
Boosting-Inspired Validation of Retrieval-Augmented Generation in Structured Scientific Knowledge Bases

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Abstract

1 Large Language Models (LLMs) enhanced with Retrieval-Augmented Generation
2 (RAG) achieve remarkable results, yet they often hallucinate or provide incomplete
3 answers. This poses critical challenges in scientific knowledge domains where
4 factuality and precision are essential. In this paper, we propose a boosting-inspired
5 evaluation framework for RAG that combines iterative error reduction with forward-
6 looking retrieval mechanisms from FLARE. Unlike existing work that primarily
7 optimizes retrieval or ranking, our focus is on the validation loop itself. We
8 validate the framework in a controlled scenario using Citavi, a structured literature
9 management system, serving as a reproducible environment for testing. Results
10 indicate that strict substring matching underestimates semantic correctness, while
11 boosting-inspired metrics highlight when expansion is necessary. This proof-
12 of-concept demonstrates technical feasibility and motivates iterative, semantic
13 validation for future scientific assistants.

14 ***Human Foreword***

15 This paper is a meta-experiment. It was created in a continuous collaboration where a human
16 researcher acted as supervisor and generative AI systems (ChatGPT-4 and GPT-5) took on the role of
17 creator of the scientific proof-of-concept. The entire workflow - from exploring the research question,
18 through drafting code and structuring the validation scenario, to producing the manuscript - was
19 conducted within a single ChatGPT chat.
20 To ensure transparency, the GitHub repository referenced in the acknowledgements provides open
21 access to the complete chat history (in German and English translation), the validation project, and
22 the Citavi test project.

23 **1 Introduction**

24 Large Language Models (LLMs) have rapidly advanced natural language processing and are increas-
25 ingly applied in scientific and industrial domains. Despite their remarkable capabilities, a persistent
26 challenge remains: LLMs tend to hallucinate, producing factually incorrect or unverifiable content
27 [1]. This shortcoming is particularly problematic in scientific knowledge bases, where accuracy,
28 reproducibility, and transparency are essential.

29 Retrieval-Augmented Generation (RAG) [2] mitigates this issue by combining parametric memory
30 stored in model weights with non-parametric memory retrieved from external corpora. While RAG
31 improves factual grounding, it lacks systematic validation loops to ensure that retrieved evidence
32 is sufficient and that generated answers remain reliable. In practice, validation is often reduced to
33 ranking metrics, leaving gaps in coverage and robustness unaddressed.

34 Boosting methods, such as Gradient Boosting [3] and XGBoost [4], demonstrate the effectiveness of
35 iteratively reducing residual errors. Similarly, FLARE [5] introduced forward-looking retrieval, in
36 which intermediate predictions guide expansion towards missing evidence. Both approaches highlight
37 the importance of iterative refinement, a principle not yet fully leveraged in RAG validation.
38 This paper is motivated by the need for reliable validation mechanisms in knowledge-intensive
39 environments. We therefore introduce a methodology that integrates boosting-inspired residual
40 tracking with FLARE-style expansion, enabling a dedicated evaluator for RAG. To examine its
41 feasibility, we conduct a pilot validation in a structured environment (Citavi), which provides
42 citations, abstracts, and hierarchical knowledge suitable for controlled testing. The results reveal
43 the limitations of strict string-matching metrics and highlight the necessity of semantic evaluation
44 for future iterations. Together, these contributions demonstrate the potential of boosting-inspired
45 validation as a new direction for improving the robustness of retrieval-augmented generation in
46 scientific knowledge bases.

47 2 Related Work

48 Our work builds on three main strands of research: ensemble learning and boosting, retrieval-
49 augmented models, and evaluation of hallucinations and factuality. Each area contributes important
50 foundations, yet none addresses the specific problem of designing validation loops for Retrieval-
51 Augmented Generation (RAG).

52 2.1 Boosting and Ensembles

53 Ensemble learning, and boosting in particular, has proven to be a powerful method for iterative
54 error reduction. Friedman introduced Gradient Boosting [3], which was later extended in practical
55 implementations such as XGBoost [4]. Further theoretical contributions, such as the comprehensive
56 review by Bühlmann and Hothorn [6], and the classic textbook by Hastie, Tibshirani, and Friedman
57 [7], emphasize the principle of repeatedly fitting residuals to improve predictive performance. This
58 principle inspires our evaluator design, which aims to detect and act upon coverage gaps in retrieved
59 evidence.

