



Article

# **Evaluating Large Language Models for Structured Science Summarization in the Open Research Knowledge Graph**

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Abstract: Structured science summaries or research contributions using properties or dimensions beyond traditional keywords enhance science findability. Current methods, such as those used by the Open Research Knowledge Graph (ORKG), involve manually curating properties to describe research papers' contributions in a structured manner, but this is labor-intensive and inconsistent among human domain-expert curators. We propose using Large Language Models (LLMs) to automatically suggest these properties. However, it is essential to assess the readiness of LLMs like GPT-3.5, Llama 2, and Mistral for this task before their application. Our study performs a comprehensive comparative analysis between the ORKG's manually curated properties and those generated by the aforementioned state-of-the-art LLMs. We evaluate LLM performance from four unique perspectives: semantic alignment with and deviation from ORKG properties, fine-grained property mapping accuracy, SciNCL embedding-based cosine similarity, and expert surveys comparing manual annotations with LLM outputs. These evaluations occur within a multidisciplinary science setting. Overall, LLMs show potential as recommendation systems for structuring science, but further fine-tuning is recommended to improve their alignment with scientific tasks and mimicry of human expertise.

Keywords: large language models; Open Research Knowledge Graph; structured summarization



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# 1. Introduction

The exponential growth in scholarly publications poses a significant challenge for researchers seeking to efficiently explore and navigate the vast landscape of the scientific literature [1]. This proliferation of publications necessitates the development of strategies that go beyond traditional keyword-based search methods to facilitate effective and strategic reading practices. In response to this challenge, the structured representation of scientific papers has emerged as a valuable approach to enhancing FAIR research discovery and comprehension. By describing research contributions in a structured, machine-actionable format with respect to the salient properties of research, also regarded as research dimensions, similarly structured papers can be easily compared, offering researchers a systematic and quick snapshot of research progress within specific domains, thus providing them with efficient ways to stay updated with research progress.

One notable initiative aimed at publishing structured representations of scientific papers is the Open Research Knowledge Graph (ORKG, https://orkg.org/ accessed on 23 April 2024) [2]. The ORKG endeavors to describe papers in terms of various research dimensions or properties. Furthermore, a distinguishing characteristic of the properties is that they are also generically applicable across various contributions on the same problem, thus making the structured paper descriptions comparable. We illustrate this with two examples. For instance, the properties "model family", "pretraining architecture", "number of parameters", "hardware used", etc., can be effectively applied to offer structured, machine-actionable summaries of research contributions on the research problem

"transformer model" in the domain of Computer Science (Figure 1). Thus, these properties can be explicitly stated as research comparison properties. As another example, papers with the research problem "DNA sequencing techniques" in the domain of Biology can be described as structured summaries based on the following properties: "sequencing platform", "read length in base pairs", "reagents cost", and "runtime in days" (Figure 2). This type of paper description provides a structured framework for understanding and contextualizing research findings.

Properties	OpenLLaMA: An Open Reproduction of LLaMA version1 - 2023	Introducing MPT-30B: Raising the bar for open-source foundation models Contribution 1 - 2023	OpenLLaMA: An Open Reproduction of LLaMA version2 - 2023
number of parameters	3B, 7B, 13B	30B	3B, 7B
maximum number of parameters (in million)	13000	30000	7000
hardware used	cloud TPU-v4	A100-40GB GPU H100-80GB GPU	cloud TPU-v4
hardware information	The models are trained on cloud TPU-v4s using EasyLM, a JAX based training pipeline we developed for training and finetuning large language models. We employ a combination of normal data parallelism and fully sharded data parallelism	The model was trained in three stages using the MosaicML Platform: (i) First it was trained on 440 A100-40GBs with a batch size of 1760. (ii) Then, on 216 A100-40GBs with a batch size of 1728. (iii) Training was completed on 256 H100-80GBs	

**Figure 1.** ORKG Comparison—Catalog of Transformer Models. This view is a snapshot of the full comparison published here https://orkg.org/comparison/R656113/, accessed on 23 April 2024.

Properties		Sequencing Techniques  Illumina Next Seq 500 - 2017	Sequencing Techniques  Illumina HiSeq 2500 RR - 2017	Sequencing Techniques  Illumina HiSeq 4000 - 2017
cost of machine in \$		250000	740000	900000
cost of resequencing a human genome with 30X coverage in \$		4410	6144	2400
cost per Gigabyte data output in \$		36.75	51.2	20
data output rate in Gigabyte per day		100	106.6	400
has research problem	*	comparison of DNA sequencing techniques	comparison of DNA sequencing techniques	comparison of DNA sequencing techniques
read length in base pairs (paired-end*)		150*	100*	150*
reads per run in Million		400	600	5000
reagents cost in \$		4410	6145	29900
runtime in days		1.2	1.125	3.5
sequencing platform	▼	Illumina Next Seq 500	Illumina HiSeq 2500 RR	Illumina HiSeq 4000

**Figure 2.** ORKG Comparison—Survey of sequencing techniques. This view is a snapshot of the full comparison published here https://orkg.org/comparison/R44668/, accessed on 23 April 2024.

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Notably, however, the predominant method in the ORKG for creating structured paper descriptions or research comparisons is manually performed by domain experts. This means that domain experts, based on their prior knowledge and experience on a research problem, select and describe the research comparison properties. While this ensures the high quality of the resulting structured papers in the ORKG, the manual annotation cycles cannot effectively scale the ORKG in practice. Specifically, the manual extraction of these salient properties of research or research comparison properties presents two significant challenges: (1) manual annotation is a time-consuming process, and (2) it introduces inconsistencies among human annotators, potentially leading to variations in interpretation and annotation.

