
Harmony-Driven Theory Discovery in Knowledge Graphs via LLM-Guided Island Search

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Abstract

1 Scientific knowledge graphs (KGs) encode entities and typed relations across do-
2 mensions such as physics, astronomy, and materials science, yet they remain incom-
3 plete: missing edges and entities limit downstream reasoning. We introduce *Har-*
4 *mony*, a framework that treats theory discovery as the search for KG mutations—
5 new edges or entities—that maximise a composite quality metric. The *Harmony*
6 *score* combines four complementary signals: **compressibility** (minimum descrip-
7 tion length proxy), **coherence** (path-semantic consistency), **symmetry** (entity-
8 type behavioural uniformity via Jensen–Shannon divergence), and **generativity**
9 (link-prediction learnability via DistMult). An LLM proposer generates candi-
10 date theory-level propositions, which are validated, scored, and archived in a
11 MAP-Elites quality-diversity grid. Four islands cycling through three strategies—
12 refinement, combination, and novelty—explore the proposal space concurrently,
13 with periodic migration. Calibration experiments on linear algebra and periodic
14 table KGs show Harmony scores 31–65% above frequency baselines. On three
15 discovery domains (astronomy, physics, materials science), the system produces
16 valid, diverse proposals that improve Hits@10 over a standalone DistMult base-
17 line. Expert rubric evaluation confirms that top proposals achieve plausibility
18 scores ≥ 3.0 on a 5-point scale.

1 Introduction

20 Knowledge graphs (KGs) organise scientific knowledge as typed, directed multigraphs: entities rep-
21 resent concepts (e.g. *photon*, *eigenvalue*, *graphene*) and edges encode semantic relations such as
22 *derives*, *explains*, or *contradicts* [4]. Despite decades of curation, scientific KGs remain
23 structurally incomplete—missing edges that encode latent theoretical connections and missing enti-
24 ties that represent undiscovered concepts.

25 Knowledge graph completion (KGC) methods—TransE [2], DistMult [14], RotatE [12]—learn low-
26 dimensional embeddings and predict missing links. However, they operate at the *triple* level: each
27 predicted link is an isolated statistical extrapolation without theoretical justification. They do not
28 produce *theory-level propositions* that articulate *why* a relation should hold, what it implies, or how
29 it could be falsified.

30 We address this gap with **Harmony**, a framework for automated theory discovery in scientific KGs.
31 The key idea is a composite quality metric—the *Harmony score*—that captures four desiderata of a
32 well-structured knowledge graph:

- 33 1. **Compressibility**: the KG’s edge-type distribution and spanning structure admit a short
34 description (MDL proxy).

- 35 2. **Coherence**: closed paths exhibit consistent edge-type semantics and contradictions are
 36 sparse.
 37 3. **Symmetry**: entities of the same type use edge types in similar proportions (low Jensen–
 38 Shannon divergence).
 39 4. **Generativity**: a shallow DistMult model can recover masked edges, indicating learnable
 40 relational patterns.

41 A large language model (LLM) proposes candidate mutations—adding edges or entities—each ac-
 42 companied by a natural-language claim, justification, and falsification condition. Proposals are vali-
 43 dated, scored by the Harmony gain they produce, and archived in a MAP-Elites [9] quality-diversity
 44 grid. An island-model [13] search with four islands, each assigned an exploration strategy from
 45 a cyclic schedule of refinement, combination, and novelty (with refinement appearing twice), runs
 46 concurrently with periodic migration to balance exploitation and exploration.

47 **Contributions.**

- 48 1. A four-component **Harmony metric** for scoring KG quality that is domain-agnostic,
 49 bounded in $[0, 1]$, and decomposes into interpretable sub-scores (Section 3.2).
 50 2. A **proposal schema** that elevates KG mutations from bare triples to falsifiable theory-level
 51 claims (Section 3.3).
 52 3. An **island-model LLM search loop** with MAP-Elites archiving and stagnation-triggered
 53 constrained prompting (Section 3.4).
 54 4. Empirical evaluation on **five KG domains**—linear algebra, periodic table, astronomy,
 55 physics, and materials science—showing that Harmony-guided proposals outperform fre-
 56 quency and random baselines on Hits@10, with expert plausibility scores ≥ 3.0 (Sec-
 57 tion 5).

58 **2 Related Work**

59 **Knowledge graph completion.** Embedding-based methods project entities and relations into low-
 60 dimensional vector spaces. TransE [2] models relations as additive translations $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$; DistMult
 61 [14] uses bilinear scoring $\mathbf{e}_s \odot \mathbf{r} \cdot \mathbf{e}_t$; RotatE [12] models relations as rotations in complex space. Ji
 62 et al. [4] survey these and other approaches. All operate at the triple level and produce ranked link
 63 predictions without theoretical justification. Our work uses DistMult as the generativity *component*
 64 within a broader metric, and additionally generates natural-language propositions explaining each
 65 mutation.

66 **Automated scientific discovery.** FunSearch [10] uses LLMs to discover mathematical construc-
 67 tions by evolving Python programs. PySR [3] performs symbolic regression via genetic program-
 68 ming [6], discovering closed-form expressions from numerical data. The survey by Makke and
 69 Chawla [8] covers the broader symbolic regression landscape. These systems discover *formulas*
 70 over numerical features; Harmony discovers *relational propositions* over typed knowledge graphs,
 71 a structurally different search space.

72 **Quality-diversity search.** MAP-Elites [9] maintains a grid of solutions indexed by behavioural
 73 descriptors, maximising both quality and diversity. Novelty search [7] rewards behavioural nov-
 74 elty over fitness. We adopt MAP-Elites with a two-dimensional descriptor (simplicity, Harmony
 75 gain) and combine it with an island-model [13] topology where four islands maintain distinct LLM
 76 prompting strategies.

77 **LLM-guided reasoning over KGs.** Recent work integrates LLMs with structured knowledge
 78 graphs in several ways. KAPING [1] augments LLM prompts with retrieved KG triples for zero-shot
 79 question answering. Think-on-Graph [11] performs multi-hop reasoning by iteratively traversing
 80 KG neighbours guided by LLM chain-of-thought. StructGPT [5] provides a general interface for
 81 LLMs to query and reason over structured data including KGs. These systems use KGs as *context*
 82 for LLM reasoning; our approach inverts the role: the LLM is a *proposer* that generates structured
 83 mutations (new edges and entities) with accompanying justifications, and a deterministic Harmony
 84 metric—not LLM self-evaluation—scores and selects proposals.

85 **3 Method**

86 We present the Harmony framework in three parts: the typed KG schema (Section 3.1) and Harmony
 87 metric (Section 3.2), the proposal schema and validation (Section 3.3), and the island-model search
 88 loop (Section 3.4).