60 2.2 Retrieval-Augmented Models

61 In parallel, retrieval-augmented models have become central to modern language technologies. Lewis
62 et al. presented RAG [2], combining parametric knowledge embedded in model weights with non-
63 parametric retrieval. Guu et al. extended this line with REALM [8], where retrieval is interleaved
64 during pretraining, and Karpukhin et al. introduced Dense Passage Retrieval (DPR) [9]. Izacard and
65 Grave proposed Fusion-in-Decoder (FiD) [10], while Borgeaud et al. scaled retrieval to trillions of
66 tokens in RETRO [11]. More recently, Izacard et al. introduced FLARE [5], which uses forward-
67 looking predictions to actively expand retrieval. Dialogue-focused systems [12] and domain-specific
68 adaptations such as scientific question answering [13] illustrate the breadth of RAG applications.
69 These advances strengthen factual grounding, but none of them explicitly incorporates validation
70 mechanisms that monitor adequacy and completeness.

71 2.3 Corrective and Adaptive Retrieval

72 Corrective and adaptive retrieval approaches show growing awareness of this gap. Corrective Retrieval
73 Augmentation (CRA) [14] integrates error signals into retrieval, and Self-RAG [15] combines
74 retrieval, generation, and reflection in a unified loop. Adaptive retrieval methods [16] explore query
75 reformulation and contextual retrieval to minimize drift. All share conceptual ground with boosting
76 in that they iteratively improve results. However, their focus remains on generation rather than on
77 dedicated validation.

78 2.4 Learning to Rank

79 Learning-to-rank methods contribute another relevant dimension. LambdaMART [17] and listwise
80 approaches [18, 19] provide effective techniques for ranking retrieval candidates, while large-scale
81 challenges such as the Yahoo! Learning to Rank dataset [20] established benchmarks for progress.

82 These methods optimize retrieval quality but do not address the broader question of whether retrieved
83 evidence is sufficient to validate generated answers.

84 **2.5 Evaluation and Hallucinations**

85 Finally, evaluation of hallucinations and factuality in natural language generation has gained in-
86 creasing attention. Ji et al. surveyed hallucination phenomena [1], while Maynez et al. [21] and
87 Zhao et al. [22] analyzed factuality in summarization and question answering. Classical metrics
88 such as precision, recall, and nDCG [23] remain standard, yet they rely on strict string matching
89 and often underestimate semantic adequacy. Surveys of retrieval-augmented methods [24–26] and
90 benchmarks like BEIR [27] provide useful overviews, but none establish explicit validation loops.
91 Recent initiatives such as FEVER [28] and Izacard et al.’s active retrieval paradigm [29] further
92 underline the need for iterative, validation-oriented approaches.

93 Taken together, the literature reveals three key insights. Boosting highlights the power of iterative
94 error reduction, retrieval-augmented models enhance factual grounding, and evaluation research
95 exposes the limitations of current metrics. What is still missing is an integrated framework that
96 connects these strands by validating retrieval adequacy through iterative mechanisms. Closing this
97 gap is the objective of the methodology described in the following section.

98 **3 Methodology**

99 The goal of this work is to develop a validation framework for Retrieval-Augmented Generation
100 (RAG) that integrates principles from boosting and FLARE. Unlike prior research that primarily
101 optimizes retrieval or generation, our focus is on the evaluation loop itself: determining whether
102 retrieved evidence is sufficient, identifying residual gaps, and deciding when expansion is necessary.
103 The methodology is designed to be dataset-agnostic and can be applied to any structured knowledge
104 base. In this section we describe the design principles, system architecture, graph representation,
105 evaluator logic, and performance indicators before introducing the validation scenario in Section 4.

106 **3.1 Design Principles**

107 As discussed in Section 2, three strands of research motivate our design: boosting demonstrates
108 the power of iterative error reduction [3, 4, 6], retrieval-augmented models such as RAG, REALM,
109 and FLARE improve factual grounding [2, 8, 5], and evaluation studies expose the limitations of
110 current metrics [1, 21]. From boosting we adopt the idea of residual tracking: in each step, what
111 remains uncovered is treated as error to be addressed. From FLARE we adopt forward-looking
112 expansion: when residuals exceed a threshold, additional retrieval is triggered. Together, these
113 principles transform validation into an iterative process rather than a static one-time assessment.

114 **3.2 System Architecture**

115 The framework is organized into four stages. First, the *ingest stage* prepares structured input and
116 artifacts. Second, the *graph construction stage* initializes a knowledge graph that captures elements
117 and relations in a compact form. Third, the *retriever stage* combines sparse retrieval (BM25) with
118 dense embeddings for semantic similarity, similar to approaches in open-domain QA [9]. Finally, the
119 *evaluator stage* applies the boosting- and FLARE-inspired logic that distinguishes our approach from
120 existing retrieval systems.

121 **3.3 Graph Representation**

122 Knowledge is represented as a graph to enable transparency and incremental updates. Nodes
123 correspond to citations, documents, or categories, while edges capture references, group membership,
124 or hierarchical relations, as is common in knowledge graph construction [? ?]. The initial graph is
125 deliberately small, containing only citations and linked documents. Expansion introduces categories
126 or additional documents as new nodes, increasing search space and recall. By tracking which nodes
127 have been covered, the graph directly supports boosting-style residual measurement.

