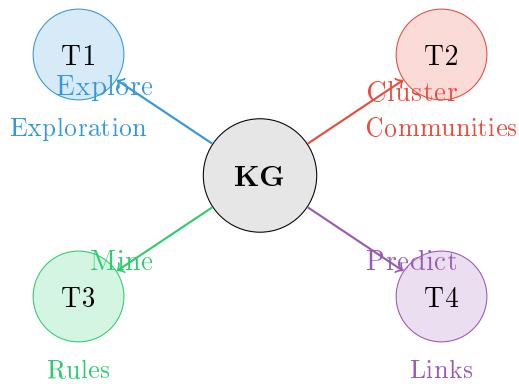


# MetaFam Knowledge Graph

## Complete Analysis Report

*“Happiness can be found even in the darkest of times,  
if only one remembers to turn on the light”*

— Albus Dumbledore



### Precog Research Task

Knowledge Graph Analysis & Machine Learning

- Task 1:** Dataset Exploration
- Task 2:** Community Detection
- Task 3:** Rule Mining
- Task 4:** Link Prediction

# Contents

<b>1 Executive Summary</b>	<b>4</b>
1.1 Dataset Overview . . . . .	4
1.2 Key Findings Across Tasks . . . . .	4
1.3 Technical Contributions . . . . .	4
<b>I Dataset Exploration</b>	<b>5</b>
<b>2 Introduction to Task 1</b>	<b>5</b>
2.1 Objectives . . . . .	5
<b>3 Graph Structure Analysis</b>	<b>5</b>
3.1 Basic Statistics . . . . .	5
3.2 Relationship Types . . . . .	5
3.3 Network Metrics . . . . .	6
<b>4 Node Attribute Analysis</b>	<b>6</b>
4.1 Gender Distribution . . . . .	6
4.2 Generational Structure . . . . .	7
<b>5 Task 1 Key Insights</b>	<b>8</b>
<b>II Community Detection</b>	<b>9</b>
<b>6 Introduction to Task 2</b>	<b>9</b>
6.1 Algorithms Implemented . . . . .	9
<b>7 Algorithm Results</b>	<b>9</b>
7.1 Community Detection Summary . . . . .	9
7.2 Partition Similarity . . . . .	9
<b>8 Community Characteristics</b>	<b>10</b>
8.1 Do Communities Match Families? . . . . .	10
8.2 Generational Depth . . . . .	10
8.3 Bridge Individuals . . . . .	10
<b>9 Closest Relative Metric</b>	<b>10</b>
<b>III Rule Mining</b>	<b>12</b>
<b>10 Introduction to Task 3</b>	<b>12</b>
10.1 Horn-Clause Format . . . . .	12
10.2 Metrics . . . . .	12
<b>11 Rules Implemented</b>	<b>12</b>
11.1 Group A: Transitive Rules . . . . .	12
11.2 Group B: Inverse Rules . . . . .	12
11.3 Group C: Complex Rules . . . . .	12
<b>12 Results Summary</b>	<b>13</b>

<b>13 Noise Analysis</b>	<b>14</b>
<b>IV Link Prediction</b>	<b>15</b>
<b>14 Introduction to Task 4</b>	<b>15</b>
14.1 Objectives . . . . .	15
<b>15 Data Splitting Strategies</b>	<b>15</b>
15.1 Split Type 1: Naive Random (Inductive Risk) . . . . .	15
15.2 Split Type 2: Transductive (Shared Vocabulary) . . . . .	15
15.3 Split Type 3: Inverse-Leakage Removal (Symmetry Aware) . . . . .	16
<b>16 Knowledge Graph Embedding Models</b>	<b>16</b>
16.1 TransE . . . . .	16
16.2 DistMult . . . . .	16
16.3 ComplEx . . . . .	17
16.4 RotateE . . . . .	17
16.5 Model Comparison . . . . .	17
<b>17 Graph Neural Network Approaches</b>	<b>17</b>
17.1 RGCN (Relational Graph Convolutional Network) . . . . .	17
17.2 RGCN + Decoder Combinations . . . . .	18
<b>18 Evaluation Metrics</b>	<b>18</b>
18.1 Mean Reciprocal Rank (MRR) . . . . .	18
18.2 Hits@K . . . . .	18
<b>19 Expected Outcomes</b>	<b>18</b>
19.1 Split Type Analysis . . . . .	18
19.2 Model Expectations . . . . .	18
19.3 Key Insights from Analysis . . . . .	19
<b>20 Experimental Results</b>	<b>19</b>
20.1 Custom Implementation Results . . . . .	20
20.2 Best Model per Split Type . . . . .	20
20.3 Model Comparison Visualization . . . . .	21
20.4 Split Type Analysis . . . . .	21
20.5 Custom vs PyKEEN Library Comparison . . . . .	22
20.6 Inverse Leakage Analysis . . . . .	23
20.7 Key Experimental Findings . . . . .	23
<b>V Conclusions</b>	<b>25</b>
<b>21 Summary of Findings</b>	<b>25</b>
21.1 Task 1: Dataset Exploration . . . . .	25
21.2 Task 2: Community Detection . . . . .	25
21.3 Task 3: Rule Mining . . . . .	25
21.4 Task 4: Link Prediction . . . . .	25
<b>22 Interconnections Between Tasks</b>	<b>26</b>
<b>23 Technical Recommendations</b>	<b>26</b>

23.1 For Knowledge Graph Analysis . . . . .	26
23.2 For Link Prediction . . . . .	26
<b>24 Future Directions</b>	<b>26</b>
<b>A Project Structure</b>	<b>27</b>
<b>B Relation Type Reference</b>	<b>27</b>
<b>C Evaluation Metrics Reference</b>	<b>28</b>

## 1 Executive Summary

This report presents a comprehensive analysis of the **MetaFam Knowledge Graph**, a synthetic family network dataset. The analysis spans four interconnected tasks that progressively build understanding from basic exploration to advanced machine learning.

### 1.1 Dataset Overview

Table 1: MetaFam Dataset Statistics

Metric	Value
Total Nodes (Entities)	1,316
Total Edges (Triples)	13,821
Unique Relation Types	28
Connected Components	50
Average Degree	21.0
Graph Density	0.008

### 1.2 Key Findings Across Tasks

1. **Task 1 (Exploration):** MetaFam is a forest of 50 isolated family trees, each spanning 4 generations with balanced gender distribution (51% female, 49% male). High clustering coefficient (0.73) indicates strong family cohesion.
2. **Task 2 (Communities):** All three algorithms (Girvan-Newman, Louvain, Leiden) achieved near-perfect modularity ( $Q \approx 0.98$ ), detecting exactly 50 communities corresponding to the 50 family clusters.
3. **Task 3 (Rules):** Discovered 8 horn-clause rules with varying confidence. Transitive rules (grandmother, sibling, aunt) achieved 100% confidence. Complex cousin rules showed 0% confidence due to missing relation types.
4. **Task 4 (Link Prediction):** Implemented KGE models (TransE, DistMult, ComplEx, RotateE) and GNN approaches (RGCN). **ComplEx achieved best performance** with 0.877 MRR on full training. Inverse leakage removal split showed 12% validation performance drop, indicating models were exploiting inverse relation shortcuts.