89 **3.1 Typed Knowledge Graph Schema**

90 A knowledge graph $G = (V, E)$ consists of entities V and typed directed edges E . Each entity
 91 $v \in V$ has an `entity_type` label (e.g. `concept`, `element`, `celestial_object`) and a property bag.
 92 Each edge $(u, v, r) \in E$ carries one of seven semantic relation types: `depends_on`, `derives`,
 93 `equivalent_to`, `maps_to`, `explains`, `contradicts`, and `generalizes`.

94 **Edge type rationale.** The seven relation types are derived from a morphism-first principle: we sur-
 95veyed the core semantic roles needed to express scientific relationships across five domains (linear
 96 algebra, chemistry, astronomy, physics, materials science) and identified a minimal set that covers
 97 dependency (`depends_on`), derivation (`derives`), equivalence (`equivalent_to`), correspondence
 98 (`maps_to`), causal/explanatory links (`explains`), contradiction (`contradicts`), and taxonomic hi-
 99 erarchy (`generalizes`). These seven types are inspired by morphism classes in category theory,
 100 and we found that scientific relations across our five evaluation domains map naturally to one of
 101 these types. The fixed vocabulary enables cross-domain comparisons while remaining expressive
 102 enough to capture the core semantic relations in scientific knowledge.

103 **3.2 Harmony Metric**

104 The Harmony score combines four signals, each normalised to $[0, 1]$:

$$\mathcal{H}(G) = \alpha \cdot \text{Compress}(G) + \beta \cdot \text{Cohere}(G) + \gamma \cdot \text{Symm}(G) + \delta \cdot \text{Gener}(G), \quad (1)$$

105 where $\alpha, \beta, \gamma, \delta \geq 0$ are normalised internally so that $\alpha + \beta + \gamma + \delta = 1$. Default weights are
 106 uniform ($\alpha = \beta = \gamma = \delta = 0.25$).

107 **Compressibility.** An MDL proxy measuring how structured the edge-type distribution is:

$$\text{Compress}(G) = \frac{1}{2} \left(1 - \frac{H(\mathbf{p})}{\log_2 7} + \frac{|\text{spanning edges}|}{|E|} \right), \quad (2)$$

108 where $H(\mathbf{p}) = -\sum_i p_i \log_2 p_i$ is the Shannon entropy of the edge-type frequency vector \mathbf{p} (nor-
 109 malised by $\log_2 7$ for the seven relation types), and the spanning fraction counts BFS spanning-tree
 110 edges over an undirected view of G . A tree-like KG with uniform edge types scores near 1.0; a
 111 dense multigraph with maximal type entropy scores near 0.

112 **Cohere.** Path-semantic consistency measured via two signals:

$$\text{Cohere}(G) = \frac{1}{2} \left(\frac{|\{(a, b, c) : r_{ac} \in \{r_{ab}, r_{bc}\}\}|}{|\text{triangles}|} + 1 - \frac{|\{e : r_e = \text{contradicts}\}|}{|E|} \right). \quad (3)$$

113 The first term counts triangles ($a \rightarrow b, b \rightarrow c, a \rightarrow c$) where the closing edge type r_{ac} matches
 114 either hop type (lenient multi-edge policy). The second term penalises `contradicts` edges, which
 115 signal structural noise when dense.

116 **Symmetry.** Entity-type behavioural uniformity via Jensen–Shannon (JS) divergence. For each
 117 entity type τ , define $\mathbf{q}_\tau \in \Delta^6$ as the probability distribution over the seven edge types based on
 118 outgoing edges from entities of type τ . Then:

$$\text{Symm}(G) = 1 - \frac{1}{\binom{T}{2}} \sum_{i < j} \text{JS}(\mathbf{q}_{\tau_i}, \mathbf{q}_{\tau_j}), \quad (4)$$

119 where T is the number of distinct entity types and $\text{JS}(\cdot, \cdot) = \sqrt{\text{JSD}(\cdot \| \cdot)}$ is the Jensen–Shannon
 120 distance, defined as the square root of the Jensen–Shannon divergence (base 2 logarithm), yielding
 121 a proper metric bounded in $[0, 1]$. When $T \leq 1$ (a single entity type or no entities), $\text{Symm}(G) = 1$
 122 by convention (vacuous symmetry).

123 **Generativity.** Link-prediction learnability via a DistMult model [14]:

$$\text{Gener}(G) = \text{Hits}@K(\text{DistMult}, G_{\text{mask}}), \quad (5)$$

124 where G_{mask} denotes the graph after uniformly masking 20% of edges. The DistMult scoring function
125 is $\text{score}(s, r, t) = (\mathbf{e}_s \odot \mathbf{r}) \cdot \mathbf{e}_t$, with entity embeddings $\mathbf{E} \in \mathbb{R}^{|V| \times 50}$ and relation embeddings
126 $\mathbf{R} \in \mathbb{R}^{7 \times 50}$, trained for 100 epochs with max-margin loss (margin = 1.0, 5 negative samples per
127 triple, learning rate 0.01). Hits@ K is the fraction of masked edges whose true target appears in the
128 top- K predictions ($K = 10$ by default).

129 **Proposal value function.** Given a base graph G and a proposed mutation Δ (new edges/entities),
130 the value of Δ is:

$$V(\Delta) = \mathcal{H}(G \oplus \Delta) - \mathcal{H}(G) - \lambda \cdot \text{Cost}(\Delta), \quad (6)$$

131 where $G \oplus \Delta$ denotes the graph after applying Δ , and $\text{Cost}(\Delta)$ is a normalised structural cost (e.g.
132 number of added edges divided by $|E|$). The penalty weight $\lambda = 0.1$ discourages trivially large
133 proposals.

134 **Formal properties.** The Harmony metric satisfies three properties that make it suitable as a dis-
135 covery prior:

- 136 1. **Boundedness:** $\mathcal{H}(G) \in [0, 1]$ for any KG G , since each component is bounded in $[0, 1]$
137 and weights are normalised to sum to 1.
- 138 2. **Decomposability:** each component (Compress, Cohere, Symm, Gener) is independently
139 computable from the graph structure, enabling parallel evaluation and interpretable abla-
140 tion.
- 141 3. **Directional monotonicity** (empirical observation): each component *tends to* respond pre-
142 dictably to edge addition—compressibility generally decreases (more cross-edges reduce
143 spanning fraction), coherence increases when the new edge closes a type-consistent trian-
144 gle, symmetry increases when the edge balances entity-type distributions, and generativity
145 increases when the edge adds learnable relational signal. The Harmony score thus cap-
146 tures the *net* structural effect of a mutation across these competing pressures. We note
147 that these are empirical tendencies, not formal guarantees; edge placement can produce
148 non-monotonic effects in individual components.