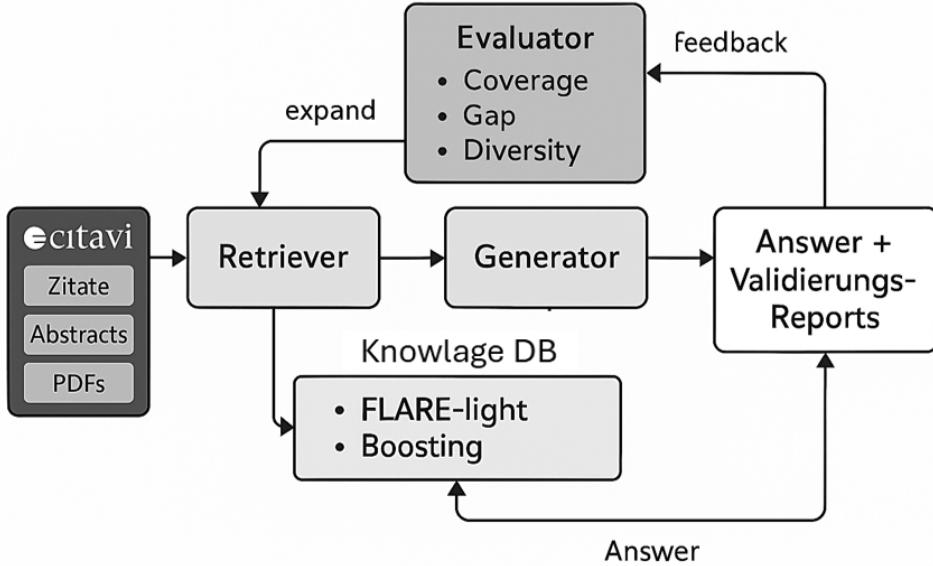


Figure 1: Workflow of the validation framework with Citavi input, RAG retrieval, and FLARE/boosting-inspired evaluation. The dataset-specific component (Citavi) is applied only in the validation scenario described in Section 4.

128 3.4 Evaluator Logic

129 The evaluator is the methodological core. Inspired by boosting, it calculates residuals by measuring
 130 the gap between retrieved evidence and gold references. Inspired by FLARE [5], it then decides
 131 whether to expand or stop: if the gap is large, the graph is expanded and retrieval is repeated; if
 132 coverage is sufficient, the loop halts. Related approaches such as Corrective Retrieval Augmentation
 133 (CRA) [14] and Self-RAG [15] share elements of this idea, but they focus on improving generation
 134 rather than providing a dedicated validation loop. Our evaluator reframes these principles as an
 135 explicit mechanism for adequacy checking.

136 3.5 Key Performance Indicators

137 Several key performance indicators operationalize validation. Coverage@ k measures whether gold
 138 evidence appears among the top- k retrieved items. Because strict matching is often too rigid, we
 139 extend this to *Semantic Coverage*, which uses cosine similarity in embedding space. Normalized
 140 Discounted Cumulative Gain (nDCG) [23] captures ranking quality and is widely applied in retrieval
 141 evaluation [27]. Two additional metrics extend FLARE principles: *Gap-FLARE* quantifies the
 142 proportion of uncovered evidence that should trigger expansion, and *Diversity-FLARE* measures
 143 the variance among retrieved results to avoid redundancy. Together, these indicators provide a
 144 multidimensional perspective on validation that goes beyond classical IR metrics.

145 3.6 Abstraction and Outlook

146 A crucial property of the methodology is that it remains independent of the specific dataset. It can be
 147 applied to enterprise document collections, scientific repositories, or any other structured corpus. In
 148 this paper, we use Citavi only as a controlled testbed to examine feasibility, not as part of the method
 149 itself. The overall workflow is illustrated in Figure 1, which also anticipates the next section where
 150 Citavi is introduced as the validation scenario.

151 4 Validation Scenario

152 The proposed methodology was validated in a controlled pilot study. The goal of this validation
 153 was not to achieve competitive performance, but to demonstrate the feasibility of boosting-inspired

154 evaluation in a structured environment. This section describes the scope and constants of the
155 experiment, the setup of the validation run, the role of Citavi as a structured testbed, the obtained
156 results, and their interpretation.

157 **4.1 Scope and Constants of the Validation**

158 The validation was deliberately constrained in order to focus on the core question of feasibility.
159 Several restrictions were imposed: iterative graph updates were disabled, the number of queries was
160 limited to five, and user feedback was excluded. These choices reduced complexity and ensured that
161 the experiment could be reproduced reliably.

162 Certain aspects of the setup were treated as constants. The graph was limited to citations and
163 documents, excluding higher-level categories. Citation types in Citavi served as proxy labels, which
164 avoided manual annotation but introduced rigidity. Retrieval was fixed to a combination of BM25
165 and embedding similarity. Together, these constants provided a stable environment, even though they
166 also introduced biases.