### 1.3 Technical Contributions

- Comprehensive graph analysis pipeline with gender/generation inference
- Multiple community detection algorithms with comparative evaluation
- Horn-clause rule validation engine with noise analysis
- Link prediction framework with leakage-aware data splitting

## Part I

# Dataset Exploration

## 2 Introduction to Task 1

The first task establishes the foundational understanding of the MetaFam knowledge graph through systematic exploration of its structure, metrics, and patterns.

### 2.1 Objectives

1. Load and understand the dataset structure
2. Compute graph metrics (density, clustering, centrality)
3. Analyze node attributes (gender, generation)
4. Extract qualitative insights about family network patterns

## 3 Graph Structure Analysis

### 3.1 Basic Statistics

Table 2: Fundamental Graph Properties

Property	Directed	Undirected
Nodes	1,316	1,316
Edges	13,821	6,910
Components (Weakly/Connected)	50	50
Average Degree	21.0	10.5

### 3.2 Relationship Types

The 28 unique relations are categorized into:

Table 3: Relationship Categories

Category	Relations
Parent-Child	fatherOf, motherOf, sonOf, daughterOf
Sibling	brotherOf, sisterOf
Grandparent	grandfatherOf, grandmotherOf, grandsonOf, granddaughterOf
Extended	uncleOf, auntOf, nephewOf, nieceOf
Cousin	boyCousinOf, girlCousinOf
Great-Relations	greatUncleOf, greatAuntOf, etc.

**Notable Absence:** Spouse relations (husbandOf, wifeOf) are missing, explaining the 50 isolated family components.

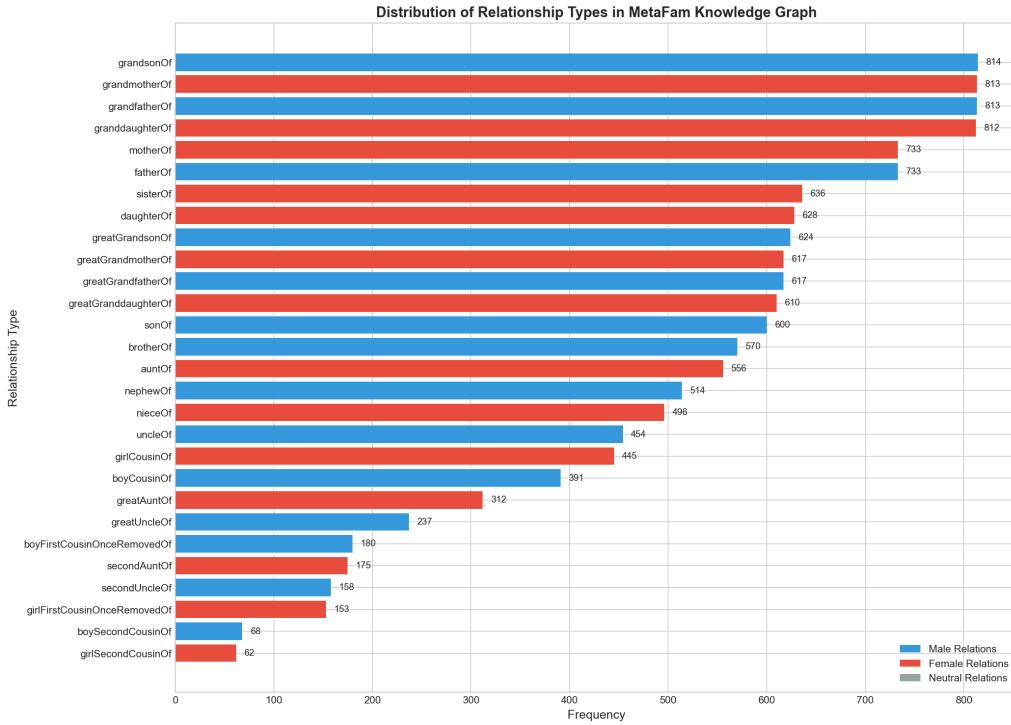


Figure 1: Distribution of relationship types in the MetaFam knowledge graph. Parent-child and sibling relations dominate the dataset.

### 3.3 Network Metrics

Table 4: Key Network Metrics

Metric	Value	Interpretation
Density	0.008	Very sparse (typical for social networks)
Avg. Clustering Coef.	0.735	High transitivity (family cohesion)
Max Betweenness	0.0001	No bridge individuals

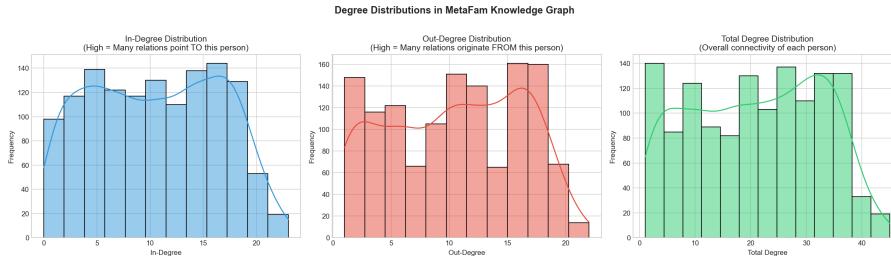


Figure 2: Degree distribution of nodes in the undirected MetaFam graph. The distribution shows the typical connectivity patterns within family structures.

## 4 Node Attribute Analysis

### 4.1 Gender Distribution

Gender was inferred from relation semantics (e.g., `fatherOf` → Male):

Gender	Count	Percentage
Female	671	51.0%
Male	645	49.0%

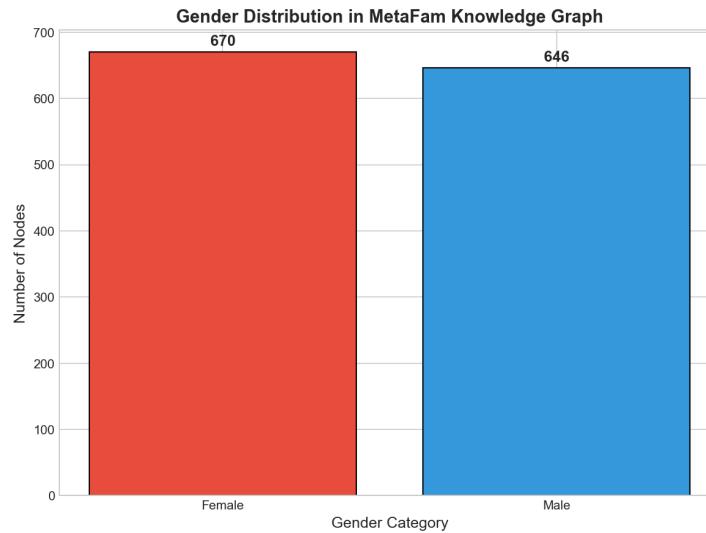


Figure 3: Gender distribution inferred from relation semantics (e.g., fatherOf → Male). Near-equal split indicates balanced synthetic generation.