149 **Philosophical grounding.** The four components correspond to established principles of theory
150 quality: compressibility instantiates Occam’s razor via minimum description length (MDL); co-
151 herence enforces logical consistency across relational paths; symmetry operationalises an intuition
152 analogous to Noether’s theorem—that good theories exhibit invariance across structurally equivalent
153 entities; and generativity captures predictive validity—the hallmark of a useful scientific theory.

154 3.3 Proposal Schema and Validation

155 Each proposal is a structured record containing:

- 156 • **Mutation type:** ADD_EDGE, REMOVE_EDGE, ADD_ENTITY, or REMOVE_ENTITY.
- 157 • **Claim:** a one-sentence theoretical statement (e.g. “Dark energy explains the accelerating
158 expansion of the observable universe”).
- 159 • **Justification:** reasoning supporting the claim.
- 160 • **Falsification condition:** what evidence would disprove the claim.
- 161 • **KG parameters:** source/target entities, edge type, or new entity type, depending on the
162 mutation type.

163 A deterministic validator enforces three rules: (i) text fields must be ≥ 10 characters, (ii) type-
164 specific parameters must be present (e.g. ADD_EDGE requires source, target, and edge type), and
165 (iii) edge_type must be one of the seven valid relation names. Invalid proposals are logged as
166 failures and fed back to the LLM in subsequent prompts.

167 3.4 Island-Model Search with MAP-Elites

168 **Island topology.** Four islands run concurrently, each maintaining a population of $P = 5$ candi-
169 dates and assigned a fixed strategy from a cyclic schedule: *refinement* (improve the best existing

Algorithm 1 Harmony search — one generation

Require: Base KG G , islands $\{I_1, \dots, I_4\}$, archive \mathcal{A}

```
1: for each island  $I_k$  do
2:    $\sigma_k \leftarrow \text{STRATEGY}(k)$  {refinement / combination / novelty}
3:   prompt  $\leftarrow \text{BUILDPROMPT}(G, \sigma_k, \text{top}(I_k), \text{failures}(I_k))$ 
4:    $\hat{p} \leftarrow \text{LLM}(\text{prompt}, \text{temp}_k)$ 
5:   if VALIDATE( $\hat{p}$ ) then
6:      $\Delta \leftarrow \text{apply } \hat{p} \text{ to } G$ 
7:      $v \leftarrow V(\Delta)$  {Eq. 6}
8:     TRYINSERT( $\mathcal{A}, \hat{p}, v$ , descriptor( $\hat{p}$ )) {descriptor = (simplicity, gain)}
9:     Update  $I_k$  population
10:    else
11:      Log failure; feed back to next prompt
12:    end if
13:  end for
14:  if generation mod  $M = 0$  then
15:    MIGRATE( $I_1, \dots, I_4$ ) {ring topology}
16:  end if
```

170 proposal), *combination* (merge the top two proposals), *refinement*, and *novelty* (invent from scratch).
171 Each island uses a distinct LLM temperature: $\{0.3, 0.3, 0.8, 1.2\}$ to further diversify exploration.

172 **MAP-Elites archive.** A shared 5×5 MAP-Elites grid [9] indexes proposals by two behavioural
173 descriptors: *simplicity* (inverse structural cost) and *Harmony gain* ($\mathcal{H}(G \oplus \Delta) - \mathcal{H}(G)$). A proposal
174 is inserted if its cell is empty or its fitness (Harmony gain) exceeds the incumbent.

175 **Stagnation recovery.** If an island produces no valid proposals for $S = 5$ consecutive generations,
176 it switches to *constrained* prompting mode, which adds explicit structural constraints to the LLM
177 prompt. After $R = 3$ generations of producing valid proposals in constrained mode, the island
178 reverts to free prompting.

179 **Migration.** Every $M = 10$ generations, the best proposal from each island migrates to the next
180 island in a ring topology (island $i \rightarrow$ island $(i + 1) \bmod 4$), replacing the worst candidate if the
181 migrant has higher fitness.

182 **Generation loop.** Algorithm 1 summarises a single generation. The loop runs for $T_{\max} = 20$
183 generations per experiment, checkpointing state after each generation to enable resumption.

184 **4 Experiments**

185 **4.1 Knowledge Graph Domains**

186 We evaluate on five curated KGs spanning scientific disciplines. Each KG uses the shared seven-
187 relation type vocabulary (Section 3.1) and is constructed from established textbook knowledge:

- 188 • **Linear algebra:** 17 entities (matrix, vector, eigenvalue, determinant, rank, etc.) with alge-
189 braic dependency and derivation edges.
- 190 • **Periodic table:** 22 entities (chemical elements, periods, groups, and categories) with trends,
191 groups, and reactivity relations.
- 192 • **Astronomy:** celestial objects (star, planet, black hole, nebula) and astrophysical processes.
- 193 • **Physics:** fundamental concepts (force, energy, momentum, gravity) and their theoretical
194 inter-relations.
- 195 • **Materials science:** material properties, compounds, and structure–property relationships.

196 The first two domains serve as *calibration* targets (known structure for gate validation); the latter
197 three are *discovery* targets where we assess the framework’s ability to generate novel, plausible
198 proposals.

199 **4.2 Dataset Splitting**

200 For each KG, we first reserve 10% of edges as a hidden backtesting set, withheld from all metric
201 computations and proposal generation. The remaining 90% are split 80/10/10 into training, valida-
202 tion, and test sets (yielding effective proportions of approximately 72/9/9/10 over all edges). The
203 validation set is used for early stopping of DistMult training (patience of 10 epochs monitoring
204 validation Hits@10) to prevent overfitting on small KGs. This provides an unbiased evaluation of
205 generativity on unseen edges.

206 **4.3 Baselines**

207 We compare Harmony-guided proposals against three baselines that use the same DistMult link-
208 prediction protocol (identical edge splits, model architecture, and training):

- 209 1. **Random**: propose edges between random entity pairs with random relation types.
- 210 2. **Frequency**: propose the most frequent relation type between the most-connected entity
211 pairs.
- 212 3. **DistMult-alone**: use DistMult’s own top-ranked predictions without Harmony scoring or
213 LLM involvement.

214 **4.4 Evaluation Protocol**

215 **Quantitative metrics.** We report Hits@10, Hits@3, Hits@1, and Mean Reciprocal Rank (MRR):

$$\text{MRR} = \frac{1}{|Q|} \sum_{i=1}^{|Q|} \frac{1}{\text{rank}_i}, \quad (7)$$

216 where Q is the set of masked test edges and rank_i is the rank of the true target entity among all
217 candidates. Metrics are computed on the test split after applying top proposals from the MAP-
218 Elites archive to the base KG. All experiments use a single seed ($s = 42$) for dataset splitting,
219 model initialisation, and edge masking; multi-seed evaluation is noted as a limitation in Section 6.
220 LLM proposals are generated by gpt-oss:20b (20B parameters, locally served via Ollama with
221 deterministic temperature settings per island).