167 Within this controlled setting, the element under validation was the evaluator. The experiment was
168 designed to test whether boosting-inspired residual tracking and FLARE-style expand/stop logic
169 could be operationalized in practice. The consistent decisions made by the evaluator serve as evidence
170 of feasibility, even if the metrics themselves reveal limitations.

171 **4.2 Experimental Setup**

172 The validation run was implemented as a snapshot experiment. At initialization, a small graph was
173 constructed containing citations and their associated documents. Retrieval was carried out using
174 BM25 and dense embeddings, with the two lists merged before evaluation. The evaluator then
175 computed Coverage@5, Semantic Coverage, nDCG@5, Gap-FLARE, and Diversity-FLARE. Logs,
176 result CSV files, and summary JSON files were generated to provide full transparency of the run. In
177 total, five queries were executed, each paired with a gold citation to serve as reference evidence.

178 **4.3 Citavi as Structured Testbed**

179 Citavi was chosen as the validation environment because of its structured organization of knowledge.
180 Citations, abstracts, and full-text PDFs are stored in a unified project file, with categories and groups
181 providing additional hierarchical structure. These features map naturally onto graph representations:
182 citations and documents become nodes, while references and categories form edges. Furthermore,
183 citation types (direct quote, summary, paraphrase) function as proxy labels for relevance, allowing
184 evaluation without manual labeling. This makes Citavi an effective testbed for feasibility studies,
185 even though it is not part of the methodology itself.

186 **4.4 Results**

187 The outcomes of the validation run are summarized in Table 1. Exact string matching yielded no
188 correct hits, while semantic inspection revealed partial correctness in one case. In all cases, the
189 evaluator returned the decision to expand.

190 **4.5 Interpretation**

191 The validation run shows that the evaluator operated consistently and as designed. All five queries
192 resulted in expand decisions, reflecting the detection of residual gaps. Coverage@5 remained at
193 zero under strict string matching, while manual semantic inspection indicated partial adequacy in
194 at least one case. The gap between exact and semantic coverage demonstrates a limitation of the
195 applied metrics. These findings establish the technical feasibility of the evaluation loop and provide
196 the empirical basis for the broader discussion in Section 5.

Table 1: Validation setup, key performance indicators, and results. Gold labels are citations from the Citavi project. Coverage is reported for exact and semantic matching.

Query	Gold Label	Exact Cov.@5	Sem. Cov.@5	nDCG@5
What is FLARE?	FLARE iteratively uses a prediction	0	1	0.0
How does RAG combine memory?	RAG combines parametric memory	0	0	0.0
What is Gradient Boosting?	Gradient boosting is a generalization	0	0	0.0
What is LambdaMART?	LambdaMART combines gradient boosting	0	0	0.0
What does REALM interleave?	REALM interleaves knowledge retrieval	0	0	0.0

197 5 Discussion and Future Work

198 The validation presented in Section 4 provides a narrow but informative demonstration of the
 199 framework. In this section, we move beyond the specific scenario and discuss what the results imply
 200 for the methodology introduced in Section 3 and for the broader research gap identified in Section 2.

201 **5.1 Implications for the Methodology (Section 3)**

202 The validation confirmed that two central design elements of the methodology are operational:
 203 boosting-inspired residual tracking and FLARE-style expand/stop decisions. These findings support
 204 the feasibility of treating adequacy as a residual and of embedding expansion as a control mechanism
 205 in validation. At the same time, the scope of the experiment revealed which aspects of the methodology
 206 remain untested. Iterative updates, semantic coverage metrics, and richer graph representations were
 207 not exercised in the pilot run. Their absence does not invalidate the design, but highlights the
 208 areas where further empirical work is required. The validation therefore partially substantiates the
 209 methodology, while pointing to open components.

210 **5.2 Connection to the Research Gap (Section 2)**

211 The limitations observed in Section 4 resonate with prior critiques in the literature. Classical metrics
 212 such as Coverage and nDCG underestimated semantic adequacy, echoing findings from hallucination
 213 and factuality research [1, 21]. Benchmarks such as BEIR [27] have already called for richer
 214 evaluation, but they lack an explicit validation loop. Our framework contributes in this direction by
 215 treating validation as an iterative process, informed by residuals and expansion. While the Citavi
 216 pilot is minimal, it illustrates that the research gap identified in Section 2 can be addressed with a
 217 concrete operational design.

218 **5.3 Limitations of the Present Study**

219 The present study is constrained by deliberate design choices: a small number of queries, reliance on
 220 proxy labels, and the exclusion of iteration and user feedback. These restrictions were necessary to
 221 ensure reproducibility in a proof-of-concept, but they limit the generalizability of the results. The
 222 implication is not that the methodology is invalid, but that further studies are required to evaluate its
 223 robustness in larger and more diverse settings.