To address the challenges associated with the manual annotation of research comparison properties, this study tests the feasibility of using pretrained Large Language Models (LLMs) to automatically suggest or recommend research dimensions as candidate properties as a viable alternative solution. Specifically, three different LLM variants, viz., GPT-3.5-turbo [3], Llama 2 [4], and Mistral [5], are tested and empirically compared for their advanced natural language processing (NLP) capabilities when applied to the task of recommending research dimensions as candidate properties. Our choice to apply LLMs is based on the following experimental consideration. The multidisciplinary nature of scientific research poses unique challenges to the identification and extraction of salient properties across domains. In this context, we hypothesize that LLMs, with their ability to contextualize and understand natural language at scale [6,7], are particularly well suited to navigate the complexities of interdisciplinary research and recommend relevant dimensions that capture the essence of diverse scholarly works. By automating the extraction process, LLMs aim to alleviate the time constraints associated with manual annotation and ensure a higher level of consistency in the specification of research dimensions by using the same system prompt or fine-tuning on gold-standard ORKG data to better align them with the task. The role of LLMs in this context is to assist human domain-expert annotators rather than replace them entirely. By leveraging the capabilities of LLMs, researchers can streamline the process of dimension extraction and enhance the efficiency and reliability of comparative analysis across diverse research fields.

In this context, the central **research question** (**RQ**) is aimed at examining the performance of state-of-the-art LLMs in recommending research dimensions: specifically, "how good are LLMs in performing this task?" Can they replace humans? To address this RQ, we compiled a *multidisciplinary*, *gold-standard dataset of human-annotated scientific papers from the Open Research Knowledge Graph (ORKG)*, detailed in the Materials and Methods Section (see Section 3.1). This dataset includes structured summary property annotations made by domain experts. We conducted a detailed comparative evaluation of domain-expertannotated properties from the ORKG against the dimensions generated by LLMs for the same papers. This dataset is the first main contribution of this work. Furthermore, our central **RQ** is examined with regard to the following four unique perspectives:

- 1. Semantic alignment and deviation assessment by GPT-3.5 between ORKG properties and LLM-generated dimensions;
- 2. The fine-grained property mapping accuracy of GPT-3.5;
- 3. SciNCL [8] embedding-based cosine similarity between ORKG properties and LLM-generated dimensions;
- 4. A survey with human experts comparing their annotations of ORKG properties with the LLM-generated dimensions.

These evaluations as well as the resulting perspectives then constitute the second main contribution of this work.

Overall, the contribution of this work is a comprehensive set of insights into the readiness of LLMs to support human annotators in the task of structuring their research contributions. Our findings reveal a moderate alignment between LLM-generated dimensions and manually annotated ORKG properties, indicating the potential for LLMs to learn from human-annotated data. However, there is a noticeable gap in the mapping of dimensions generated by LLMs

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versus those annotated by domain experts, highlighting the need for fine-tuning LLMs on domain-specific datasets to reduce this disparity. Despite this gap, LLMs demonstrate the ability to capture the semantic relationships between LLM-generated dimensions and ORKG properties, particularly in a zero-shot setting, as evidenced by the strong correlation results of embedding similarity. In the survey, the human experts noted that while they were not ready to change their existing property annotations based on the LLM-generated dimensions, they highlighted the utility of the auto-LLM recommendation service at the time of creating the structured summary descriptions. This directly informs a future research direction for making LLMs fit for structured science summarization.

The structure of the rest of this paper is as follows: Section 2 provides a brief summary of related work. In Section 3—the Materials and Methods Section—we start by detailing our materials, including the creation of an evaluation dataset. We then describe our methodology, beginning with brief technical introductions to the three language models selected for this study. We also discuss the evaluation methods that we used, outlining three key types of similarity assessments performed between ORKG properties and LLM-generated research dimensions. Additionally, we introduce a human assessment survey that compares ORKG properties with LLM-generated dimensions. In Section 4—the Results and Discussion Section—we provide an in-depth analysis of each evaluation's outcomes. Finally, Section 5 summarizes our findings, discusses their implications, and proposes future research avenues.

#### 2. Related Work

LLMs in Scientific Literature Analysis. The utilization of LLMs for various NLP tasks has seen widespread adoption in recent years [9,10]. Within the realm of scientific literature analysis, researchers have explored the potential of LLMs for tasks such as generating summaries and abstracts of research papers [11,12], extracting insights and identifying patterns [13], aiding in literature reviews [14], enhancing knowledge integration [15], etc. However, the specific application of LLMs for recommending research dimensions to obtain structured representations of research contributions is a relatively new area of investigation that we explore in this work. Furthermore, to offer insights into the readiness of LLMs for our novel task, we perform a comprehensive set of evaluations comparing the LLM-generated research dimensions and the human-expert-annotated properties. As a straightforward preliminary evaluation, we measure the semantic similarity between the LLM and human-annotated properties. To this end, we employ a specialized language model tuned for the scientific domain to create embeddings for the respective properties.

Various Scientific-Domain-Specific Language Models. The development of domain-specific language models has been a significant advancement in NLP. In the scientific domain, a series of specialized models have emerged. SciBERT, introduced by Beltagy et al. [16], was the first language model tailored for scientific texts. This was followed by SPECTER, developed by Cohan et al. [17]. More recently, Ostendorff et al. introduced SciNCL [8], a language model designed to capture the semantic similarity between scientific concepts by leveraging pretrained BERT embeddings. In this study, to ensure comprehensiveness, we tested all the mentioned variants of language models. Our goal was to project ORKG properties and LLM-generated dimensions into a scientific embedding space, which served as a tool to evaluate their similarity.

Evaluating LLM-Generated Content. In the context of evaluating LLM-generated dimensions against manually curated properties, several studies have employed similarity measures to quantify the relatedness between the two sets of textual data. One widely used metric is cosine similarity, which measures the cosine of the angle between two vectors representing the dimensions [18]. This measure has been employed in various studies, such as Yasunaga et al. [19], who used cosine similarity to assess the similarity between summaries automatically generated by LLMs and human-written annotations. Similarly, Banerjee et al. [20] employed cosine similarity as a metric to benchmark the accuracy of LLM-generated answers of autonomous conversational agents. In contrast to

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cosine similarity, other studies have explored alternative similarity measures for evaluating LLM-generated content. For instance, Jaccard similarity measures the intersection over the union of two sets, providing a measure of overlap between them [21]. This measure has been employed in tasks such as document clustering and topic modeling [22,23]. Jaccard similarity offers a distinct perspective on the overlap between manually curated and LLM-generated properties, as it focuses on the shared elements between the two sets rather than their overall similarity. We considered both cosine and Jaccard similarity in our evaluation; however, based on our embedding representation, we ultimately chose to use cosine similarity as our distance measure.