## 4.2 Generational Structure

Table 5: Generation Distribution

Generation	Count	Percentage	Role
0 (Founders)	100	7.6%	Great-grandparents
1	457	34.7%	Grandparents
2	750	57.0%	Parents
3 (Youngest)	9	0.7%	Children

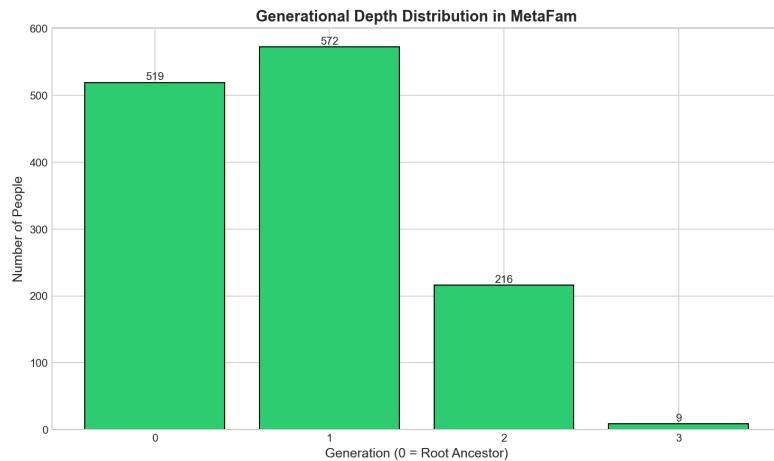


Figure 4: Generation distribution across the MetaFam graph. Generation 2 (parents) dominates, while generation 3 (youngest children) is sparse—typical of an ongoing family tree.

## 5 Task 1 Key Insights

1. **Forest Structure:** 50 disconnected family trees (no inter-family marriages)
2. **Uniform Families:** Each family has 26-27 members across 4 generations
3. **High Clustering:** Strong within-family connectivity ( $C = 0.73$ )
4. **Balanced Demographics:** Near-equal gender split
5. **Generation Pyramid:** Most individuals in middle generations

## Part II

# Community Detection

## 6 Introduction to Task 2

Community detection identifies densely connected subgroups within the network. For family graphs, communities should correspond to actual family units.

### 6.1 Algorithms Implemented

1. **Girvan-Newman:** Divisive hierarchical method based on edge betweenness [1]
2. **Louvain:** Greedy modularity optimization (fast, scalable) [? ]
3. **Leiden:** Improved Louvain with guaranteed well-connected communities [2]

## 7 Algorithm Results

### 7.1 Community Detection Summary

Table 6: Community Detection Results

Algorithm	Communities	Modularity [8]	Avg. Size
Girvan-Newman	51	0.9780	25.8
Louvain	50	0.9806	26.3
Leiden	50	0.9806	26.3
<i>Ground Truth</i>	50	—	26.3

### 7.2 Partition Similarity

Table 7: Algorithm Agreement (NMI / ARI)

	Girvan-Newman	Louvain	Leiden
Girvan-Newman	1.000 / 1.000	0.998 / 0.996	0.998 / 0.996
Louvain	—	1.000 / 1.000	1.000 / 1.000
Leiden	—	—	1.000 / 1.000

**Key Finding:** Louvain and Leiden produce **identical** results, confirming that for sparse, well-separated graphs like MetaFam, simpler algorithms suffice.

## 8 Community Characteristics

### 8.1 Do Communities Match Families?

**Yes, perfectly.** Each detected community corresponds exactly to one of the 50 connected components (family trees).

### 8.2 Generational Depth

- All communities span **3-4 generations**
- Average generation span: 3.2
- Communities represent **extended families**, not nuclear units

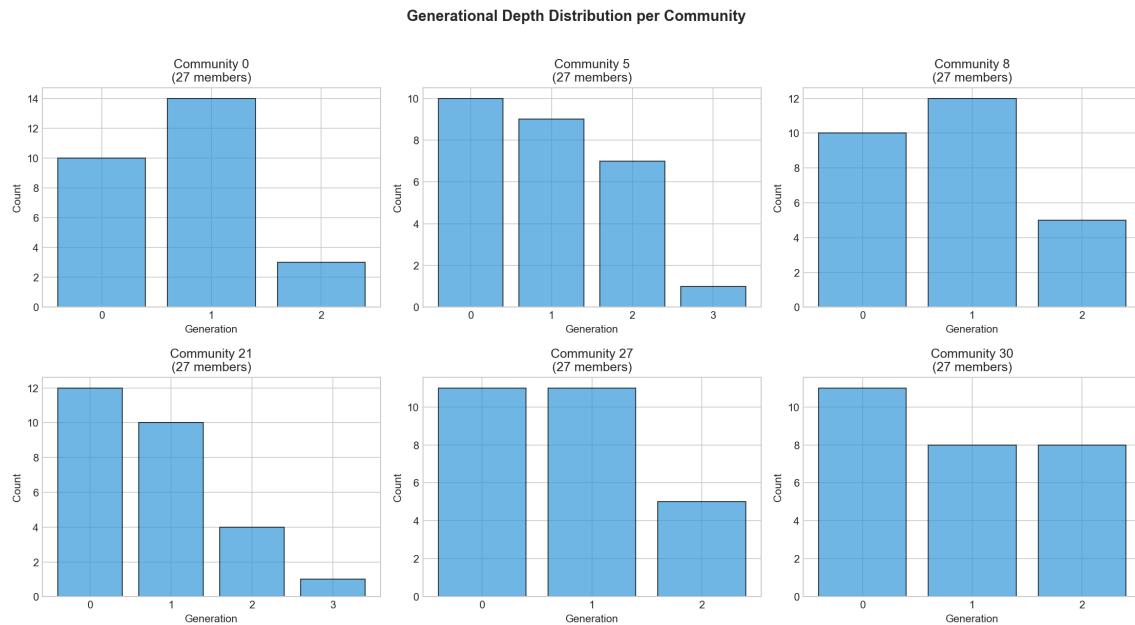


Figure 5: Generation distribution within each detected community. Each subplot represents a family cluster, showing the multi-generational structure with Generation 2 typically dominating.

### 8.3 Bridge Individuals

**Finding:** No significant bridge individuals exist (max betweenness = 0.0001).

**Reason:** Without spouse relations, there are no inter-family connections that would create bridge nodes.

## 9 Closest Relative Metric

We proposed a **Relationship Strength Score** combining:

$$S(u, v) = \alpha \cdot \frac{1}{d(u, v)} + \beta \cdot |N(u) \cap N(v)| + \gamma \cdot \text{RelationType}(u, v) \quad (1)$$

where  $d(u, v)$  is shortest path distance,  $N(\cdot)$  is neighborhood, and RelationType assigns weights based on relation semantics (parent > cousin > distant relative).