224 **6 Conclusion**

225 **6.1 Summary**

226 This paper proposed a validation framework for Retrieval-Augmented Generation (RAG) that inte-
 227 grates boosting-inspired residual tracking with FLARE-style expand/stop logic. The methodology

shifts the focus from optimizing retrieval or generation to validating adequacy itself, treating uncovered evidence as residuals and using expansion as a control mechanism.

A pilot validation in a Citavi-based testbed confirmed technical feasibility. The evaluator consistently identified residual gaps and triggered expand decisions, demonstrating that the two guiding principles of the methodology can be implemented in practice. At the same time, the restricted scope—five queries, proxy labels, no iterative updates—revealed limitations: classical string-based metrics such as Coverage@ k and nDCG underestimated semantic adequacy, and expand decisions could not influence retrieval outcomes. These findings establish a foundation for iterative, feedback-driven validation but stop short of a full performance benchmark.

6.2 Future Work

Future work will extend the framework along several directions. First, iterative cycles must be enabled so that residuals and expansion interact dynamically across multiple retrieval rounds. Second, semantic similarity measures will be integrated to capture adequacy beyond surface-level matching, ensuring that paraphrases and equivalent formulations are recognized. Third, richer graph structures should be employed, incorporating categories and cross-document relations to broaden coverage. Fourth, user feedback can be leveraged as an additional residual signal, bridging automated evaluation with practical relevance. Finally, the framework should be applied to larger and more diverse benchmarks such as BEIR as well as to industrial document collections, to assess robustness and scalability.

Taken together, these steps will move the approach from a controlled proof-of-concept toward a practical methodology for improving the reliability of retrieval-augmented generation in scientific and industrial contexts.

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315 **A Technical Appendices and Supplementary Material**

316 Technical appendices with additional results, figures, graphs and proofs may be submitted with the
317 paper submission before the full submission deadline, or as a separate PDF in the ZIP file below
318 before the supplementary material deadline. There is no page limit for the technical appendices.

319 **Agents4Science AI Involvement Checklist**

320 This checklist is designed to allow you to explain the role of AI in your research. This is important for
321 understanding broadly how researchers use AI and how this impacts the quality and characteristics
322 of the research. **Do not remove the checklist! Papers not including the checklist will be desk**
323 **rejected.** You will give a score for each of the categories that define the role of AI in each part of the
324 scientific process. The scores are as follows:

- 325 • **[A] Human-generated:** Humans generated 95% or more of the research, with AI being of
326 minimal involvement.
- 327 • **[B] Mostly human, assisted by AI:** The research was a collaboration between humans and
328 AI models, but humans produced the majority (>50%) of the research.
- 329 • **[C] Mostly AI, assisted by human:** The research task was a collaboration between humans
330 and AI models, but AI produced the majority (>50%) of the research.
- 331 • **[D] AI-generated:** AI performed over 95% of the research. This may involve minimal
332 human involvement, such as prompting or high-level guidance during the research process,
333 but the majority of the ideas and work came from the AI.

334 These categories leave room for interpretation, so we ask that the authors also include a brief
335 explanation elaborating on how AI was involved in the tasks for each category. Please keep your
336 explanation to less than 150 words.

337 **IMPORTANT,** please:

- 338 • **Delete this instruction block, but keep the section heading “Agents4Science AI Involve-**
339 **ment Checklist”,**
- 340 • **Keep the checklist subsection headings, questions/answers and guidelines below.**
- 341 • **Do not modify the questions and only use the provided macros for your answers.**

342 1. **Hypothesis development:** Hypothesis development includes the process by which you
343 came to explore this research topic and research question. This can involve the background
344 research performed by either researchers or by AI. This can also involve whether the idea
345 was proposed by researchers or by AI.

346 Answer: **[B]**

347 Explanation: The central idea – combining boosting-inspired validation with RAG and
348 using Citavi as the structured testbed – originated from the human researcher. Generative
349 AI contributed by exploring alternative framings and drafting formulations, but it required
350 significant clarification and supervision before aligning with the intended approach. Thus,
351 hypothesis development was primarily human-driven, with AI providing supportive input.

352 2. **Experimental design and implementation:** This category includes design of experiments
353 that are used to test the hypotheses, coding and implementation of computational methods,
354 and the execution of these experiments.

355 Answer: **[C]**

356 Explanation: The experimental design and implementation were generated mostly by AI.
357 Generative AI produced the Docker Compose setup, Python application code, and evaluator
358 logic for the validation loop. The human researcher supervised, ensured executability, and
359 applied minimal adjustments (e.g., correct handling of SQLite rows from Citavi and path
360 alignment). Thus, while the technical foundation came from AI, the human role was critical
361 for validation and final operability.

362 3. **Analysis of data and interpretation of results:** This category encompasses any process to
363 organize and process data for the experiments in the paper. It also includes interpretations of
364 the results of the study.