Furthermore, aside from the straightforward similarity computations between the two sets of properties, we also leverage the capabilities of LLMs as evaluators. The utilization of LLMs as evaluators in various NLP tasks has been proven to be a successful approach in a number of recent publications. For instance, Kocmi and Federmann [24] demonstrated the effectiveness of GPT-based metrics for assessing translation quality, achieving state-of-the-art accuracy in both reference-based and reference-free modes. Similarly, the Eval4NLP 2023 shared task, organized by Leiter et al. [25], explored the use of LLMs as explainable metrics for machine translation and summary evaluation, showcasing the potential of prompting and score extraction techniques to achieve results on par with or even surpassing recent reference-free metrics. In our study, we employ the GPT-3.5 model as an evaluator, leveraging its capabilities to assess the quality, from its own judgment of semantic correspondence, of LLM-generated research dimensions with the human-curated properties in the ORKG.

In summary, previous research has laid the groundwork for evaluating LLMs' performance in scientific literature analysis, and our study builds upon these efforts by exploring the application of LLMs for recommending research dimensions and evaluating their quality using specialized language models and similarity measures.

# 3. Materials and Methods

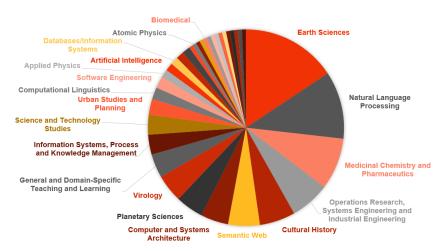
This section is organized into three subsections. In the first subsection, the creation of the gold-standard evaluation dataset from the ORKG with human-domain-expertannotated research comparison properties used to assess their similarity to LLM-generated properties is described. The second subsection provides an overview of the three LLMs, viz., GPT-3.5, Llama 2, and Mistral, applied to automatically generate the research comparison properties, highlighting their respective technical characteristics. Lastly, the third subsection discusses the various evaluation methods used in this study, offering differing perspectives on the similarity comparison of ORKG properties for the instances in our gold-standard dataset versus those generated by the LLMs.

# 3.1. Material: Our Evaluation Dataset

As alluded to in the Introduction, answering the central **RQ** of this work requires comparing the research dimensions generated by three different LLMs with the human-annotated research comparison properties in the ORKG. For this, we created an evaluation dataset of annotated research dimensions based on the ORKG. As a starting point, we curated a selection of ORKG Comparisons from <a href="https://orkg.org/comparisons">https://orkg.org/comparisons</a> (accessed on 23 April 2024) that were created by experienced ORKG users. These users had varied research backgrounds. The selection criteria for comparisons from these users were as follows: the comparisons had to have at least 3 properties and contain at least 5 contributions, since we wanted to ensure that the properties were not too sparse a representation of a research problem but were those that generically reflected a research comparison over several works. Upon the application of these criteria, the resulting dataset comprised 103 ORKG Comparisons. These selected gold-standard comparisons contained 1317 papers from 35 different research fields addressing over 150 distinct research problems. The gold-standard dataset can be downloaded from the Leibniz University Data Repository at <a href="https://doi.org/10.25835/6oyn9d1n">https://doi.org/10.25835/6oyn9d1n</a> (accessed on 23 April 2024). The selection of compar-

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isons ensured the diversity of the research fields' distribution, comprising Earth Sciences, Natural Language Processing, Medicinal Chemistry and Pharmaceutics, Operations Research, Systems Engineering, Cultural History, Semantic Web, and others. See Figure 3 for the full distribution of research fields in our dataset.



**Figure 3.** Research field distribution of the selected papers in our evaluation dataset containing human-domain-expert-annotated properties that were applied to represent the paper's structured contribution descriptions in the Open Research Knowledge Graph (ORKG).

Once we had the comparisons, we then looked at the individual structured papers within each comparison and extracted their human-annotated properties. Thus, our resulting dataset is highly multidisciplinary, comprising structured paper instances from the ORKG with their corresponding domain-expert property annotations across different fields of research. For instance, the properties listed below were extracted from the comparison "A Catalog of Transformer Models" (Figure 1):

```
["has model", "model family", "date created", "organization", "innovation", "pretraining architecture", "pretraining task", "fine-tuning task", "training corpus", "optimizer", "tokenization", "number of parameters", "maximum number of parameters (in million)", "hardware used", "hardware information", "extension", "has source code", "blog post", "license", "research problem"]
```

Another example of structured papers' properties in the comparison "Survey of sequencing techniques" (Figure 2) is as follows:

```
["cost of machine in $", "cost of resequencing a human genome with 30% coverage in $", "cost per Gigabyte data output in $", "data output rate in Gigabyte per day", "has research problem", "read length in base pairs (paired-end*) ", "reads per run in Million", "reagents cost in $", "runtime in days", "sequencing platform", "total data output yield in Gigabyte"]
```

The aforementioned dataset is now the gold standard that we use in the evaluations for the LLM-generated research dimensions. In this section, we provide a clear distinction between the terms *ORKG properties* and *LLM-generated research dimensions*. According to our hypothesis, ORKG properties are not necessarily identical to research dimensions. Contribution properties within the ORKG relate to specific attributes or characteristics associated with individual research papers in a comparison, outlining aspects such as authorship, publication year, methodology, and findings. Conversely, research dimensions encapsulate the multifaceted aspects of a given research problem, constituting the nuanced

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themes or axes along which scholarly investigations are conducted. ORKG contribution properties offer insights into the attributes of individual papers, whereas research dimensions operate at a broader level, revealing the finer-grained thematic fundamentals of research endeavors. While ORKG contribution properties focus on the specifics of research findings, research dimensions offer a more comprehensive context for analyzing a research question that can be used to find similar papers that share the same dimensions. In order to test the alignment of LLM-generated research dimensions with ORKG properties, several LLMs were selected for comparison, as described in the next section.

#### 3.2. Method: Three Large Language Models Applied for Research Dimension Generation

In this section, we discuss the LLMs applied for automated research dimension generation as well as the task-specific prompt that was designed as the input to the LLM.