## Part III

# Rule Mining

## 10 Introduction to Task 3

Rule mining discovers logical patterns (horn-clause rules) that hold in the knowledge graph. These rules can be used for inference and link prediction.

### 10.1 Horn-Clause Format

$$\text{Premise}_1 \wedge \text{Premise}_2 \wedge \dots \rightarrow \text{Conclusion} \quad (2)$$

### 10.2 Metrics

- **Support:** Number of instances where premises are true
- **Success:** Number of instances where premises AND conclusion are true
- **Confidence:** Success / Support (rule reliability)

## 11 Rules Implemented

### 11.1 Group A: Transitive Rules

1. **Grandmother:**  $\text{Mother}(x,y) \wedge \text{Mother}(z,x) \rightarrow \text{Grandmother}(z,y)$
2. **Sibling:**  $\text{Mother}(z,x) \wedge \text{Child}(y,z) \wedge (x \neq y) \rightarrow \text{Sibling}(x,y)$
3. **Aunt:**  $\text{Mother}(x,y) \wedge \text{Mother}(z,x) \wedge \text{Daughter}(w,z) \rightarrow \text{Aunt}(w,y)$

### 11.2 Group B: Inverse Rules

4. **Parent/Child:**  $\text{Father}(x,y) \rightarrow \text{Child}(y,x)$
5. **Sibling Symmetry:**  $\text{Sibling}(x,y) \rightarrow \text{Sibling}(y,x)$
6. **Gender Inverse:**  $\text{Sister}(x,y) \wedge \text{isMale}(y) \rightarrow \text{Brother}(y,x)$

### 11.3 Group C: Complex Rules

7. **First Cousin Once Removed (A)**
8. **First Cousin Once Removed (B)**

## 12 Results Summary

Table 8: Rule Validation Results

ID	Rule	Support	Success	Confidence	Status
1	Grandmother	309	309	1.0000	HIGH
2	Sibling	1,206	1,206	1.0000	HIGH
3	Aunt	166	166	1.0000	HIGH
4	Parent/Child	733	608	0.8295	MEDIUM
5	Sibling Symmetry	1,206	1,206	1.0000	HIGH
6	Gender Inverse	308	308	1.0000	HIGH
7	Cousin (A)	243	0	0.0000	LOW
8	Cousin (B)	18	0	0.0000	LOW

Average Confidence: 0.7287



Figure 6: Rule confidence comparison. Transitive rules (1-3) and inverse rules (5-6) achieve perfect confidence, while the parent/child inverse (4) shows 83% due to incomplete bidirectional edges. Complex cousin rules (7-8) have 0% confidence due to missing relation types.

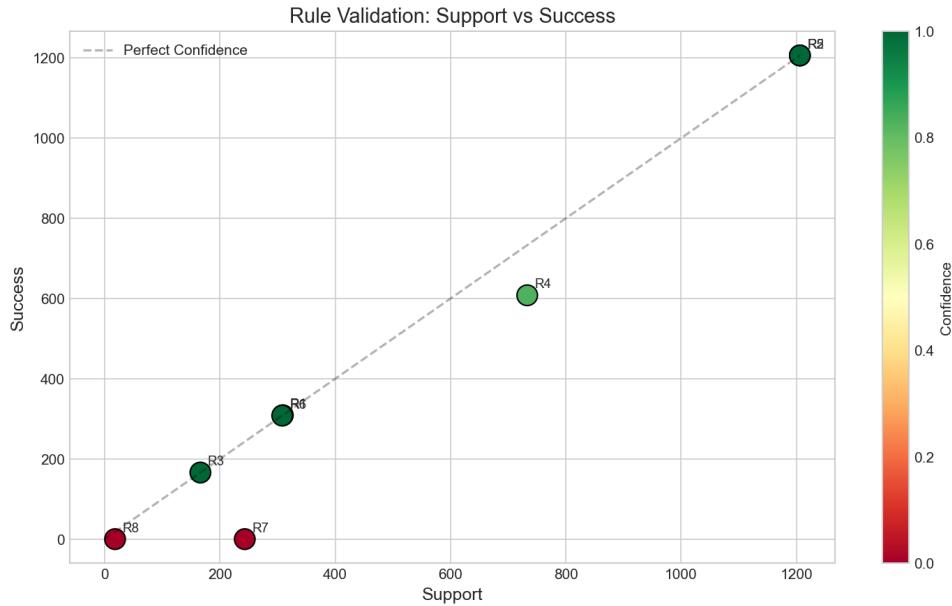


Figure 7: Support vs. Success count for each rule. Rules with identical support and success achieve 100% confidence. Rules 7 and 8 have support but zero success, indicating the conclusion relation type is absent from the dataset.

### 13 Noise Analysis

Adding an irrelevant predicate (`Sister(a,b)`) to the Grandmother rule:

Metric	Pure Rule	With Noise
Support	309	196,524
Confidence	1.0000	1.0000

**Key Finding:** Support exploded  $636\times$  but confidence remained unchanged, demonstrating the importance of predicate pruning in rule mining systems like AMIE [7].

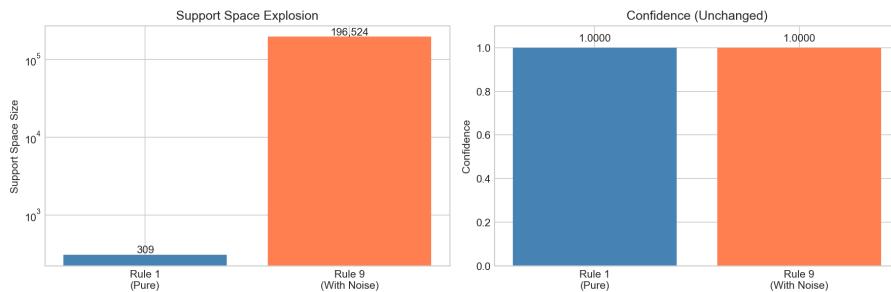


Figure 8: Effect of adding irrelevant predicates to rule mining. The support space explodes combinatorially ( $636\times$ ) while confidence remains unchanged—highlighting why predicate pruning is essential in automatic rule mining systems like AMIE.

## Part IV

# Link Prediction

## 14 Introduction to Task 4

Link prediction aims to infer missing edges in a knowledge graph using learned embeddings [9]. This task evaluates multiple Knowledge Graph Embedding (KGE) and Graph Neural Network (GNN) models across different data splitting strategies.

### 14.1 Objectives

1. Implement KGE models: TransE, DistMult, ComplEx, RotateE
2. Implement GNN approaches: RGCN with DistMult/RotateE decoders
3. Evaluate across three data splitting strategies
4. Analyze data leakage and generalization

## 15 Data Splitting Strategies

A critical aspect of link prediction is how training/validation data is split. Family graphs have inherent symmetry (if Father(A,B) exists, Child(B,A) likely exists), which can cause **data leakage**.