365 Answer: **[D]**

366 Explanation: The analysis of data and the interpretation of the results were carried out
367 exclusively by the generative AI. The AI processed the outputs of the validation experiments,
368 produced explanations, and articulated the interpretation of adequacy and gaps in coverage.

369 The human researcher did not perform independent analysis but only supervised the process
370 from a meta-level. Thus, data analysis and interpretation were exclusively AI-driven.

- 371 4. **Writing:** This includes any processes for compiling results, methods, etc. into the final
372 paper form. This can involve not only writing of the main text but also figure-making,
373 improving layout of the manuscript, and formulation of narrative.

374 Answer: **[D]**

375 Explanation: The entire writing process—including generation of text, creation of figures and
376 tables, and compilation of the reference list—was carried out exclusively by the generative
377 AI. The human researcher did not contribute to the manuscript text itself but acted only in a
378 supervisory role. Thus, the writing of the paper was exclusively AI-driven.

- 379 5. **Observed AI Limitations:** What limitations have you found when using AI as a partner or
380 lead author?

381 Description: The observed limitations of generative AI in this project were varied, but the
382 documentation also allows the reader to grasp them for themselves. The link to Github
383 with the entire chat history with ChatGPT, as well as the validation scenario and the paper,
384 is published in the acknowledgements for this paper. Because this chat history already
385 showed a strong trend toward a scientific feasibility review of a concept before the call was
386 launched, it was logical to make it available to your project. The following points from
387 the conversation were particularly noticeable: On the one hand, ChatGPT had difficulty
388 consistently reusing information throughout the entire workflow. For example, towards
389 the end, results from the beginning of the chat history were hardly considered during the
390 paper creation process. ChatGPT frequently relied on its pre-trained background knowledge
391 instead of using the provided project files. Only after explicit inquiries did ChatGPT indicate
392 that it would only superficially review the file. Particularly with papers used for training
393 and also considered in this project, it was impossible to deviate from existing knowledge.
394 Taking the direct approach without critically questioning assumptions, even though critical
395 doubt and methodological rigor are essential in scientific work, was the greatest difficulty in
396 this project. Towards the end of the process, repeated inquiries from the human supervisor
397 were necessary to ensure that the AI had partially considered the provided information
398 and integrated it into the paper. Post-correction for the paper was deliberately omitted.
399 The overall quality of the results was complete and assessable as an independent work
400 with strong support for, for example, an academic paper, but was more reminiscent of a
401 satisfactory bachelor's thesis grade 3.0, as it severely lacked depth, consistency, and critical
402 reflection. This was also influenced by the special setup: the entire workflow was carried
403 out in a single chat, from the brief idea of a term, its contextualization, deriving possible
404 synergies, identifying the use case and research question, and finally creating the paper itself.
405 In cases where individual steps are examined over several sessions, the process of creating a
406 scientific paper was deliberately followed from start to finish in a continuous dialogue. This
407 structure created a workflow similar to supervised student work: The human took on the role
408 of supervisor, while the AI took on the role of the students and was guided to do scientific
409 work. The AI was able to create depth for clearly defined sub-goals, but often lost the overall
410 overview and rushed into creating final versions, which is why several loops were created.
411 The ChatGPT fluctuated between superficial overviews and repeated refinements of simple
412 to-dos with limited added value. These dynamics—including strengths and weaknesses—are
413 documented in the chat transcript included in the repository formatted for readability.

414 **Agents4Science Paper Checklist**

415 The checklist is designed to encourage best practices for responsible machine learning research,
416 addressing issues of reproducibility, transparency, research ethics, and societal impact. Do not remove
417 the checklist: **Papers not including the checklist will be desk rejected.** The checklist should
418 follow the references and follow the (optional) supplemental material. The checklist does NOT count
419 towards the page limit.

420 Please read the checklist guidelines carefully for information on how to answer these questions. For
421 each question in the checklist:

- 422 • You should answer [Yes] , [No] , or [NA] .
- 423 • [NA] means either that the question is Not Applicable for that particular paper or the
424 relevant information is Not Available.
- 425 • Please provide a short (1–2 sentence) justification right after your answer (even for NA).

426 **The checklist answers are an integral part of your paper submission.** They are visible to the
427 reviewers and area chairs. You will be asked to also include it (after eventual revisions) with the final
428 version of your paper, and its final version will be published with the paper.

429 The reviewers of your paper will be asked to use the checklist as one of the factors in their evaluation.
430 While "[Yes]" is generally preferable to "[No]", it is perfectly acceptable to answer "[No]" provided
431 a proper justification is given. In general, answering "[No]" or "[NA]" is not grounds for rejection.
432 While the questions are phrased in a binary way, we acknowledge that the true answer is often more
433 nuanced, so please just use your best judgment and write a justification to elaborate. All supporting
434 evidence can appear either in the main paper or the supplemental material, provided in appendix.
435 If you answer [Yes] to a question, in the justification please point to the section(s) where related
436 material for the question can be found.