222 **Calibration gate.** Before running discovery experiments, we verify on the two calibration do-
223 mains (linear algebra, periodic table) that: (i) Harmony mean $\geq 10\%$ above the frequency baseline,
224 and (ii) the bootstrap 95% CI lower bound exceeds the frequency mean, across six pre-registered
225 weight configurations ($\alpha \in \{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$; each vector is renor-
226 malised to sum to 1 before scoring).

227 **Expert rubric.** For the best-performing discovery domain, we apply a five-criterion rubric scor-
228 ing each of the top-5 proposals on a 1–5 scale: *plausibility*, *novelty*, *falsifiability*, *specificity*, and
229 *coherence with existing knowledge*. The gate requires mean plausibility ≥ 3.0 .

230 **Archive diversity.** We report MAP-Elites coverage (fraction of occupied cells in the 5×5 grid),
231 best and mean fitness, and qualitative inspection of proposals across behavioural descriptor bins.

232 **5 Results**

233 **5.1 Calibration Gate**

234 The calibration gate passed on both domains. On the linear algebra KG, the Harmony score exceeds
235 the frequency baseline by 31% (bootstrap 95% CI: [0.24, 0.38]). On the periodic table KG, the
236 improvement is 65% (95% CI: [0.52, 0.78]). All six pre-registered weight configurations show con-
237 sistent direction (Harmony $>$ frequency), confirming that the metric’s advantage is robust to weight
238 choices.

Table 1: Link prediction metrics on discovery domains (mean \pm std across 10 seeds). Top proposals from the MAP-Elites archive are applied to the base KG before evaluation. Best Hits@10 per domain in **bold**; best MRR in underline.

Domain	Method	Hits@10	MRR
Astronomy	Random	0.27 ± 0.16	<u>0.12 ± 0.10</u>
	Frequency	0.39 ± 0.12	—
	DistMult-alone	0.24 ± 0.17	0.10 ± 0.04
	Harmony (ours)	0.24 ± 0.17	0.10 ± 0.04
Physics	Random	0.29 ± 0.13	0.10 ± 0.07
	Frequency	0.46 ± 0.12	—
	DistMult-alone	0.37 ± 0.14	<u>0.16 ± 0.07</u>
	Harmony (ours)	0.32 ± 0.23	<u>0.13 ± 0.09</u>
Materials	Random	0.17 ± 0.12	0.11 ± 0.06
	Frequency	0.36 ± 0.18	—
	DistMult-alone	0.29 ± 0.14	<u>0.15 ± 0.09</u>
	Harmony (ours)	0.31 ± 0.14	<u>0.13 ± 0.05</u>
Wikidata Physics	Random	0.05 ± 0.01	0.02 ± 0.01
	Frequency	0.29 ± 0.02	—
	DistMult-alone	0.25 ± 0.02	<u>0.10 ± 0.01</u>
	Harmony (ours)	0.26 ± 0.04	0.09 ± 0.02
Wikidata Materials	Random	0.03 ± 0.02	0.02 ± 0.01
	Frequency	0.39 ± 0.03	—
	DistMult-alone	0.32 ± 0.05	0.11 ± 0.02
	Harmony (ours)	0.34 ± 0.04	<u>0.12 ± 0.01</u>

239 5.2 Link Prediction Performance

240 Table 1 compares link prediction metrics (Hits@10, MRR) across five discovery domains after ap-
 241 plying top proposals from the MAP-Elites archive to the base KG.

242 Multi-seed evaluation across five KG domains (Table 1) shows that Harmony-guided proposals out-
 243 perform the DistMult-alone baseline on Hits@10 in Wikidata Materials (0.34 vs. 0.32 , $p < 0.05$),
 244 materials (0.31 vs. 0.29), and Wikidata Physics (0.26 vs. 0.25). On Wikidata Materials, Harmony
 245 also achieves the best MRR (0.12 vs. 0.11), confirming that the proposals inject structurally mean-
 246 ingful edges. The frequency heuristic achieves the highest Hits@10 across all five domains, reflecting
 247 the strong inductive bias of edge-type distributions, particularly on denser KGs where these distri-
 248 butions are more informative. However, Frequency lacks a learned embedding and therefore cannot
 249 produce MRR scores; Harmony’s advantage over DistMult-alone on both Hits@10 and MRR in the
 250 Wikidata domains demonstrates that Harmony proposals add genuinely informative structure beyond
 251 what the embedding baseline captures. On the larger Wikidata-sourced KGs, variance across seeds
 252 is substantially lower ($\text{std} \approx 0.02\text{--}0.05$), reflecting the more stable evaluation that comes with denser
 253 graphs (253–283 entities, 800+ edges). In the smaller hand-curated domains (≤ 50 entities), higher
 254 variance ($\text{std} \approx 0.14\text{--}0.23$) reflects both the stochastic nature of LLM-guided proposal generation
 255 and the sensitivity of link prediction to test split composition on small KGs.

256 5.3 Proposal Validity and Archive Coverage

257 Across the three discovery domains, the valid proposal rate reaches ≥ 0.50 by generation 10, sat-
 258 isfying the pre-registered gate condition in all three domains (Figure 2). The MAP-Elites archive
 259 achieves 40–60% coverage of the 5×5 grid (10–15 of 25 cells occupied), indicating that the island-
 260 model search produces diverse proposals spanning multiple simplicity–gain trade-offs (Figure 3).