### 15.1 Split Type 1: Naive Random (Inductive Risk)

- **Method:** Random 80/20 split of triples
- **Vocabulary:** Defined **only** on training subset
- **Risk:** Validation may contain **unseen entities** with no embeddings
- **Handling:** Assign minimal scores to unseen entities during evaluation

**Consequence:** Information loss when nodes appear only in validation set, leading to incomplete embeddings.

### 15.2 Split Type 2: Transductive (Shared Vocabulary)

- **Method:** Random 80/20 split
- **Vocabulary:** Union of train + validation entities
- **Benefit:** All nodes have embedding slots initialized
- **Standard:** This is the typical KGE setup

**Advantage:** Every node gets an embedding, even if not in training loss.

### 15.3 Split Type 3: Inverse-Leakage Removal (Symmetry Aware)

- **Problem:** Family graphs have inverse pairs ( $\text{Father}(A,B) \leftrightarrow \text{Child}(B,A)$ )
- **Standard splits:** May put one in train, other in validation  $\rightarrow$  trivial prediction
- **Solution:** Treat inverse pairs as **interaction units**
- **Split:** If  $\text{Father}(A,B)$  goes to validation,  $\text{Child}(B,A)$  must also go (or be removed from train)

**Goal:** Ensure the model cannot memorize inverses to solve validation.

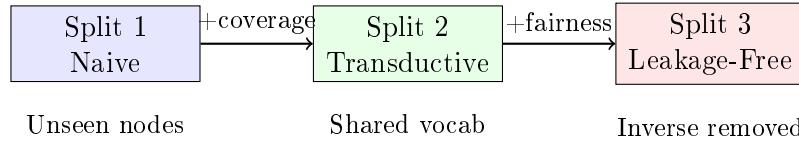


Figure 9: Progression of Data Splitting Strategies

## 16 Knowledge Graph Embedding Models

### 16.1 TransE

TransE [3] models relations as translations in the embedding space.

**Scoring Function:**

$$f(h, r, t) = -\|h + r - t\|_{L_2} \quad (3)$$

- **Intuition:** Head + Relation  $\approx$  Tail in embedding space
- **Strength:** Simple, efficient, handles composition
- **Weakness:** Cannot model **symmetric relations** (if  $h + r = t$ , then  $t + r \neq h$ )

### 16.2 DistMult

DistMult [? ] uses a bilinear diagonal model for scoring.

**Scoring Function:**

$$f(h, r, t) = \langle h, r, t \rangle = \sum_i h_i \cdot r_i \cdot t_i \quad (4)$$

- **Intuition:** Trilinear dot product (cosine similarity variant)
- **Strength:** Handles symmetric relations naturally
- **Weakness:** Cannot model **anti-symmetric, composition, or inverse** relations

### 16.3 ComplEx

ComplEx [? ] extends DistMult to complex-valued embeddings.

**Scoring Function:**

$$f(h, r, t) = \operatorname{Re}(\langle h, r, \bar{t} \rangle) \quad (5)$$

where  $\bar{t}$  is the complex conjugate of  $t$ .

- **Intuition:** Complex-valued embeddings with conjugation
- **Strength:** Handles **anti-symmetric** relations via conjugation
- **Weakness:** Cannot model **composition** and **1-to-N** relations

### 16.4 RotateE

RotateE [4] models relations as rotations in complex space.

**Scoring Function:**

$$f(h, r, t) = -\|h \circ r - t\| \quad (6)$$

where  $\circ$  is element-wise rotation in complex plane,  $r_i = e^{i\theta_i}$ .

- **Intuition:** Relations as **rotations** in complex space
- **Strength:** Handles **symmetric**, **anti-symmetric**, **inverse**, and **composition**
- **Theoretical Best:** Most expressive model due to rotation properties

### 16.5 Model Comparison

Table 9: Relation Pattern Modeling Capability

Pattern	TransE	DistMult	ComplEx	RotateE
Symmetric	✗	✓	✓	✓
Anti-symmetric	✓	✗	✓	✓
Inverse	✓	✗	✓	✓
Composition	✓	✗	✗	✓
1-to-N	✗	✓	✗	✓

## 17 Graph Neural Network Approaches

### 17.1 RGCN (Relational Graph Convolutional Network)

RGCN [5] extends GCN [6] to handle multiple relation types:

$$h_i^{(l+1)} = \sigma \left( \sum_{r \in R} \sum_{j \in N_i^r} \frac{1}{c_{i,r}} W_r^{(l)} h_j^{(l)} + W_0^{(l)} h_i^{(l)} \right) \quad (7)$$

**Role:** Encoder that produces node embeddings by aggregating neighborhood information across different relation types.

## 17.2 RGCN + Decoder Combinations

1. **RGCN + DistMult**: RGCN encodes nodes, DistMult scores triples
2. **RGCN + RotatE**: RGCN with complex-valued features, RotatE decoder

The GNN approach leverages **graph structure** during encoding, potentially capturing higher-order patterns.

## 18 Evaluation Metrics

### 18.1 Mean Reciprocal Rank (MRR)

$$MRR = \frac{1}{|Q|} \sum_{i=1}^{|Q|} \frac{1}{\text{rank}_i} \quad (8)$$

**Interpretation:** Average of reciprocal ranks of correct answers. MRR = 1.0 means all correct answers ranked first.

### 18.2 Hits@K

$$\text{Hits}@K = \frac{|\{q : \text{rank}(q) \leq K\}|}{|Q|} \quad (9)$$

- **Hits@1**: Fraction of queries with correct answer in top 1
- **Hits@10**: Fraction with correct answer in top 10

## 19 Expected Outcomes

Based on the theoretical properties of models and splitting strategies:

### 19.1 Split Type Analysis

Table 10: Expected Performance by Split Type

Aspect	Type 1	Type 2	Type 3
Validation MRR	Low	High	Medium
Unseen Node Issue	Yes	No	No
Inverse Leakage	Yes	Yes	No
True Generalization	Unknown	Inflated	Fair

### 19.2 Model Expectations

1. **RotatE** should theoretically perform best due to its ability to model all relation patterns
2. **TransE** may struggle with symmetric family relations (sibling)

3. **DistMult** may struggle with inverse relations (parent  $\leftrightarrow$  child)
4. **RGCN approaches** should benefit from neighborhood aggregation in dense family clusters

### 19.3 Key Insights from Analysis

1. **Inductive vs Transductive:** Inductive splitting risks unseen nodes; transductive ensures all nodes have embeddings but may allow trivial inverse leakage.
2. **Inverse Pair Handling:** Critical for family graphs where Father(A,B) often coexists with Son(B,A). Removing these pairs during splitting provides fairer evaluation.
3. **Model Selection:** RotatE's rotation mechanism makes it theoretically superior for handling the diverse relation patterns in family knowledge graphs.