437 **IMPORTANT**, please:

- 438 • **Delete this instruction block, but keep the section heading "Agents4Science Paper**
439 **Checklist",**
- 440 • **Keep the checklist subsection headings, questions/answers and guidelines below.**
- 441 • **Do not modify the questions and only use the provided macros for your answers.**

442 **1. Claims**

443 Question: Do the main claims made in the abstract and introduction accurately reflect the
444 paper's contributions and scope?

445 Answer: [No]

446 Justification: The idea and solution approach are well structured, and the validation scenario
447 was chosen with a very strong scope. However, the results did not provide evidence that this
448 approach delivers clear added value.

449 Guidelines:

- 450 • The answer NA means that the abstract and introduction do not include the claims
451 made in the paper.
- 452 • The abstract and/or introduction should clearly state the claims made, including the
453 contributions made in the paper and important assumptions and limitations. A No or
454 NA answer to this question will not be perceived well by the reviewers.
- 455 • The claims made should match theoretical and experimental results, and reflect how
456 much the results can be expected to generalize to other settings.
- 457 • It is fine to include aspirational goals as motivation as long as it is clear that these goals
458 are not attained by the paper.

459 **2. Limitations**

460 Question: Does the paper discuss the limitations of the work performed by the authors?

461 Answer: [Yes]

462 Justification: The paper reflects openly on boundaries and challenges of the chosen proof-of-
463 concept scope, but these are discussed mainly in a general scientific reflection rather than
464 presented as method-specific limitations.

465 Guidelines:

- 466 • The answer NA means that the paper has no limitation while the answer No means that
467 the paper has limitations, but those are not discussed in the paper.
- 468 • The authors are encouraged to create a separate "Limitations" section in their paper.
- 469 • The paper should point out any strong assumptions and how robust the results are to
470 violations of these assumptions (e.g., independence assumptions, noiseless settings,
471 model well-specification, asymptotic approximations only holding locally). The authors
472 should reflect on how these assumptions might be violated in practice and what the
473 implications would be.
- 474 • The authors should reflect on the scope of the claims made, e.g., if the approach was
475 only tested on a few datasets or with a few runs. In general, empirical results often
476 depend on implicit assumptions, which should be articulated.
- 477 • The authors should reflect on the factors that influence the performance of the approach.
478 For example, a facial recognition algorithm may perform poorly when image resolution
479 is low or images are taken in low lighting.
- 480 • The authors should discuss the computational efficiency of the proposed algorithms
481 and how they scale with dataset size.
- 482 • If applicable, the authors should discuss possible limitations of their approach to
483 address problems of privacy and fairness.
- 484 • While the authors might fear that complete honesty about limitations might be used by
485 reviewers as grounds for rejection, a worse outcome might be that reviewers discover
486 limitations that aren't acknowledged in the paper. Reviewers will be specifically
487 instructed to not penalize honesty concerning limitations.

488 **3. Theory assumptions and proofs**

489 Question: For each theoretical result, does the paper provide the full set of assumptions and
490 a complete (and correct) proof?

491 Answer: [NA]

492 Justification: This paper does not contain formal theoretical results or proofs. It presents a
493 proof-of-concept study with generative AI and human supervision rather than theorem-driven
494 research.

495 Guidelines:

- 496 • The answer NA means that the paper does not include theoretical results.
- 497 • All the theorems, formulas, and proofs in the paper should be numbered and cross-
498 referenced.
- 499 • All assumptions should be clearly stated or referenced in the statement of any theorems.
- 500 • The proofs can either appear in the main paper or the supplemental material, but if
501 they appear in the supplemental material, the authors are encouraged to provide a short
502 proof sketch to provide intuition.

503 **4. Experimental result reproducibility**

504 Question: Does the paper fully disclose all the information needed to reproduce the main ex-
505 perimental results of the paper to the extent that it affects the main claims and/or conclusions
506 of the paper (regardless of whether the code and data are provided or not)?

507 Answer: [No]

508 Justification: The validation presented in the paper is rudimentary and yields only weak
509 results; reproducibility of the experiments is not ensured within the paper itself. While
510 the supplementary chat log and Citavi test project, as well as the GitHub reference in
511 the acknowledgements, provide useful material for further research on AI workflows, the
512 scientific question is only conceptually outlined and not supported by reproducible, verifiable
513 results.

514 Guidelines:

- 515 • The answer NA means that the paper does not include experiments.
 516 • If the paper includes experiments, a No answer to this question will not be perceived
 517 well by the reviewers: Making the paper reproducible is important.
 518 • If the contribution is a dataset and/or model, the authors should describe the steps taken
 519 to make their results reproducible or verifiable.
 520 • We recognize that reproducibility may be tricky in some cases, in which case authors
 521 are welcome to describe the particular way they provide for reproducibility. In the case
 522 of closed-source models, it may be that access to the model is limited in some way
 523 (e.g., to registered users), but it should be possible for other researchers to have some
 524 path to reproducing or verifying the results.