#### 3.2.1. The Three LLMs

To test the automated generation of research dimensions, we tested and compared the outputs of three different state-of-the-art LLMs with comparable parameter counts, namely, GPT-3.5, Llama 2, and Mistral.

GPT-3.5, developed by OpenAI, is one of the most influential LLMs to date. Its number of parameters is not publicly disclosed [26]. In comparison, its predecessor GPT-3 models come in different sizes and contain from 125 million parameters for the smallest model to 175 billion for the largest [10]. GPT-3.5 has demonstrated exceptional performance on a range of NLP tasks, including translation, question answering, and text completion. Notably, the capabilities of this model are accessed through the OpenAI API since the model is closed-source, which limits direct access to its architecture for further exploration or customization.

Llama 2 by Meta AI [4], the second iteration of the Llama LLM, represents a significant advancement in the field. Featuring twice the context length of its predecessor, Llama 1 [27], Llama 2 offers researchers and practitioners a versatile tool for working with NLP. Importantly, Llama 2 is available free of charge for both research and commercial purposes, with multiple parameter configurations available, including a 13-billion-parameter option. In addition, the model supports fine-tuning and self-hosting, which enhances its adaptability to a variety of use cases.

Mistral, developed by Mistral AI, is a significant competitor in the landscape of LLMs. With a parameter count of 7.3 billion, Mistral demonstrates competitive performance on various benchmarks, often outperforming Llama 2 despite its smaller size [5]. In addition, Mistral is distinguished by its open-source code, released under the Apache 2.0 license, making it easily accessible for research and commercial applications. Notably, Mistral has an 8k context window, which allows for a more complete understanding of context compared to the 4k context window of Llama 2 [28].

Overall, GPT-3.5, despite its closed-source nature, remains influential in NLP research, with a vast number of parameters that facilitate its generic task performance in the context of a wide variety of applications. Conversely, Llama 2 and Mistral, with their open-source nature, provide flexibility and accessibility to researchers and developers while displaying similar performance characteristics to GPT [29]. Released shortly after Llama 2, Mistral, in particular, shows notable performance advantages over Llama 2, highlighting the rapid pace of innovation and improvement in the development of LLMs. These differences between models lay the groundwork for assessing their alignment with manually curated properties from the ORKG and determining their potential for automated research metadata creation and the retrieval of related work.

To effectively utilize the capabilities of these LLMs, we employed various computational resources and APIs. GPT-3.5 was accessed via the OpenAI API, which allowed us to harness its extensive capabilities through cloud-based infrastructure. This setup facilitated efficient and scalable interactions with the model. For the Llama 2 and Mistral models, we used the GPU cluster at our organization at TIB and the L3S Research Centre.

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This cluster includes a range of GPUs, such as NVIDIA series 1080 ti, 2080 ti, RTX 8000, and RTX A5000. The LLMs were accessed through the Ollama API (accessed on 23 April 2024), enabling the deployment and execution of the LLMs on our dedicated hardware. This GPU cluster provided the necessary computational power to meet the demands of running these models, ensuring robust performance for our evaluation tasks. The GPUs were selected based on the resources available in our server at the time of each specific experiment. By integrating these APIs and computational infrastructures, we were able to efficiently leverage the strengths of each LLM within the constraints of our resources.

#### 3.2.2. Research Dimension Generation Prompts for the LLMs

An LLM's performance on a particular task is highly dependent on the quality of the prompt. To find the optimal prompt methodology, our study explores various established prompting techniques, including zero-shot [30], few-shot [10], and chain-of-thought prompting [31]. The simplest type of prompt is a zero-shot approach, wherein pretrained LLMs, owing to the large-scale coverage of human tasks within their pretraining datasets, demonstrate competence in task execution without prior exposure to specific examples. While zero-shot prompting provides satisfactory results for certain tasks, some of the more complex tasks require few-shot prompting. By providing the model with several examples, few-shot prompting enables in-context learning, potentially enhancing model performance. Another popular technique is chain-of-thought prompting, which instructs the model to think step-by-step. Guiding the LLM through sequential steps helps to break down complex tasks into manageable components that are easier for the LLM to complete.

In this study, the task involves providing the LLM with a research problem, and based on this input, the model should suggest research dimensions that it finds relevant to structure contributions from similar papers that address the research problem. Our system prompts for each technique, along with examples of output for the research problem "Automatic text summarization" from GPT-3.5, are shown in Table 1.

**Table 1.** Prompt variations utilizing different prompt engineering techniques to instruct LLMs for the research dimension generation task.

Prompting Technique	System Prompt	Output Example
Zero-Shot	You will be provided with a research problem, your task is to list dimensions that are relevant to find similar papers for the research problem.  Respond only in the format of a python list.	["Natural Language Processing", "Text Analysis", "Machine Learning", "Deep Learning", "Information Retrieval", "Artificial Intelligence", "Language Models", "Document Summarization"]
Few-Shot	You will be provided with a research problem, your task is to list dimensions that are relevant to find similar papers for the research problem. Respond only in the format of a python list. The following are two successfully completed task examples.  Research problem: "Transformer models" Research dimensions: ["model", "date created", "pretraining architecture", "pretraining task", "training corpus", "optimizer", "tokenization", "number of parameters", "license"]  Research problem: "Liposomes as drug carriers" Research dimensions: ["Type of nanocarrier", "Nanoparticle preparation method", "Lipid composition", "Drug type", "Particle size"]	["Summarization approach", "Document type", "Language", "Evaluation metric", "Model type", "Training dataset", "Compression ratio", "Summary length"]

Table 1. Cont.

Prompting Technique	System Prompt	Output Example
Chain-of-Thought	You will be provided with a research problem, your task is to list dimensions that are relevant to find similar papers for the research problem. Provide justification why each dimension is relevant for finding similar papers. Think step-by-step. At the end combine all the relevant dimensions in the format of a python list.	["Task/Methodology", "Domain/Genre", "Evaluation Metrics", "Language", "Input/Output Format", "Deep Learning/Traditional Methods", "Applications"]

Our analysis shows that the utilization of more advanced prompting techniques did not necessarily result in superior outcomes, which leads us to believe that our original zero-shot prompt is sufficient for our task's completion. The absence of discernible performance improvements with the adoption of more complex prompting techniques highlights the effectiveness of the initial zero-shot prompt in aligning with the objectives of research dimension extraction. Consequently, we apply the zero-shot prompt methodology.