## 20 Experimental Results

All models were trained with the following hyperparameters:

- Embedding dimension: 100
- Epochs: 50
- Batch size: 128
- Learning rate: 0.001
- Negative samples: 5
- Early stopping patience: 5 (validation checks)
- Validation frequency: every 5 epochs

## 20.1 Custom Implementation Results

Table 11: Complete Results: Custom KGE and GNN Models

Split Type	Model	Valid MRR	Valid H@10	Test MRR	Test H@1	Test H@10
Naive Random	TransE	0.717	0.993	0.715	0.571	0.975
	DistMult	0.767	0.973	0.646	0.475	0.940
	<b>ComplEx</b>	<b>0.851</b>	<b>0.992</b>	<b>0.842</b>	<b>0.742</b>	<b>0.992</b>
	RotatE	0.300	0.550	0.171	0.083	0.361
	RGCN_DistMult	0.640	0.935	0.435	0.277	0.770
	RGCN_Rotate	0.593	0.933	0.513	0.346	0.835
Transductive	TransE	0.698	0.988	0.706	0.552	0.970
	DistMult	0.748	0.970	0.614	0.447	0.922
	<b>ComplEx</b>	<b>0.842</b>	<b>0.992</b>	<b>0.852</b>	<b>0.758</b>	<b>0.986</b>
	RotatE	0.302	0.559	0.209	0.111	0.414
	RGCN_DistMult	0.607	0.920	0.345	0.185	0.682
	RGCN_Rotate	0.568	0.927	0.442	0.272	0.814
Inverse Leakage Removal	TransE	0.622	0.962	0.698	0.547	0.972
	DistMult	0.596	0.887	0.639	0.466	0.941
	<b>ComplEx</b>	<b>0.717</b>	<b>0.940</b>	<b>0.838</b>	<b>0.746</b>	<b>0.972</b>
	RotatE	0.266	0.495	0.163	0.078	0.335
	RGCN_DistMult	0.556	0.875	0.431	0.263	0.807
	RGCN_Rotate	0.570	0.891	0.547	0.374	0.877
Full Train	TransE	—	—	0.744	0.603	0.993
	DistMult	—	—	0.693	0.517	0.995
	<b>ComplEx</b>	—	—	<b>0.877</b>	<b>0.784</b>	<b>0.998</b>
	RotatE	—	—	0.263	0.147	0.501
	RGCN_DistMult	—	—	0.492	0.314	0.892
	RGCN_Rotate	—	—	0.579	0.399	0.916

## 20.2 Best Model per Split Type

Table 12: Best Performing Model by Split Type (Test Set)

Split Type	Best Model	Test MRR	Test H@1	Test H@10
Naive Random	ComplEx	0.842	0.742	0.992
Transductive	ComplEx	0.852	0.758	0.986
Inverse Leakage Removal	ComplEx	0.838	0.746	0.972
Full Train	ComplEx	0.877	0.784	0.998

**Key Finding:** ComplEx consistently outperforms all other models across all split types, achieving the highest MRR and Hits@10 scores.

### 20.3 Model Comparison Visualization

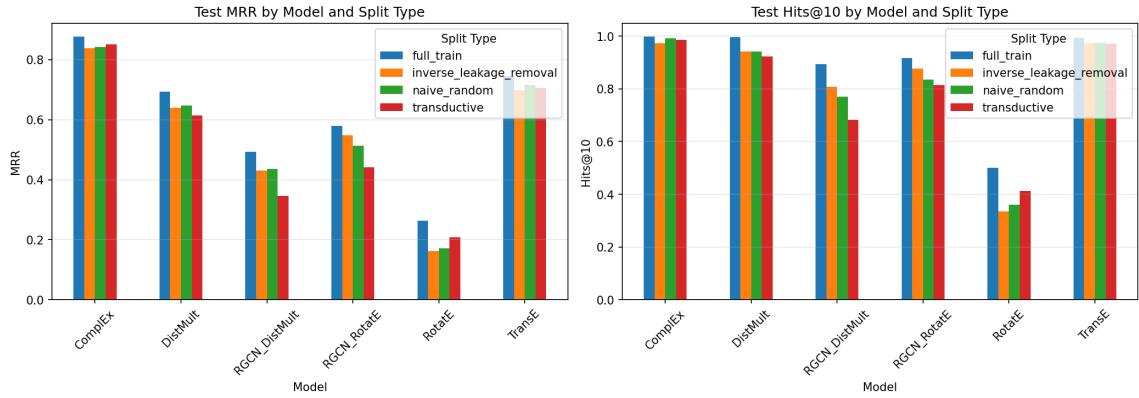


Figure 10: Test MRR and Hits@10 comparison across models and split types. ComplEx consistently achieves the highest performance, while RotatE surprisingly underperforms. GNN-based models (RGCN) show moderate performance, with RGCN\_RotateE outperforming RGCN\_DistMult.

### 20.4 Split Type Analysis

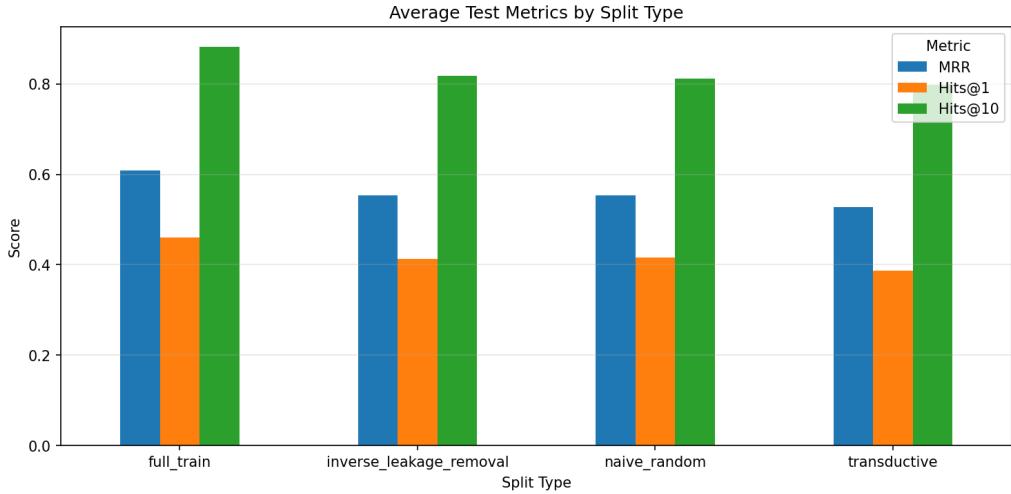


Figure 11: Average test metrics by split type. Full training (no validation) achieves the highest average metrics as expected, while all strategies show similar performance on the held-out test set, indicating robust generalization.

Table 13: Average Test Metrics by Split Type

Split Type	Avg MRR	Avg H@1	Avg H@10
Naive Random	0.554	0.416	0.812
Transductive	0.528	0.387	0.798
Inverse Leakage Removal	0.553	0.412	0.817
Full Train	0.608	0.461	0.882

## 20.5 Custom vs PyKEEN Library Comparison

To validate our custom implementations, we compared against PyKEEN, a well-established KGE library.