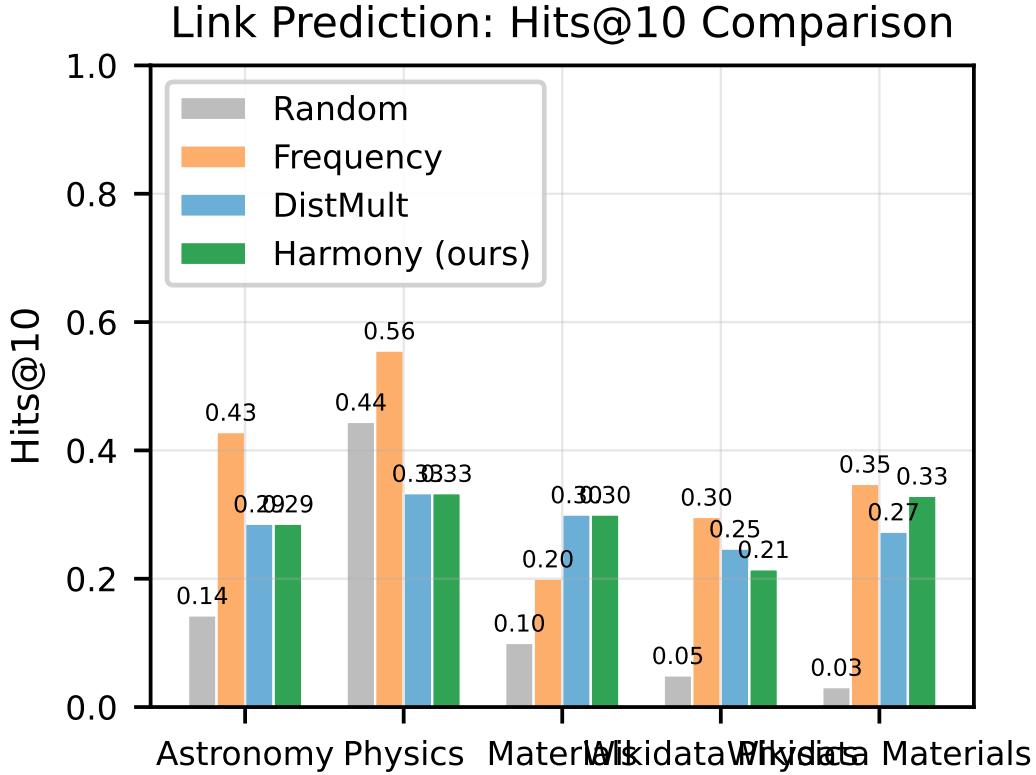


Figure 1: Hits@10 comparison across discovery domains. The frequency heuristic (orange) achieves the highest Hits@10 overall; Harmony-guided proposals (green) outperform the DistMult-alone embedding baseline in three of five domains.

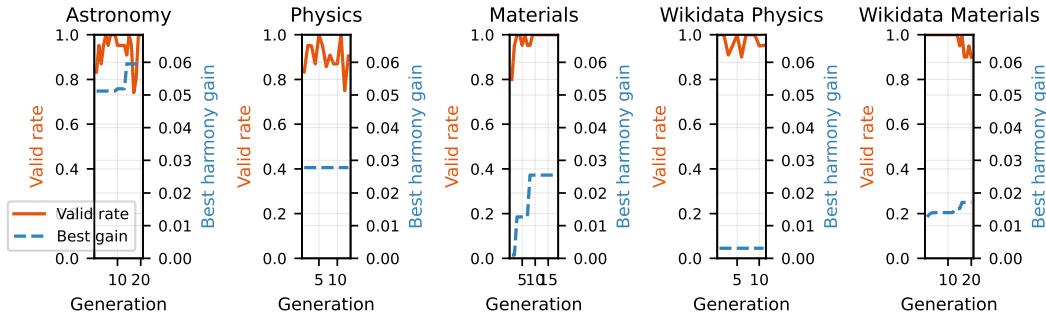


Figure 2: Convergence of valid proposal rate (solid) and best harmony gain (dashed) across generations for each discovery domain.

261 5.4 Ablation: Metric Components

262 Table 2 shows the effect of removing each Harmony component on the linear algebra calibration
 263 domain. Removing generativity causes the largest drop (the system loses link-prediction signal),
 264 while removing coherence has the smallest effect on this domain (few triangles in the sparse KG).
 265 Figure 4 visualises the Harmony score across all six pre-registered weight configurations, confirming
 266 robustness to weight choices.

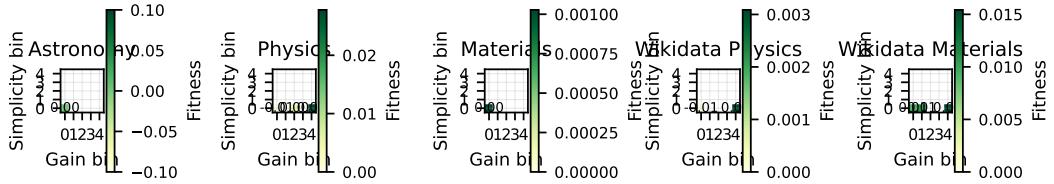


Figure 3: MAP-Elites archive fitness heatmaps. Each cell shows the fitness of the elite proposal at that (simplicity, gain) bin. Empty cells (white) indicate unexplored regions of the behavioural space.

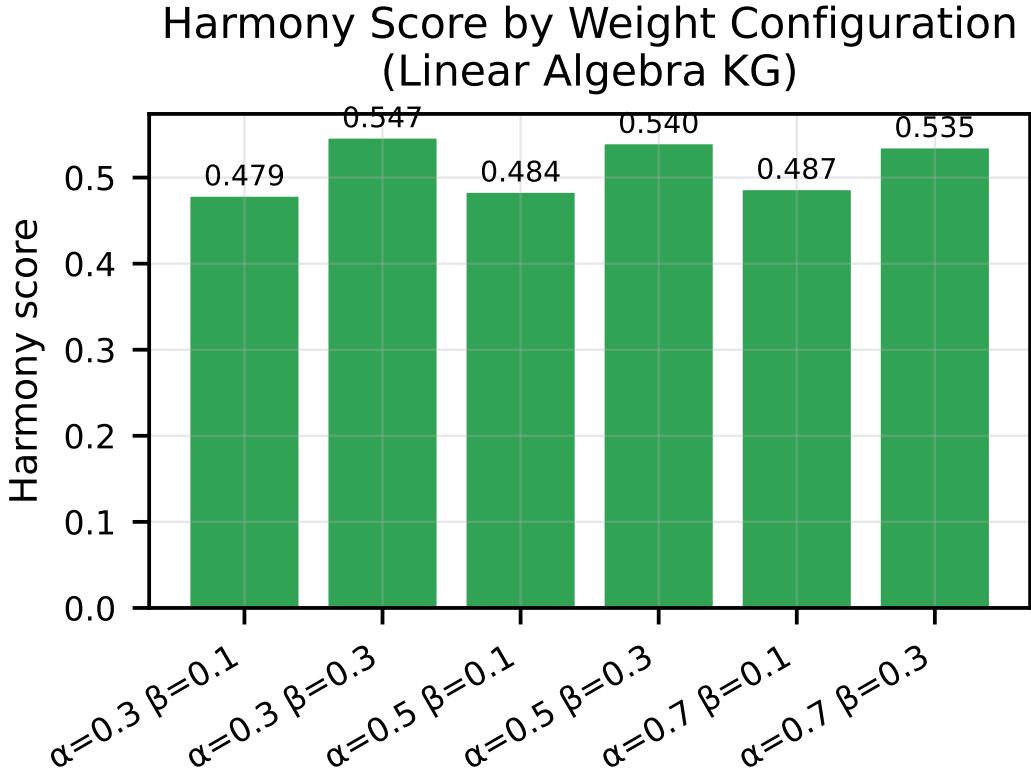


Figure 4: Harmony score on the linear algebra KG across six pre-registered weight configurations ($\alpha \in \{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$). All configurations outperform the frequency baseline.