525 **5. Open access to data and code**

526 Question: Does the paper provide open access to the data and code, with sufficient instruc-
 527 tions to faithfully reproduce the main experimental results, as described in supplemental
 528 material?

529 Answer: [Yes]

530 Justification: The GitHub repository provides open access to the validation project, the
 531 complete chat history with ChatGPT, and the Citavi test project, along with instructions.
 532 These resources allow other researchers to faithfully reproduce the experimental setup and
 533 verify the main claims.

534 Guidelines:

- 535 • The answer NA means that paper does not include experiments requiring code.
 536 • Please see the Agents4Science code and data submission guidelines on the conference
 537 website for more details.
 538 • While we encourage the release of code and data, we understand that this might not be
 539 possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not
 540 including code, unless this is central to the contribution (e.g., for a new open-source
 541 benchmark).
 542 • The instructions should contain the exact command and environment needed to run to
 543 reproduce the results.
 544 • At submission time, to preserve anonymity, the authors should release anonymized
 545 versions (if applicable).

546 **6. Experimental setting/details**

547 Question: Does the paper specify all the training and test details (e.g., data splits, hyper-
 548 parameters, how they were chosen, type of optimizer, etc.) necessary to understand the
 549 results?

550 Answer: [Yes]

551 Justification: The paper specifies the relevant experimental setting for the proof-of-concept,
 552 including the restricted scope (five queries, no user feedback, no iterative tuning) and the
 553 use of a Citavi test project. While continuous retraining of data was not implemented in the
 554 validation, the conditions under which the presented results were obtained are sufficiently
 555 described.

556 Guidelines:

- 557 • The answer NA means that the paper does not include experiments.
 558 • The experimental setting should be presented in the core of the paper to a level of detail
 559 that is necessary to appreciate the results and make sense of them.
 560 • The full details can be provided either with the code, in appendix, or as supplemental
 561 material.

562 **7. Experiment statistical significance**

563 Question: Does the paper report error bars suitably and correctly defined or other appropriate
 564 information about the statistical significance of the experiments?

565 Answer: [No]

566 Justification: This paper does not report error bars or statistical significance measures.
567 However, the restricted scope of the validation (five queries, no feedback, no retraining) was
568 explicitly defined and used consistently to evaluate the proposed method.

569 Guidelines:

- 570 • The answer NA means that the paper does not include experiments.
571 • The authors should answer "Yes" if the results are accompanied by error bars, confi-
572 dence intervals, or statistical significance tests, at least for the experiments that support
573 the main claims of the paper.
574 • The factors of variability that the error bars are capturing should be clearly stated
575 (for example, train/test split, initialization, or overall run with given experimental
576 conditions).

577 8. Experiments compute resources

578 Question: For each experiment, does the paper provide sufficient information on the com-
579 puter resources (type of compute workers, memory, time of execution) needed to reproduce
580 the experiments?

581 Answer: [No]

582 Justification: The validation scenario was lightweight and could be executed on standard
583 computing resources, that why the paper does not provide explicit details on hardware type,
584 memory, or runtime.

585 Guidelines:

- 586 • The answer NA means that the paper does not include experiments.
587 • The paper should indicate the type of compute workers CPU or GPU, internal cluster,
588 or cloud provider, including relevant memory and storage.
589 • The paper should provide the amount of compute required for each of the individual
590 experimental runs as well as estimate the total compute.

591 9. Code of ethics

592 Question: Does the research conducted in the paper conform, in every respect, with the
593 Agents4Science Code of Ethics (see conference website)?

594 Answer: [Yes]

595 Justification: This paper is conforms fully with the Agents4Science Code of Ethics.

596 Guidelines:

- 597 • The answer NA means that the authors have not reviewed the Agents4Science Code of
598 Ethics.
599 • If the authors answer No, they should explain the special circumstances that require a
600 deviation from the Code of Ethics.

601 10. Broader impacts

602 Question: Does the paper discuss both potential positive societal impacts and negative
603 societal impacts of the work performed?

604 Answer: [No]

605 Justification: The paper is the direct outcome of a ChatGPT-assisted scientific writing
606 process and does not include a dedicated discussion of potential positive or negative societal
607 impacts.

608 Guidelines:

- 609 • The answer NA means that there is no societal impact of the work performed.
610 • If the authors answer NA or No, they should explain why their work has no societal
611 impact or why the paper does not address societal impact.
612 • Examples of negative societal impacts include potential malicious or unintended uses
613 (e.g., disinformation, generating fake profiles, surveillance), fairness considerations,
614 privacy considerations, and security considerations.
615 • If there are negative societal impacts, the authors could also discuss possible mitigation
616 strategies.