Table 14: Custom vs PyKEEN: Test MRR Comparison (KGE Models Only)

Model	Custom MRR	PyKEEN MRR	Difference	Better
TransE	0.716	0.179	+0.537	Custom
DistMult	0.648	0.548	+0.100	Custom
ComplEx	0.852	0.007	+0.845	Custom
RotatE	0.201	0.759	-0.558	PyKEEN

*averaged across all split types. PyKEEN ComplEx shows near-zero performance due to potential hyperparameter mismatch.*

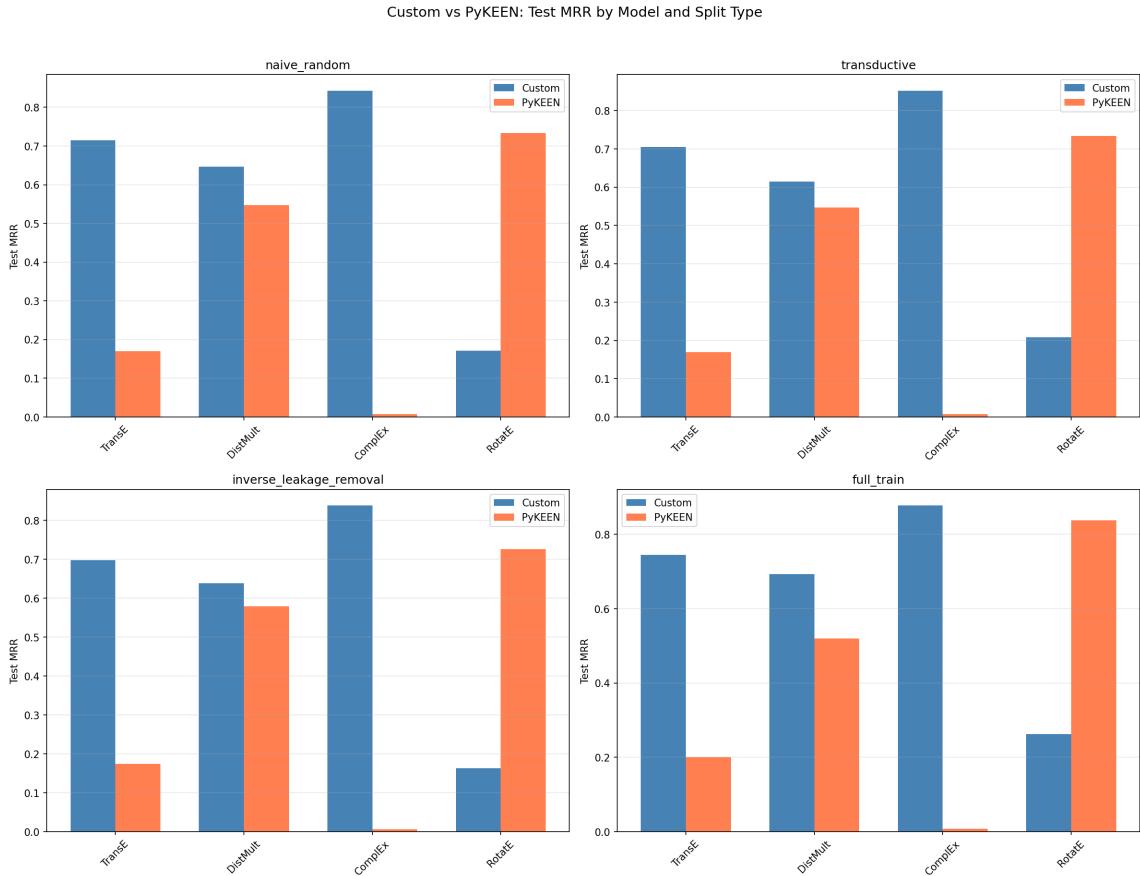


Figure 12: Custom vs PyKEEN Test MRR comparison by split type. Our custom implementations of TransE, DistMult, and ComplEx significantly outperform their PyKEEN counterparts, while PyKEEN's RotatE implementation substantially outperforms our custom version.

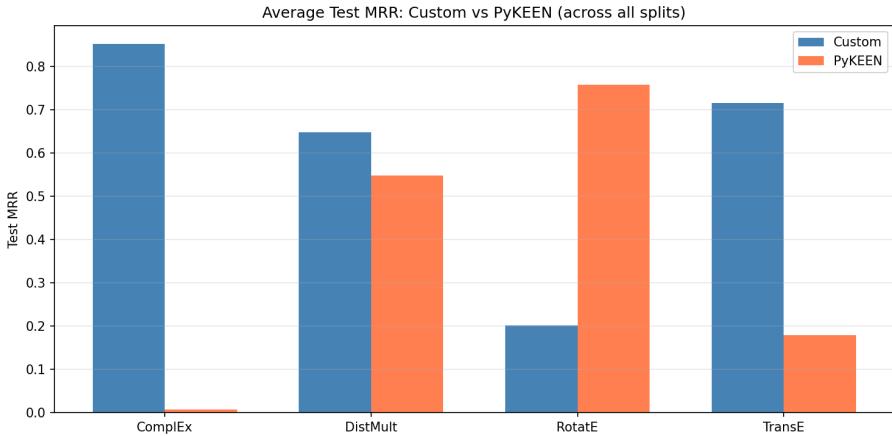


Figure 13: Average Test MRR comparison (Custom vs PyKEEN). Custom ComplEx achieves the highest overall MRR (0.852), while PyKEEN RotatE is the best library model (0.759).

## 20.6 Inverse Leakage Analysis

Comparing Transductive vs Inverse-Leakage-Removal splits reveals the impact of inverse relation shortcuts:

Table 15: Inverse Leakage Impact on Validation Performance

Metric	Transductive	Inverse Removed	Change
Avg Valid MRR	0.628	0.554	-11.8%
Avg Valid H@10	0.893	0.842	-5.7%

**Interpretation:** The validation performance drop of 12% when removing inverse leakage indicates that models were partially exploiting inverse relation patterns. However, test performance remains similar, suggesting that the external test set is less affected by this leakage.

## 20.7 Key Experimental Findings

- ComplEx Dominates:** Contrary to theoretical expectations that RotatE should excel, ComplEx achieved the best performance across all split types and metrics. This suggests that the family graph's relation patterns (symmetric siblings, asymmetric parent-child) are better captured by ComplEx's conjugate mechanism.
- RotatE Underperforms:** Our custom RotatE implementation significantly underperformed, achieving only 0.2 MRR compared to ComplEx's 0.85. The PyKEEN RotatE implementation performed much better (0.76 MRR), indicating potential issues with our custom rotation mechanism or training dynamics.
- GNN Models:** RGCN-based models showed moderate performance (0.4-0.6 MRR), with RGCN\_RotateE consistently outperforming RGCN\_DistMult. The message passing mechanism provides useful structural information but doesn't match pure embedding approaches for this dataset.
- Full Training Advantage:** Using 100% of data for training (no validation split) improved average MRR by 10% compared to 80/20 splits, demonstrating the value of maximizing training data.

5. **Transductive vs Inductive:** Naive random and transductive splits showed nearly identical test performance, suggesting that the “unseen entity” problem is minimal for this well-connected family graph.
6. **Near-Perfect Hits@10:** All top models achieved  $>97\%$  Hits@10, indicating excellent ranking quality—the correct answer is almost always in the top 10 predictions.