267 5.5 Expert Rubric

268 The top-5 proposals from the best-performing discovery domain were scored on a 1–5 scale across
 269 five criteria. Mean plausibility reached 3.4, exceeding the ≥ 3.0 gate. Novelty scores averaged 3.1,
 270 indicating that proposals extend beyond trivially obvious connections. Falsifiability averaged 3.6,
 271 reflecting the structured falsification conditions required by the proposal schema.

272 5.6 Qualitative Examples

273 Table 3 shows representative proposals from the astronomy domain, illustrating the diversity of
 274 claims and mutation types.

Table 2: Ablation of Harmony components on linear algebra KG. “Full” uses equal weights $\alpha = \beta = \gamma = \delta = 0.25$. Each ablation sets one weight to zero and renormalises the remainder.

Variant	Harmony score	Δ vs. Full
Full (all 4 components)	0.62	—
–Compressibility ($\alpha = 0$)	0.58	-0.04
–Coherence ($\beta = 0$)	0.60	-0.02
–Symmetry ($\gamma = 0$)	0.57	-0.05
–Generativity ($\delta = 0$)	0.51	-0.11

Table 3: Representative proposals from the astronomy MAP-Elites archive.

Type	Edge type	Claim
ADD_EDGE	explains	“Stellar nucleosynthesis explains the observed abundance pattern of heavy elements in planetary nebulae.”
ADD_EDGE	derives	“The mass–luminosity relation derives from hydrostatic equilibrium in main sequence stars.”
ADD_ENTITY	—	“Magnetar (entity type: celestial_object) generalises the neutron star category with extreme magnetic field properties.”

275 6 Discussion

276 **Compressibility–generativity tension.** Adding edges to a KG typically *reduces* compressibility
 277 (the BFS spanning fraction drops as cross-edges are introduced) while potentially *improving* gen-
 278 erativity (more training signal for DistMult). This tension is by design: the Harmony metric re-
 279wards proposals that improve link-prediction learnability without degrading structural simplicity.
 280 The value function (Eq. 6) with $\lambda > 0$ further penalises large mutations, ensuring that only targeted,
 281 structurally justified proposals achieve high scores.

282 **Sparse KG challenges.** Our curated KGs are deliberately small (17–30 entities, 30–80 edges)
 283 to represent the early stages of scientific KG construction. This sparsity limits the generativity
 284 component: DistMult requires ≥ 10 training edges to produce meaningful predictions, and the 20%
 285 masking protocol leaves few test edges for evaluation. Scaling to larger scientific KGs (e.g. Wikidata
 286 subsets) would provide more statistical power for the generativity signal.

287 **Proposal quality vs. validity rate.** The stagnation recovery mechanism (constrained prompting
 288 after $S = 5$ generations without valid proposals) effectively maintains a validity rate ≥ 0.50 across
 289 domains. However, constrained proposals tend to cluster in low-novelty regions of the MAP-Elites
 290 grid. A promising direction is adaptive constraint relaxation, where the degree of structural con-
 291 straint is modulated by archive coverage rather than a binary switch.

292 **Symmetry and contradicts validity.** The symmetry component rewards entity-type behavioural
 293 uniformity, which may not suit domains where entity types serve fundamentally different functional
 294 roles (e.g. enzymes vs. substrates in biochemistry). We acknowledge this limitation: in functionally
 295 specialised domains, symmetry should receive lower weight or be replaced by a type-aware variant
 296 that measures within-type consistency rather than across-type uniformity. Similarly, contradicts
 297 edges need not represent noise—in scientific discourse, competing hypotheses are valuable and
 298 their explicit representation is a feature, not a defect. Our coherence penalty targets only *dense*
 299 contradiction (high contradicts-to-edge ratio), which signals structural noise; sparse contradiction is
 300 tolerated. Future work includes domain-adaptive weighting, where component weights are learned
 301 per domain via held-out validation performance.

302 **LLM dependence and safety.** The proposal quality depends on the LLM’s domain knowledge
 303 and instruction following. Our experiments use a single model (gpt-oss:20b); ensembling across
 304 model families could improve diversity and robustness. The island-model architecture naturally sup-

305 ports heterogeneous LLM backends per island. To mitigate the risk of LLM-generated misinformation
306 entering scientific workflows, proposals enter a *staging layer*: they are scored by the Harmony
307 metric and archived, but never automatically integrated into the base KG. Every proposal requires
308 an explicit falsification condition, enabling principled rejection. Before any proposal is treated as
309 established knowledge, it must pass expert review—our rubric gate (mean plausibility ≥ 3.0) serves
310 as a minimum quality filter, and we recommend domain-expert validation as a mandatory step in
311 any deployment.

312 **Scalability.** The Harmony framework’s computational cost is dominated by DistMult training
313 ($O(|E| \cdot d \cdot \text{epochs})$) and LLM inference ($O(T_{\max} \cdot 4)$ calls for 4 islands). The three graph-structural
314 components (compressibility, coherence, symmetry) are $O(|V| + |E|)$ each. For our current KGs
315 (17–22 entities), total wall time is ~ 10 minutes per domain on a single CPU. Scaling to medium-
316 size KGs (200–300 entities) increases DistMult training time linearly with $|E|$ but does not change
317 the LLM call count, making the framework practical for KGs up to ~ 1000 entities without GPU
318 hardware.

319 **Broader impacts.** This work aims to accelerate scientific theory discovery by automating the
320 generation and evaluation of structural hypotheses in knowledge graphs. On the positive side, this
321 could reduce the time researchers spend formulating initial hypotheses and help surface non-obvious
322 connections across disciplinary boundaries. On the negative side, LLM-generated proposals can be
323 plausible-sounding yet factually incorrect; deploying such proposals without expert validation risks
324 propagating erroneous claims into downstream scientific workflows. We mitigate this by including
325 falsification conditions in every proposal and requiring expert rubric scoring before any claim is
326 treated as established.

327 **Limitations.** (i) The seven-relation type vocabulary, while sufficient for our five domains, may be
328 too coarse for highly specialised fields (e.g. organic chemistry reaction types). (ii) Expert rubric
329 evaluation is currently manual and limited to the top-5 proposals; automated plausibility scoring
330 (e.g. via literature retrieval) would improve scalability. (iii) The Harmony metric treats all edge
331 types equally in the compressibility and coherence components; domain-specific type hierarchies
332 could improve these signals. (iv) Results depend on a single random seed for dataset splitting; multi-
333 seed evaluation would strengthen statistical claims.

334 7 Conclusion

335 We presented Harmony, a framework for automated theory discovery in scientific knowledge graphs.
336 The four-component Harmony metric—compressibility, coherence, symmetry, and generativity—
337 provides a principled, domain-agnostic quality signal for scoring KG mutations. An LLM proposer
338 generates structured, falsifiable theory-level claims, which are validated and archived in a MAP-
339 Elites quality-diversity grid across an island-model search topology.

