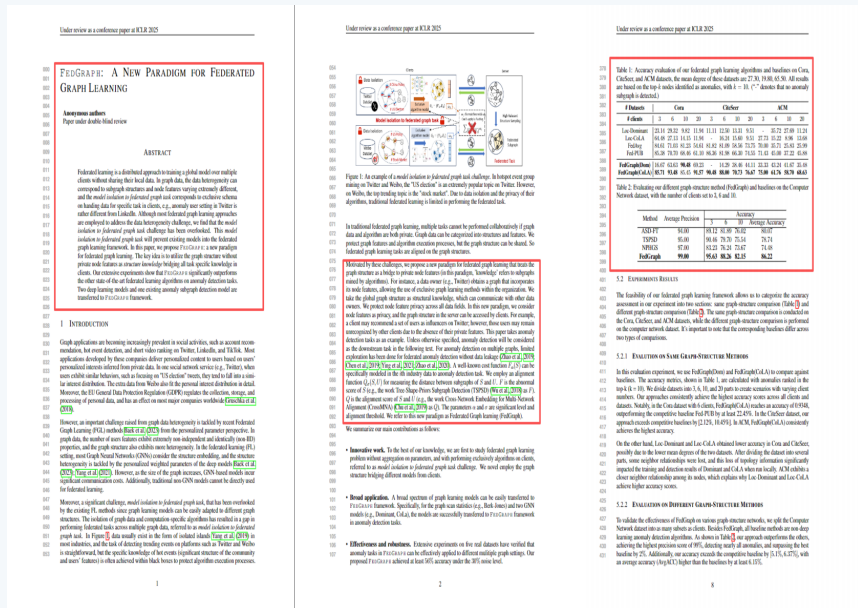
Type: Within-Sample

[illegible]

Explanation: The paper's evidence is based entirely on preclinical models (simulations, mice, rabbits, ex vivo porcine tissue). The edits in the Abstract and Discussion make strong, unhedged claims about setting a “new standard for clinical bioimaging” that is “ready for immediate adoption” in “human surgery.” These conclusions are a gross overstatement, as the preclinical data do not support such direct and immediate claims of clinical efficacy and adoption.

Type: Witin-Generate

Example2: 875



Question: Evaluate Abstract, Introduction and Experiment section for issues in Inference & Conclusions.

Explanation: The paper’s claims of generality are not supported by its evidence. The title and abstract introduce “FedGraph: A New Paradigm for Federated Graph Learning” (page 1), suggesting a broadly applicable framework. However, the methodology is heavily tailored to, and the experiments are exclusively focused on, the single downstream task of anomaly detection. For example, a stated contribution is “Broad application,” but this is immediately qualified with “the models are successfully transferred to FEDGRAPH framework in anomaly detection tasks” (page 2). Furthermore, Section 5, “EXPERIMENTS”, exclusively reports results on anomaly detection tasks. This discrepancy represents an issue of Inference & Conclusions, as the broad conclusion of having created a new “paradigm” for FGL is an overstatement that exceeds what the narrow experimental results can support.

Error Type: IC (Inference & Conclusions)

Type: Within-Sample

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3.2 BLOCK PARALLELISM WITH A GENERALIZED ASYNCHRONOUS TEMPLATE

THUNDERKITTENS helps developers reduce overheads by coordinating howworkers in block asynchronously overlap execution. Though the GPU hierarchy might suggest the wide variety of techniques, we propose a single concise template that we find enables manance on a surprisingly broad range of AI workloads. We first define the template, we steps – load compute-store-finish (LCSF) for short – and builds on the classical prod paradigm (Dijkstra, 1968; Bauer et al., 2011). We show how the LCSF template can be the tradeoffs between occupancy and efficiency (reducing CHM, Cores in Section 2).

Figure 5: A simplified depiction of attention in the LCSF template to highlight the role of different specialized workers. Left is executed by workers that manage HBM to SRAM memory movement, and right by parallel compute workers, which operate in fast memory, registers and SRAM.

1. **Load function.** Specifies the data that load workers should load from HBM to shared memory, and when to signal to compute workers that this memory is ready for use.
2. **Compute function.** Specifies the kernel instructions that compute workers should execute, using the data structure and operation primitives from Section 3.1.
3. **Store function.** Specifies what data workers need to store to HBM.
4. **Finish function.** At the end of the kernel, the workers store any final state and exit.