To test the alignment of LLM-generated research dimensions with ORKG properties, each of the LLMs was given the same prompt to create a list of dimensions that are relevant for finding similar papers based on the provided research problem. Table 2 shows the comparison between some of the manually created properties from the ORKG and the research dimensions provided by GPT-3.5, Llama 2, and Mistral.

**Table 2.** A comparison of manually created ORKG properties with LLM-generated research dimensions for the same papers.

Research Problem	ORKG Properties	GPT-3.5 Dimensions	Llama 2 Dimensions	Mistral Dimensions
https://orkg.org/ comparison/R141123/ (accessed on 23 April 2024), Limestone mineral identification using Hyperion imagery	"Data used", "Research problem", "Study Area", "Software", "Analysis", "Processing", "Field instrument", "Reference"	"Mineralogy", "Limestone", "Hyperion imagery", "Identification"	"Remote Sensing", "Hyperspectral Imaging", "Mineral Identification", "Limestone", "Hyperion Imagery", "Geological Mapping", "Image Classification", "Spectral Analysis", "Earth Observation", "Geoscience"	"Limestone", "Mineral identification", "Remote sensing", "Hyperion imagery", "Spectral signatures", "Band ratios", "Textural features", "Shape descriptors", "Machine learning algorithms", "Support Vector Machines", "Decision trees", "Random forests"
https://orkg.org/ comparison/R204005/ (accessed on 23 April 2024), Do human noroviruses infect animals	"Material", "Method", "Symptoms and signs", "Research problem", "Species", "Location", "Antigen used", "Immunoglobulin class", "Primers"', "Noroviruses found', "Norovirus genotype"	"viral infectivity", "host range", "cross-species transmission", "zoonotic potential"	"Host species", "Viral genotype", "Transmission route", "Infection prevalence", "Pathogenesis", "Diagnostic methods", "Epidemiology", "Evolutionary history", "Interaction with other pathogens", "Public health implications"	"Norovirus", "Animals", "Transmission", "Species", "Symptoms", "Epidemiology", "Serotypes", "Immunity", "Detection methods", "Genome analysis"

3.3. Method: Three Types of Similarity Evaluations between ORKG Properties and LLM-Generated Research Dimensions

This section outlines the methodology used to evaluate our dataset, namely, the automated evaluation of semantic alignment and deviation, as well as mapping between ORKG properties and LLM-generated research dimensions performed by GPT-3.5. Additionally,

we present our approach to calculating the embedding similarity between properties and research dimensions.

#### 3.3.1. Semantic Alignment and Deviation Evaluations Using GPT-3.5

To measure the semantic similarity between ORKG properties and LLM-generated research dimensions, we conducted semantic alignment and deviation assessments using an LLM-based evaluator. In this context, semantic alignment refers to the degree to which two sets of concepts share similar meanings, whereas semantic deviation assesses how far apart they are in terms of meaning. As the LLM evaluator, we leveraged GPT-3.5. As input, it was provided with both the lists of properties from ORKG and the dimensions extracted by the LLMs in a string format per research problem. Semantic alignment was rated on a scale from 1 to 5, using the following system prompt to perform this task:

You will be provided with two lists of strings, your task is to rate the semantic alignment between the lists on the scale form 1 to 5. Your response must only include an integer representing your assessment of the semantic alignment, include no other text.

Additionally, the prompt included a detailed description of the scoring system shown in Table 3.

**Table 3.** Descriptions of the semantic alignment scores provided in the GPT-3.5 system prompt.

Score	Description
1—Strongly Disaligned	The strings in the lists have minimal or no semantic similarity.
2—Disaligned	The strings in the lists have limited semantic alignment.
3—Neutral	The semantic alignment between the lists is moderate or average.
4—Aligned	The strings in the lists show substantial semantic alignment.
5—Strongly Aligned	The strings in the lists exhibit high semantic coherence and alignment.

To further validate the accuracy of our alignment scores, we leveraged GPT-3.5 as an evaluator again but this time to generate semantic deviation scores. By using this contrastive alignment versus deviation evaluation method, we can cross-reference where the LLM evaluator displays a strong agreement in its evaluation and assess the evaluations for reliability. Specifically, we evaluate the same set of manually curated properties and LLM-generated research dimensions using both agents, with the expectation that the ratings will exhibit an inverse relationship. In other words, high alignment scores should correspond to low deviation scores, and vice versa. The convergence of these opposing measures would provide strong evidence for the validity of our evaluation results. Similar to the task of alignment rating, the system prompt below was used to instruct GPT-3.5 to measure semantic deviation, and the ratings described in Table 4 were also part of the prompt.

You will be provided with two lists of strings, your task is to rate the semantic deviation between the lists on the scale form 1 to 5. Your response must only include an integer representing your assessment of the semantic deviation, include no other text.

Table 4. Descriptions of the semantic deviation scores provided in the GPT-3.5 system prompt.

Score	Description
1—Minimal Deviation	The strings in the lists show little or no semantic difference.
2—Low Deviation	The semantic variance between the lists is limited.
3—Moderate Deviation	There is a moderate level of semantic difference between the strings in the lists.
4—Substantial Deviation 5—Significant Deviation	The lists exhibit a considerable semantic gap or difference. The semantic disparity between the lists is pronounced and substantial.

By combining these two evaluations, we can gain a more nuanced understanding of the relationship between the ORKG properties and LLM-generated research dimensions.

#### 3.3.2. ORKG Property and LLM-Generated Research Dimension Mappings by GPT-3.5

To further analyze the relationships between ORKG properties and LLM-generated research dimensions, we used GPT-3.5 to find the mappings between individual properties and dimensions. This approach diverges from the previous semantic alignment and deviation evaluations, which considered the lists as a whole. Instead, we instructed GPT-3.5 to identify the number of properties that exhibit similarity to individual research dimensions. This was achieved by providing the model with the two lists of properties and dimensions and prompting it to count the number of similar values between the lists.