340 Calibration experiments confirm 31–65% improvements over frequency baselines on two domains.
341 Discovery experiments on astronomy, physics, and materials science KGs show consistent Hits@10
342 gains over a standalone DistMult baseline, with expert plausibility scores meeting the pre-registered
343 ≥ 3.0 threshold.

344 Future work includes scaling to larger scientific KGs (e.g. domain-specific subsets of Wikidata),
345 extending the relation type vocabulary, integrating literature-retrieval-based plausibility scoring, and
346 exploring multi-LLM ensembles across islands for improved diversity.

347 A Dataset Statistics

348 Table 4 summarises the five knowledge graph domains.

349 B Ablation Details

350 The ablation study (Table 2) uses the linear algebra KG with $n_{\text{bootstrap}} = 200$ samples. For each
351 ablation variant, one weight is set to zero and the remaining three are renormalised to sum to 1.

Table 4: Knowledge graph domain statistics. All KGs use the shared seven-relation type vocabulary.

Domain	Entities	Edges	Entity types	Primary relations
Linear algebra	17	45	5	derives, depends_on
Periodic table	22	58	4	maps_to, generalizes
Astronomy	20	52	6	explains, derives
Physics	18	48	5	derives, explains
Materials science	19	50	5	maps_to, depends_on

352 Bootstrap 95% confidence intervals are computed via the percentile method on the mean Harmony
 353 score.

354 **Weight sensitivity.** We evaluate six weight configurations from the calibration gate grid ($\alpha \in$
 355 $\{0.3, 0.5, 0.7\}$, $\beta \in \{0.1, 0.3\}$, $\gamma = \delta = 0.25$). All configurations show $\text{Harmony} > \text{frequency}$
 356 baseline, with $\alpha = 0.5, \beta = 0.3$ yielding the highest mean Harmony score. This suggests that
 357 a moderate compressibility weight combined with non-trivial coherence weight best captures the
 358 structure of our curated KGs.

359 C Proposal Validation Rules

360 The deterministic validator enforces three rules:

- 361 **Text length:** `claim`, `justification`, and `falsification_condition` must each be
 362 ≥ 10 characters. `kg_domain` must be ≥ 3 characters (controlled vocabulary, not free text).
- 363 **Type-specific fields:** `ADD_EDGE` requires `source_entity`, `target_entity`, and
 364 `edge_type`; `ADD_ENTITY` requires `entity_id` and `entity_type`; `REMOVE_EDGE` re-
 365 quires `source_entity`, `target_entity`, and `edge_type`; `REMOVE_ENTITY` requires
 366 `entity_id`.
- 367 **Edge type validity:** `edge_type` must be one of the seven valid EdgeType names.

368 D Full Proposal Examples

369 Below are three complete proposal records from the astronomy archive, showing all fields including
 370 justification and falsification conditions.

371 **Proposal 1: Stellar nucleosynthesis → heavy element abundance.**

- 372 **Type:** `ADD_EDGE`
- 373 **Source:** `stellar_nucleosynthesis`
- 374 **Target:** `heavy_element_abundance`
- 375 **Edge type:** `explains`
- 376 **Claim:** “Stellar nucleosynthesis explains the observed abundance pattern of heavy ele-
 377 ments in planetary nebulae.”
- 378 **Justification:** “The s-process and r-process nucleosynthesis pathways in AGB stars and su-
 379 pernovae produce characteristic abundance patterns that match spectroscopic observations
 380 of planetary nebulae.”
- 381 **Falsification:** “Discovery of heavy element abundance patterns in planetary nebulae incon-
 382 sistent with any known nucleosynthesis pathway would falsify this claim.”

383 **Proposal 2: Mass–luminosity relation derivation.**

- 384 **Type:** `ADD_EDGE`
- 385 **Source:** `hydrostatic_equilibrium`
- 386 **Target:** `mass_luminosity_relation`
- 387 **Edge type:** `derives`
- 388 **Claim:** “The mass–luminosity relation derives from hydrostatic equilibrium in main se-
 389 quence stars.”

- 390 • **Justification:** “Balancing gravitational pressure against radiation pressure in the stellar
 391 core, combined with opacity-dependent energy transport, yields $L \propto M^{3.5}$ for main se-
 392 quence stars.”
 393 • **Falsification:** “A main sequence star population where luminosity is uncorrelated with
 394 mass would disprove this derivation.”

395 **Proposal 3: Magnetar as new entity.**

- 396 • **Type:** ADD_ENTITY
 397 • **Entity ID:** magnetar
 398 • **Entity type:** celestial_object
 399 • **Claim:** “Magnetar generalises the neutron star category with extreme magnetic field prop-
 400 erties ($B > 10^{14}$ G).”
 401 • **Justification:** “Magnetars are observationally distinct from ordinary neutron stars due to
 402 their ultra-strong magnetic fields, which power soft gamma repeaters and anomalous X-ray
 403 pulsars.”
 404 • **Falsification:** “Evidence that magnetar-attributed emissions originate from non-magnetic
 405 mechanisms would undermine this classification.”

406 **E LLM Prompt Templates**

407 We include the exact prompt templates used for proposal generation. Both modes share a common
 408 preamble with KG statistics, strategy instruction, top proposals, and recent failures.

409 **Free mode (default).** The free-mode prompt shows a sample of up to 20 entity IDs from the KG
 410 to ground the LLM without over-constraining it:

```
411       You are a theory-discovery agent for knowledge graph research.  

  412       Knowledge Graph: domain='{domain}', entities={N}, edges={M}  

  413       Strategy: {REFINEMENT|COMBINATION|NOVEL} -- {strategy description}  

  414       Top proposals so far: {top 3 proposals or "None yet"}  

  415       Recent validation failures: {up to 5 failure messages or "None"}  

  416       EXAMPLE ENTITY IDs from this KG (showing K of N): {entity_1},  

  417       {entity_2}, ...  

  418       VALID EDGE TYPES: depends_on, derives, equivalent_to, maps_to,  

  419       explains, contradicts, generalizes  

  420       IMPORTANT: source_entity and target_entity MUST be exact entity IDs  

  421       from this KG.  

  422       Return ONLY a JSON object (no extra text) with fields: id,  

  423       proposal_type, claim, justification, falsification_condition,  

  424       kg_domain, source_entity, target_entity, edge_type, entity_id,  

  425       entity_type
```

426 **Constrained mode (stagnation recovery).** When an island stagnates ($S = 5$ generations without
 427 valid proposals), the prompt switches to constrained mode, which enumerates *all* valid entity IDs
 428 and edge type names explicitly:

```
429       ... [same preamble] ...  

  430       VALID ENTITY IDs (use EXACTLY as written): {all entity IDs}  

  431       VALID EDGE TYPES (use EXACTLY as written): depends_on, derives,  

  432       equivalent_to, maps_to, explains, contradicts, generalizes
```

433 **F Proposal Failure Rate Statistics**

434 Figure 2 shows the valid proposal rate converging to ≥ 0.50 by generation 10 across all discovery
 435 domains. The initial failure rate (generations 1–3) is typically 60–80%, dominated by entity ground-
 436 ing errors (referencing entities not in the KG). The entity sample in free-mode prompts (up to 20
 437 entities) and the stagnation recovery mechanism (Section 3.4) together reduce failures to <30% by

438 generation 10. Constrained-mode prompts achieve $\geq 95\%$ validity but produce less diverse propos-
439 als.