Multi-stage buffer: The template maintains N stage pipeline buffers in shared memory, which are used for loads and stores from IBM. Load/store workers address the buffers in the buffer list, which contains the indices of compute workers. With a single stage, load workers would need to wait for all compute workers to finish execution before replacing the input tile. A 2-stage buffer can be used to reduce the wait time. The input tile can asynchronously load, while the compute workers execute on the current tile. Deep buffers can reduce the synchronization required across compute workers, allowing them to operate on multiple tiles concurrently. TK lets the user set a single number for the number of buffers to use for the user. For example, if the user sets 2 for the number of buffers, Section 3.2 we vary the number of stages $N \in \{1, 2, 3, 4\}$ for our GEMM kernel.	4096	2	484
	4096	3	683
	4096	4	760

Published as a conference paper at ICLR 2025

Tradeoffs between occupancy and efficiency TP parametrizes the number of load/store and compute workers (or occupancy) providing a simple way for developers tune their kernels. As discussed in Section 2, higher occupancy increases overlapping, but creates contention over limited hardware resources (e.g., registers). With fewer registers, workers need to operate on smaller tiles of data, resulting in more instruction issues, SRAM to register ID, and potentially higher synchronization overheads due to the increased data partitioning across workers.

We find the general LCSF template to be effective across a range of AI workloads. We keep the template lightweight and simple by making opinionated design choices. However, we don't want TK to get in the way of achieving peak GPU performance – TK is *embedded*, meaning developers can use the full power of CUDA to extend the library as warranted.

TK makes it easier for users to quickly try varied grid layouts and coordinate thread block launches. This can help reduce the setup and tear-down costs for each thread block (C_{setup} in Section 3), and encourage memory reuse between thread blocks, to avoid slow HBM accesses (C_{reuse} in Section 2).

4096	64	93	108	69
4096	128	161	184	133
4096	256	271	309	242
4096	512	414	450	407
4096	1024	565	600	633

L2 reuse and block launch order Recall that thread blocks need to communicate via HBM. As introduced in Section 3, when thread blocks reuse memory, the data is often available in L2 cache, which is significantly faster than HBM. However, cache eviction means that these reuse qualities depend on the order in which blocks get launched. For our attention and GEMM kernels, we measure efficiency as we vary block order, summarized in Table 3. Block order substantially affects L2 reuse (measured through HBM bandwidth), which in turn can control kernel performance.

Explanation: The paper introduces a key contribution, the ‘load-compute-store-finish’ template, and its acronym ‘LCSF’. This error introduces inconsistencies in this critical term: it’s defined as ‘LCS-F’ on page 6, called ‘LCFS’ in a figure title on page 7, and written out in full in the conclusion on page 10, while the original ‘LCSF’ acronym remains elsewhere. This terminological inconsistency for a central, paper-defined concept creates ambiguity and undermines the paper’s precision.

Type: Within-Generate

Example2: 293

Under review as a conference paper at ICLR 2025

REGULARIZED OPTIMAL TRANSPORT FOR SINGLE-CELL TEMPORAL TRAJECTORY ANALYSIS

Anonymous authors
Paper under double-blind review

ABSTRACT

The temporal relationship between different cellular states and lineages is only partially understood and has major significance for cell differentiation and cancer progression. However, two pain points persist and limit learning-based solutions: (i) lack of real datasets and standardized benchmark for early cell development; (ii) the complicated transcriptional data fed classic temporal analysis. We integrate *Recover-102*, a large-scale mouse retinal ganglion cell dataset with annotations for 9 time stages and 20,000 gene expressions. Existing approaches show a limited generalization of our datasets. To tackle the modeling bottleneck, we then translate this fundamental biology problem into a machine learning formulation (i.e., one-point trajectory analysis). An innovative regularized optimal transport algorithm, *TRIOPT*, is proposed to fill in the research gap, consisting of (1) continuous ranked autoencoder to extract high-quality cell representations; (2) cost function regularization through biology priors for distribution transport; (3) continuous temporal trajectory optimization based on discrete matched time stages. Extensive empirical investigations demonstrate that our framework produces superior cell lineages and pseudotime, compared to existing approaches on *Recover-102*, and another two public benchmarks. Moreover, *TRIOPT* is capable of identifying biologically meaningful gene sets along with the developmental trajectory, and its standard gene knockout results echo the findings in physical wet lab validation.