The system prompt used for this task was as follows:

You will be provided with two lists of strings, your task is to count how many values from list1 are similar to values of list2.

Respond only with an integer, include no other text.

By leveraging GPT-3.5's capabilities in this manner, we were able to count the number of LLM-generated research dimensions that are related to individual ORKG properties. The mapping count provides a more fine-grained insight into the relationships between the properties and dimensions.

### 3.3.3. Scientific Embedding-Based Semantic Distance Evaluations

To further examine the semantic relationships between ORKG properties and LLM-generated research dimensions, we employed an embedding-based approach. Specifically, we utilized SciNCL to generate vector embeddings for both the ORKG properties and the LLM-generated research dimensions. These embeddings were then compared using cosine similarity as a measure of semantic similarity. We evaluated the similarity of ORKG properties to the research dimensions generated by GPT-3.5, Llama 2, and Mistral. Additionally, we compared the LLM-generated dimensions to each other, providing insights into the consistency and variability of the research dimensions generated by different LLMs. By leveraging embedding-based evaluations, we were able to quantify the semantic similarity between the ORKG properties and the LLM-generated research dimensions, as well as among the dimensions themselves.

# 3.3.4. Human Assessment Survey Comparing ORKG Properties with LLM-Generated Research Dimensions

We conducted a survey to evaluate the utility of LLM-generated dimensions in the context of domain-expert-annotated ORKG properties. The survey was designed to solicit the impressions of domain experts when shown their original annotated properties versus the research dimensions generated by GPT-3.5. We selected participants who are experienced in creating structured paper descriptions in the ORKG. These participants included ORKG curation grant participants (https://orkg.org/about/28/Curation\_Grants (accessed on 23 April 2024)), ORKG employees, and authors whose comparisons were displayed on the ORKG Featured Comparisons page at https://orkg.org/featured-comparisons, accessed on 23 April 2024. Each participant was given up to 5 surveys, one for each of 5 different papers that they structured. Each survey evaluated the properties of a paper against it's research dimensions. Participants could choose to complete one, some, or all of the surveys. At the end, we received 23 total responses to our survey, corresponding to 23 different papers.

The survey itself consisted of five questions, most of which were designed on a Likert scale, to gauge the domain expert's assessment of the effectiveness of the LLM-generated research dimensions. For each survey, as evaluation data, participants were presented with two tables: one including their annotated ORKG property names and values (Figure 4) and another one consisting of the research dimension name, its description, and value

generated by GPT-3.5 from a title and abstract of the same paper (Figure 5). Following these data was the survey questionnaire. The questions asked participants to rate the relevance of LLM-generated research dimensions, consider making edits to the original ORKG structured contribution, and evaluate the usefulness of LLM-generated content as suggestions before creating their structured contributions. Additionally, participants were asked to describe how LLM-generated content would have been helpful and rate the alignment of LLM-generated research dimensions with the original ORKG structured contribution. The survey questionnaire is shown below:

- 1. How many of the properties generated by ChatGPT are relevant to your ORKG structured contribution? (Your answer should be a number)
- 2. Considering the ChatGPT-generated content, would you consider making edits to your original ORKG structured contribution?
- 3. If the ChatGPT-generated content were available to you as suggestions before you created your structured contribution, would it have been helpful?
  - (a) If you answered "Yes" to the question above, could you describe how it would have been helpful?
- 4. On a scale of 1 to 5, please rate how well the ChatGPT-generated response aligns with your ORKG structured contribution.
- 5. We plan to release an AI-powered feature to support users in creating their ORKG contributions with automated suggestions. In this context, please share any additional comments or thoughts you have regarding the given ChatGPT-generated structured contribution and its relevance to your ORKG contribution.

ļ	Property Name	Property Value	
	data source research problem Data coverage Data domains	Journal of Biological Chemistry (JBC) extract text fragments to support the annotation of a given protein- GO term association Scholarly article full-text Molecular Biology	
l	Coarse-grained Entity types Number of training data mentions	Biological process   Biological Process GO Terms	l
i	Number of test data mentions	Protein	İ
-	Annotation type	Gold-standard data	1

Figure 4. An example of ORKG properties shown to survey respondents.

ļ	Property Name	Property Description	Property Value	
ĺ	Research Theme   Background		Evaluation of BioCreAtIVE assessment of task 2 Large scale analysis approaches using bioinformatics or experimental techniques	
	Need	Text mining tools to facilitate extra	Useable in real world scenarios to assist database curators	i
- 1	Results   Participants		Based on triplets of protein-GO term-article passage More than 15,000 individual results provided	
į	Evaluation	Expert curators evaluated annotation	Promising results but still far from required performance	ĺ
	Difficulties   Dataset		Various strategies used to tackle the task Allows new possibilities for training information extraction methods	

Figure 5. An example of GPT dimensions shown to survey respondents.

The subsequent section will present the results obtained from these methodologies, providing insights into the similarity between ORKG properties and LLM-generated research dimensions.

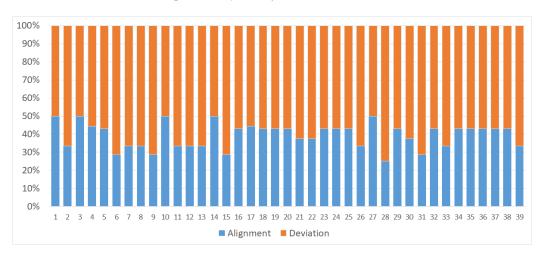
# 4. Results and Discussion

This section presents the results of our evaluation, which aimed to assess the LLMs' performance in the task of recommending research dimensions by calculating the similarity between ORKG properties and LLM-generated research dimensions. We employed three types of similarity evaluations: semantic alignment and deviation assessments, property and research dimension mappings using GPT-3.5, and embedding-based evaluations using SciNCL.