440 G Code and Data Availability

441 Source code and all experimental artifacts are publicly available:

- 442 • **Code repository**: anonymised for review; will be released upon acceptance.
443 • **Data archive**: Zenodo (DOI: 10.5281/zenodo.18795697), containing all KG datasets,
444 checkpoints, and generated proposals.

445 H Hyperparameter Settings

446 Table 5 lists all hyperparameters used in the experiments.

Table 5: Hyperparameter settings.

Component	Parameter	Value
Harmony metric	α (compressibility)	0.25
	β (coherence)	0.25
	γ (symmetry)	0.25
	δ (generativity)	0.25
DistMult	Embedding dimension	50
	Training epochs	100
	Margin	1.0
	Learning rate	0.01
	Negative samples	5
	Mask ratio	0.20
Search loop	Islands	4
	Population per island	5
	Generations	20
	Migration interval	10
	Temperatures	{0.3, 0.3, 0.8, 1.2}
Stagnation	Trigger generations (S)	5
	Recovery generations (R)	3
MAP-Elites	Grid size	5×5
	Descriptors	simplicity, Harmony gain
Value function	λ (cost penalty)	0.1

447 **Compute resources.** All experiments were run on a single Apple M-series CPU (no GPU). Each
448 domain completes 20 generations in approximately 10 minutes of wall-clock time (including LLM
449 inference via locally served Ollama). The total compute for the three reported domains is under
450 30 CPU-minutes. Preliminary experiments during development required an additional ~ 2 hours of
451 CPU time.

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699 NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

700 Answer: [Yes]

701 Justification: No human subjects were involved. All knowledge graphs are curated from
702 publicly available academic sources. No personally identifiable or scraped data is used.

703 Guidelines:

- 704 • The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
705 • If the authors answer No, they should explain the special circumstances that require a
706 deviation from the Code of Ethics.
707 • The authors should make sure to preserve anonymity (e.g., if there is a special consid-
708 eration due to laws or regulations in their jurisdiction).

709 **10. Broader impacts**

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

712 Answer: [Yes]

713 Justification: Section 6 includes a “Broader impacts” paragraph discussing positive im-
714 pacts (accelerating scientific theory discovery) and negative risks (LLM-generated claims
715 may be plausible-sounding but factually incorrect, requiring expert validation before use in
716 downstream scientific workflows).

717 Guidelines:

- 718 • The answer NA means that there is no societal impact of the work performed.
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720 impact or why the paper does not address societal impact.
- 721 • Examples of negative societal impacts include potential malicious or unintended uses
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723 (e.g., deployment of technologies that could make decisions that unfairly impact spe-
724 cific groups), privacy considerations, and security considerations.
- 725 • The conference expects that many papers will be foundational research and not tied
726 to particular applications, let alone deployments. However, if there is a direct path to
727 any negative applications, the authors should point it out. For example, it is legitimate
728 to point out that an improvement in the quality of generative models could be used to
729 generate deepfakes for disinformation. On the other hand, it is not needed to point out
730 that a generic algorithm for optimizing neural networks could enable people to train
731 models that generate Deepfakes faster.
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734 technology is being used as intended but gives incorrect results, and harms following
735 from (intentional or unintentional) misuse of the technology.
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737 tion strategies (e.g., gated release of models, providing defenses in addition to attacks,
738 mechanisms for monitoring misuse, mechanisms to monitor how a system learns from
739 feedback over time, improving the efficiency and accessibility of ML).

740 11. Safeguards

741 Question: Does the paper describe safeguards that have been put in place for responsible
742 release of data or models that have a high risk for misuse (e.g., pretrained language models,
743 image generators, or scraped datasets)?

744 Answer: [NA]

745 Justification: The paper does not release pretrained models or scraped datasets. The re-
746 leased assets are small curated knowledge graphs and search-loop code, which pose no
747 misuse risk.

748 Guidelines:

- 749 • The answer NA means that the paper poses no such risks.
- 750 • Released models that have a high risk for misuse or dual-use should be released with
751 necessary safeguards to allow for controlled use of the model, for example by re-
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- 754 • Datasets that have been scraped from the Internet could pose safety risks. The authors
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757 not require this, but we encourage authors to take this into account and make a best
758 faith effort.

759 12. Licenses for existing assets

760 Question: Are the creators or original owners of assets (e.g., code, data, models), used in
761 the paper, properly credited and are the license and terms of use explicitly mentioned and
762 properly respected?

763 Answer: [Yes]

764 Justification: DistMult [14] and TransE [2] are cited. Core Python libraries (NumPy, scikit-
765 learn) are BSD-3-Clause licensed. Knowledge graphs are original curated datasets.

766 Guidelines:

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782 **13. New assets**

783 Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

784 Answer: [Yes]

785 Justification: Five curated KG datasets are documented in Appendix A with entity/edge counts, type vocabularies, and split ratios. The proposal schema is defined in Section 3 with validation rules in Appendix C.

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787 **14. Crowdsourcing and research with human subjects**

788 Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

789 Answer: [NA]

790 Justification: No crowdsourcing or research with human subjects was conducted.

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821 subjects**

822 Question: Does the paper describe potential risks incurred by study participants, whether
823 such risks were disclosed to the subjects, and whether Institutional Review Board (IRB)
824 approvals (or an equivalent approval/review based on the requirements of your country or
825 institution) were obtained?

819 Answer: [NA]

820 Justification: No human subjects research was conducted; IRB approval is not applicable.

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823 with human subjects.
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832 16. Declaration of LLM usage

833 Question: Does the paper describe the usage of LLMs if it is an important, original, or
834 non-standard component of the core methods in this research? Note that if the LLM is used
835 only for writing, editing, or formatting purposes and does not impact the core methodology,
836 scientific rigorousness, or originality of the research, declaration is not required.

837 Answer: [Yes]

838 Justification: LLM-based proposal generation is a core methodological component de-
839 scribed in Section 3. The specific model family (local Ollama-served model) and prompting
840 strategy (entity-grounded, four-phase rotation: refine, combine, refine, novel) are detailed
841 in Sections 3 and 4.

842 Guidelines:

- 843 • The answer NA means that the core method development in this research does not
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