1 INTRODUCTION

Since first introduced in 2009, large-scale single-cell RNA sequencing (scRNA-seq) has presented enormous opportunities for researchers in various research fields (Pau et al., 2014; Satija et al., 2015; Tsim et al., 2019). It helps reveal detailed information on transcriptional patterns in different cell and tissue types as well as disease models (Eisenstein et al., 2020; Izquierdo et al., 2022). Equipped with scRNA-seq, we are able to discover significant heterogeneities that would never be found with bulk analysis within the cell population, which contributes to understanding biology questions with higher cellular resolution. The first-adopting technology and increased recognition of different cell subtypes also naturally lead us to ask: “How and when are the cell subtypes established?” “Could we predict the developmental trajectory of each cell and predict the cell ‘jour’ based on current states?” “But could we find the key regulator that controls this type of establishment?” Answer to these questions are important for cell differentiation research in developmental biology (Hiro et al., 2017; Han et al., 2018; Galati et al., 2020) and can provide promising pipelines to demystify the cellular response during disease progression (Zhang et al., 2022; Jia et al., 2022). In the past decade, although a great amount of effort (Trapnell et al., 2014; Qin et al., 2017; Ji et al., 2018; Street et al., 2018; Cao et al., 2019) has been put into developing trajectory inference methods using single-cell sequencing data, it remains extremely challenging. This is because, with current technologies, we can not trace the same population of cells over developmental time. It only allows us to collect the transcriptional information of cells for a specific time point as a

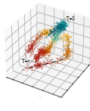


Figure 1: Demo Cell Temporal Trajectory Inference. The plot shows the developmental trajectory of cells, with the color gradient representing different time stages. The axes are labeled 'Time' and 'Gene Expression'.

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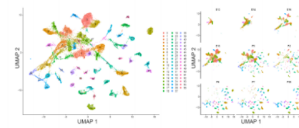


Figure 3: (Left) Clustering results for 50 kinds of cell types and projecting them into a 2D space via UMAP. (Right) Decomposing the clustering results by their time stage labels. Zoom in for better reliability.

Data Collection. For the *Recover-102* dataset, we extract 30K mouse neuron cells from previously published datasets (Shekhar et al., 2022; Whitney et al., 2023) and newly formed data. The developmental time stages of E13.5, E14, E16, E18, P0, P2, P4, P7, P14 (Figure 4). Then, the corresponding gene expressions are measured by the RNA sequencing technique as previously defined. Single-cell libraries were prepared using the single-cell gene expression 3' kit on the Chromium platform (10X Genomics, Pleasanton, CA) following the manufacturer’s protocol. To be specific, single cells were partitioned into Gel beads in Emulsion (GEMs) in the 10X Chromium instrument followed by cell lysis and barcoded reverse transcription of RNA, amplification, cDNA fragmentation, 7’ adapter attachment, and sample indexing. On average, around 8,000 ~ 12,000 single cells were loaded on each channel, and around 3,000 ~ 7,000 cells were recovered. Libraries were sequenced on the Illumina HiSeq 2,500 platforms.

3.2 SINGLE CELL DATA PROCESS

Preprocess and Properties. After we collected the raw signals, the following single-cell sequencing data preprocessing was done using the Scanpy package (Hao et al., 2023). Sample quality control was performed on each sample individually. For each sample, doublets were removed using DoubletFinder (McGinnis et al., 2019). We retained cells that expressed at least 1,500 genes and less than 11,000 genes. Meanwhile, we removed cells that have more than 5% mitochondrial genes and genes expressed in fewer than 10 cells. The resulting n cells \times g genes matrix of UMI counts were subject to downstream analysis. The UMI-based gene expression matrix was normalized using scranNorm (Hafemeister & Satija, 2019). After that, the batch correction was done with canonical correlation analysis (Hochberg, 1992; Anderson et al., 1958), using the top 4,000 anchor genes.