# 4.1. Semantic Alignment and Deviation Evaluations

The average alignment between paper properties and research field dimensions was found to be 2.9 out of 5, indicating a moderate level of alignment. In contrast, the average

deviation was 4.1 out of 5, suggesting a higher degree of deviation. When normalized, the proportional values translate to 41.2% alignment and 58.8% deviation (Figure 6). These results imply that, while there is some alignment between paper properties and research field dimensions, there is also a significant amount of deviation, highlighting the difference between the concepts of structured papers' properties and research dimensions. This outcome supports our hypothesis that LLM-based research dimensions generated solely from a research problem, relying on LLM-encoded knowledge, may not fully capture the nuanced inclinations of domain experts when they annotate ORKG properties to structure their contributions, where the domain experts have the full paper at hand. We posit that an LLM not explicitly tuned to the scientific domain, despite its vast parameter space, is not able to emulate a human expert's subjectivity to structure contributions.



**Figure 6.** Proportional values of semantic alignment and deviation between ORKG properties and GPT-generated dimensions.

# 4.2. Property and Research Dimension Mappings

We examine our earlier posited claim in a more fine-grained manner by comparing the property versus research dimension mappings. The average number of mappings was found to be 0.33, indicating a low number of mappings between paper properties and research field dimensions. The average ORKG property count was 4.73, while the average GPT dimension count was 8. These results suggest that LLMs can generate a more diverse set of research dimensions than the ORKG properties, but with a lower degree of similarity. Notably, the nature of ORKG properties and research dimensions differs in their scope and focus. Common ORKG properties like "research problem", "method", "data source", and others provide valuable information about a specific paper, but they cannot be used to comprehensively describe a research field as a whole. In contrast, research dimensions refer to the shared properties of a research question, rather than focus on an individual paper. This difference contributes to the low number of mappings between paper properties and research field dimensions, which further supports our conjecture that an LLM based only on its own knowledge applied to a given research problem might not be able to completely emulate a human expert's subjectivity in defining ORKG properties. These results, therefore, are not a direct reflection of the inability of the LLMs tested to recommend suitable properties to structure contributions on the theme. This then opens the avenue for future work to explore how LLMs fine-tuned on the scientific domain perform in the task as a direct extension of our work.

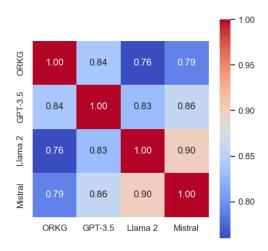
#### 4.3. Embedding-Based Evaluations

The embedding-based evaluations provide a more nuanced perspective on the semantic relationships between the ORKG properties and the LLM-generated research dimensions. By leveraging the SciNCL embeddings, we were able to quantify the cosine similarity between these two concepts, offering insights into their alignment. The results indicate a high

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degree of semantic similarity, with the cosine similarity between ORKG properties and the LLM-generated dimensions reaching 0.84 for GPT-3.5, 0.79 for Mistral, and 0.76 for Llama 2. These values suggest that the LLM-generated dimensions exhibit a strong correlation with the manually curated ORKG properties, signifying a substantial semantic overlap between the two.

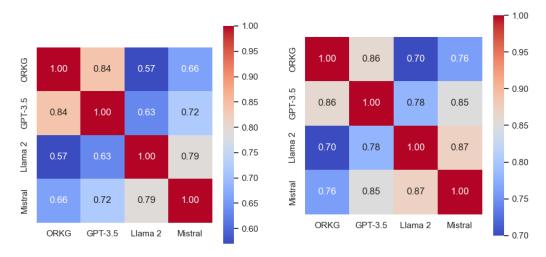
Furthermore, the correlation heatmap (Figure 7) provides a visual representation of these similarities, highlighting the strongest correlations between ORKG properties and LLM-generated dimensions. The embedding-based evaluations indicate that GPT-3.5 demonstrates the highest similarity to the ORKG properties, outperforming both Llama 2 and Mistral. When comparing LLM-generated dimensions between these models, the strong similarity observed between the Llama 2 and Mistral dimensions highlights the remarkable consistency in the research dimensions generated by these two models.



**Figure 7.** Correlation heatmap of cosine similarity between SciNCL embeddings of ORKG properties and LLM-generated dimensions.

To further validate our findings, we extended our evaluations using SciBERT and SPECTER embeddings in addition to SciNCL. These additional embeddings provided similar results, reinforcing the reliability of our conclusions. Specifically, using SPECTER embeddings, the cosine similarity between the ORKG properties and the LLM-generated dimensions was 0.86 for GPT-3.5, 0.70 for Llama 2, and 0.76 for Mistral. With SciBERT embeddings, the cosine similarity values were 0.84 for GPT-3.5, 0.57 for Llama 2, and 0.66 for Mistral (Figure 8). These consistent results across different embedding models highlight the robustness of the LLMs' capacity to generate research dimensions that are semantically aligned with the manually curated ORKG properties.

Overall, the embedding-based evaluations provide a quantitative representation of the semantic relationships between the ORKG properties and the LLM-generated research dimensions. These results suggest that, while there are notable differences between the two, the LLMs exhibit a strong capacity to generate dimensions that are semantically aligned with the manually curated ORKG properties, particularly in the case of GPT-3.5. This finding highlights the potential of LLMs to serve as valuable tools for automated research metadata creation and the retrieval of related work.



(a) SciBERT embeddings

(b) SPECTER embeddings

**Figure 8.** Correlation heatmap of cosine similarity between embeddings of ORKG properties and LLM-generated dimensions.

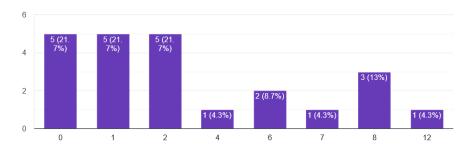
#### 4.4. Human Assessment Survey

To further evaluate the utility of the LLM-generated research dimensions, we conducted a survey to solicit feedback from domain experts who annotated the properties to create structured science summary representations or structured contribution descriptions in the ORKG. The survey was designed to assess the participants' impressions when presented with their original ORKG properties alongside the research dimensions generated by GPT-3.5.