Clustering. In this research, we are interested in the evolution of different cell types of mouse neurons. Therefore, we built a nearest-neighbor graph to cluster cells based on their transcriptional similarity. Specifically, the number of nearest neighbors was chosen to be 50, according to the rich experiences of biology scientists. The edges were weighted based on the Jaccard overlap metric, and graph clustering was performed using the Leiden algorithm (Hendrick et al., 2020). In the end, as demonstrated in Figure 3 (Left), the cell clusters were then projected onto a nonlinear 2D space using the Uniform Manifold Approximation and Projection (UMAP) algorithm (McInnes et al., 2018). For temporal trajectory analysis, we further decomposed the cell clusters by their time stage labels like Figure 3 (Right). Our goal is to diversify the neuron evolution path across these 9 time stages. Referring Appendix B.2 for more details.

Question: Review the Abstract and Methods sections for Language & Expression problems.

Explanation: The paper uses the phrase “gene expressions” ambiguously, creating confusion about the size and composition of the dataset. The abstract mentions integrating a dataset with “30,000 gene expressions” (page 1, line 016), which is repeated on page 2 (contains 30,000 gene expressions). This phrasing could be misinterpreted as 30,000 unique genes being measured. The Data Collection section later clarifies that the dataset actually consists of “30K mouse neuron cells” (page 4, line 181). This inconsistent terminology affects the meaning of a critical domain quantity (the number of samples), making it a Language & Expression error.

Error Type: LE (Language & Expression)

Type: Within-Sample

F HUMAN-MACHINE CONSISTENCY EVALUATION

As described in Section 4.1, we employ GPT-4.1 to extract detailed information (*e.g.* evidence sets, reasoning chains) from the responses generated by the models under evaluation. Subsequently, based on the formulas presented in Section 4.1, we calculate S_{location} and $S_{\text{reasoning}}$, which are then used to derive S_{total} for each model’s response to the given question.

To evaluate whether GPT-4.1 accurately extracts detailed information from the model responses, we conduct a human-Machine consistency evaluation. We first randomly sampled 200 questions from the dataset. Then, we invited human experts to analyze the corresponding model-generated responses for these questions and to manually extract key information, including evidence sets, reasoning chains, and the number of unrelated errors.

	S_{total}	S_{location}	$S_{\text{reasoning}}$	$P_{\text{unrelated_err}}$
Spearman’s correlation coefficients	0.841	0.806	0.842	0.954

Table 4: Spearman’s correlation coefficients for: S_{total} , S_{location} , $S_{\text{reasoning}}$, and $P_{\text{unrelated_err}}$.

Using the information extracted by the human experts, we perform the following calculations:

- (1) The $\vec{S}_{\text{location}}$ vector for the 200 questions is calculated based on the evidence sets and Equation 3.
- (2) The $\vec{S}_{\text{reasoning}}$ vector is computed from the reasoning chains and Equation 4.
- (3) The $\vec{P}_{\text{unrelated_err}}$ vector is obtained from the count of unrelated errors.
- (4) The \vec{S}_{total} vector is calculated for the 200 questions using Equation 6.

Subsequently, these human-derived vectors ($\vec{S}_{\text{location}}$, $\vec{S}_{\text{reasoning}}$, $\vec{P}_{\text{unrelated_err}}$, and \vec{S}_{total}) are compared against their counterparts generated by GPT-4.1. Spearman’s correlation coefficient is then calculated for these four metrics. The results are presented in Table 4.

Among the four Spearman correlation coefficients, the metric $P_{\text{unrelated_err}}$ exhibits the highest correlation. This indicates that GPT-4.1’s extraction of unrelated errors closely aligns with that of human experts, making it the most precise among the three types of extracted information (*i.e.* evidence sets, reasoning chains, and unrelated errors).

Although the correlation coefficients for the *evidence location score* and *reasoning process score* are relatively lower than $P_{\text{unrelated_err}}$, they still fall within the range of strong positive correlation. This demonstrates a high degree of consistency in the numerical trends of the scores calculated from GPT-4.1 and human expert extractions, respectively, proving that GPT-4.1 is capable of extracting the majority of effective evidence sets and reasoning chains.

The correlation for the *total score* also lies within the strong positive range and slightly surpasses the correlations for the evidence location score. This also reflects a high level of agreement between GPT-4.1 and human experts.

In summary, GPT-4.1 can extract relevant evidence and reasoning steps with considerable accuracy, leading to precise evaluation scores. This validates the effectiveness of our methodology, which uses GPT-4.1 to parse the responses of the models under evaluation.