For the first question in the questionnaire assessing the relevance of LLM-generated dimensions for creating a structured paper summary or structuring the contribution of a paper, on average, 36.3% of the research dimensions generated by LLMs were considered highly relevant (Figure 9). This suggests that LLM-generated dimensions can provide useful suggestions for creating structured contributions in the ORKG. For the second question, the majority of participants (60.9%) did not think it was necessary to make changes to their existing ORKG structured paper property annotations based on the LLM-generated dimensions, indicating that, while the suggestions were relevant, they may not have been sufficient to warrant significant changes (Figure 10). However, based on the third question, the survey also revealed that the majority of authors (65.2%) believed that having LLMgenerated content as suggestions before creating the structured science summaries or structured contributions would have been helpful (Figure 11). The respondents noted that such LLM-based dimension suggestions could serve as a useful starting point, provide a basis for improvement, and aid in including additional properties. Based on the fourth question, the alignment between LLM-generated research dimensions and the original ORKG structured contribution properties was rated as moderate, with an average rating of 2.65 out of 5 (Figure 12). This indicates that, while there is some similarity between the two, there is room for further alignment. As such, participants raised concerns about the specificity of generated dimensions potentially diverging from the actual goal of the paper. For the final question on the release of such an LLM-based feature, the respondents emphasized the importance of aligning LLMs based on the domain-expert property names while allowing descriptions to be generated, ensuring relevance across different research domains and capturing specific details like measurement values and units.

How many of the properties generated by ChatGPT are relevant to your ORKG structured contribution? (Your answer should be a number)

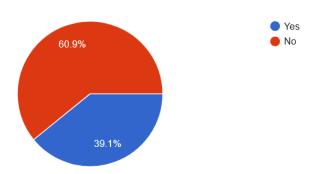
23 responses



**Figure 9.** Counts of the number of relevant LLM-generated research dimensions for structuring a paper's contribution or creating a structured science summary.

Considering the ChatGPT-generated content, would you consider making edits to your original ORKG structured contribution?

23 responses



**Figure 10.** The willingness of the participants to make changes to their existing annotated ORKG properties when shown the LLM-generated research dimensions.

If the ChatGPT-generated content were available to you as suggestions before you created your structured contribution, would it have been helpful?

23 responses

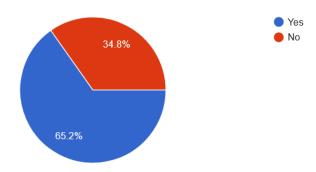


Figure 11. The utility of LLM-generated dimensions as suggestions.

On a scale of 1 to 5, please rate how well the ChatGPT-generated response aligns with your ORKG structured contribution.

22 responses

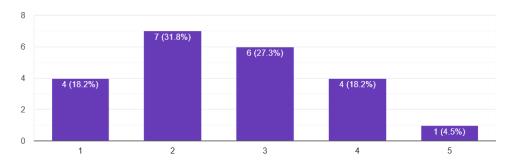


Figure 12. The alignment of LLM-generated dimensions with ORKG structured contributions.

Overall, the findings of the survey indicate that LLM-generated dimensions exhibited a moderate alignment with manually extracted properties. Although the generated properties did not perfectly align with the original contributions, they still provided valuable suggestions that authors found potentially helpful in various aspects of creating structured contributions for the ORKG. For instance, the suggestions were deemed useful in facilitating the creation of comparisons, identifying relevant properties, and providing a starting point for further refinement. However, concerns regarding the specificity and alignment of the generated properties with research goals were noted, suggesting areas for further refinement. These concerns highlight the need for LLMs to better capture the nuances of research goals and objectives in order to generate more targeted and relevant suggestions. Nonetheless, the overall positive feedback from participants suggests that AI tools, such as LLMs, hold promise for assisting users in creating structured research contributions and comparisons within the ORKG platform.

# 5. Conclusions

In this study, we investigated the performance of state-of-the-art Large Language Models (LLMs) in recommending research dimensions, aiming to address the central research question: How effectively do LLMs perform in the task of recommending research dimensions? Through a series of evaluations, including semantic alignment and deviation assessments, property and research dimension mappings, embedding-based evaluations, and a human assessment survey, we sought to provide insights into the capabilities and limitations of LLMs in this domain.

The findings of our study elucidated several key aspects of LLM performance in recommending research dimensions. First, our semantic alignment and deviation assessments revealed a moderate level of alignment between manually curated ORKG properties and LLM-generated research dimensions, accompanied by a higher degree of deviation. While LLMs demonstrate some capacity to capture semantic similarities, there are notable differences between the concepts of structured paper properties and research dimensions. This suggests that LLMs may not fully emulate the nuanced inclinations of domain experts when structuring contributions.

Second, our property and research dimension mapping analysis indicated a low number of mappings between paper properties and research dimensions. While LLMs can generate a more diverse set of research dimensions than ORKG properties, the degree of similarity is lower, highlighting the challenges in aligning LLM-generated dimensions with human-expert-curated properties.

Third, our embedding-based evaluations showed that GPT-3.5 achieved the highest semantic similarity between ORKG properties and LLM-generated research dimensions, outperforming Mistral and Llama 2 in that order.

Fourth and finally, our human assessment survey provided valuable feedback from domain experts, indicating a moderate alignment between LLM-generated dimensions and manually annotated properties. While the suggestions provided by LLMs were deemed potentially helpful in various aspects of creating structured contributions, concerns regarding specificity and alignment with research goals were noted, suggesting areas for improvement.

While this study provides valuable insights into the performance of LLMs in generating research dimensions, there are several limitations that should be acknowledged. Firstly, the LLMs used in this research are trained on a wide range of text, not exclusively the scientific literature, which may affect their ability to accurately generate research dimensions. Secondly, due to hardware limitations, we were unable to test larger LLM models, restricting our evaluation to small and medium-sized models. Furthermore, this work represents the first empirical investigation into this novel research problem, defining a preliminary paradigm for future research in this area. As such, our evaluation focused on state-of-the-art LLMs, serving as a stepping stone for future studies to explore a broader range of LLM architectures and scales. Moving forward, researchers should consider testing a diverse array of LLMs, including larger models and those specifically fine-tuned for scientific domains, to gain a more comprehensive understanding of their capabilities and limitations in generating research dimensions.

In conclusion, our study contributes to a deeper understanding of LLM performance in recommending research dimensions to create structured science summary representations in the ORKG. While LLMs show promise as tools for automated research metadata creation and the retrieval of related work, further development is necessary to enhance their accuracy and relevance in this domain. Future research may explore the fine-tuning of LLMs on scientific domains to improve their performance in recommending research dimensions.

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