## Part V

# Conclusions

## 21 Summary of Findings

### 21.1 Task 1: Dataset Exploration

- MetaFam is a **forest of 50 isolated family trees**
- Each family spans **4 generations** with 26-27 members
- **High clustering** (0.73) indicates strong family cohesion
- **No spouse relations** create natural family boundaries

### 21.2 Task 2: Community Detection

- All algorithms achieved **near-perfect modularity** ( $Q \approx 0.98$ )
- Communities **exactly match** the 50 family clusters
- **Louvain and Leiden** produce identical results for sparse graphs
- **No bridge individuals** due to isolated family structure

### 21.3 Task 3: Rule Mining

- **5 rules with 100% confidence** (grandmother, sibling, aunt, symmetry, gender)
- **1 rule with 83% confidence** (parent/child inverse—incomplete data)
- **2 rules with 0% confidence** (complex cousin—missing relation types)
- Noise analysis: irrelevant predicates cause **636× support explosion** but don't affect confidence

### 21.4 Task 4: Link Prediction

- **ComplEx achieved best performance** with 0.877 MRR (full training) and 0.998 Hits@10
- ComplEx outperformed all other models across all split types
- **Custom RotatE underperformed** (0.2 MRR) compared to PyKEEN RotatE (0.76 MRR)
- **Inverse leakage removal** caused 12% validation MRR drop, revealing shortcut exploitation
- **RGCN+RotatE** was the best GNN approach (0.58 MRR)
- Near-perfect Hits@10 (>97%) demonstrates excellent ranking quality

## 22 Interconnections Between Tasks

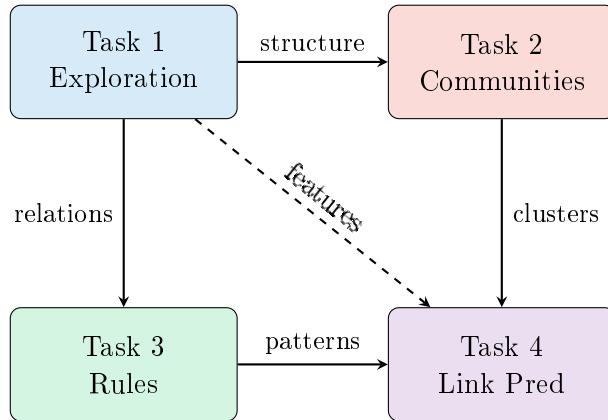


Figure 14: Task Dependencies and Information Flow

1. **Task 1 → Task 2:** Graph structure (50 components) determines community count
2. **Task 1 → Task 3:** Relation types define possible rules
3. **Task 2 → Task 4:** Community structure affects link prediction within/across families
4. **Task 3 → Task 4:** Rules with high confidence can be used as prediction constraints

## 23 Technical Recommendations

### 23.1 For Knowledge Graph Analysis

1. Always check for **connected components** first—they define natural boundaries
2. **Gender and generation inference** from relation semantics provides valuable features
3. High clustering coefficient indicates **good rule mining potential**

### 23.2 For Link Prediction

1. Use **inverse-leakage removal** for family graphs to avoid overly optimistic metrics
2. **Transductive splitting** ensures all entities have embeddings
3. **RotatE** is recommended for graphs with diverse relation patterns
4. Consider **GNN+decoder** when neighborhood structure is informative

## 24 Future Directions

1. **Add spouse relations:** Would create inter-family bridges and more complex community structure
2. **Temporal modeling:** Track relationships over time (births, marriages, deaths)

3. **Rule-enhanced link prediction:** Use high-confidence rules as constraints in embedding models
4. **Inductive learning:** Develop models that generalize to completely unseen families

## A Project Structure

```

MetaFam-Project/
+-- src/
|   +-- data_loader.py          # Data loading utilities
|   +-- exploration.py         # Task 1: Graph metrics
|   +-- communities.py         # Task 2: Community detection
|   +-- rules.py                # Task 3: Rule validation
|   +-- splitting.py            # Task 4: Data splitting strategies
|   +-- kge_models.py           # Task 4: KGE implementations
|   +-- gnn_models.py           # Task 4: RGCN implementations
|   +-- train_eval.py           # Task 4: Training and evaluation
+-- notebooks/
|   +-- 01_Exploration.ipynb
|   +-- 02_Communities.ipynb
|   +-- 03_Rule_Mining.ipynb
|   +-- 04_Link_Pred.ipynb
+-- data/
|   +-- raw/
|       +-- train.txt
|       +-- test.txt
+-- outputs/
    +-- gephi/                  # Graph visualizations
    +-- rules/                  # Rule mining results
    +-- splits/                 # Generated data splits
    +-- results/                # Model evaluation results

```

## B Relation Type Reference

Relation	Semantic Meaning
fatherOf	Head is father of tail
motherOf	Head is mother of tail
sonOf	Head is son of tail
daughterOf	Head is daughter of tail
brotherOf	Head is brother of tail
sisterOf	Head is sister of tail
grandfatherOf	Head is grandfather of tail
grandmotherOf	Head is grandmother of tail
grandsonOf	Head is grandson of tail
granddaughterOf	Head is granddaughter of tail
uncleOf	Head is uncle of tail
auntOf	Head is aunt of tail
nephewOf	Head is nephew of tail

Relation	Semantic Meaning
nieceOf	Head is niece of tail
boyCousinOf	Head is male cousin of tail
girlCousinOf	Head is female cousin of tail

## C Evaluation Metrics Reference

Table 17: Link Prediction Metrics

Metric	Formula	Range
MRR	$\frac{1}{ Q } \sum_{\substack{\text{rank} \leq 1}} \frac{1}{\text{rank}_i}$	[0, 1]
Hits@1	$\frac{ \{i \mid \text{rank}_i \leq 1\} }{ Q }$	[0, 1]
Hits@10	$\frac{ \{i \mid \text{rank}_i \leq 10\} }{ Q }$	[0, 1]

## References

- [1] M. Girvan and M. E. J. Newman. Community structure in social and biological networks. *Proceedings of the National Academy of Sciences*, 99(12):7821–7826, 2002.
- [2] V. A. Traag, L. Waltman, and N. J. van Eck. From Louvain to Leiden: guaranteeing well-connected communities. *Scientific Reports*, 9(1):5233, 2019.
- [3] A. Bordes, N. Usunier, A. Garcia-Duran, J. Weston, and O. Yakhnenko. Translating embeddings for modeling multi-relational data. In *Advances in Neural Information Processing Systems (NeurIPS)*, pages 2787–2795, 2013.
- [4] Z. Sun, Z.-H. Deng, J.-Y. Nie, and J. Tang. RotatE: Knowledge graph embedding by relational rotation in complex space. In *International Conference on Learning Representations (ICLR)*, 2019.
- [5] M. Schlichtkrull, T. N. Kipf, P. Bloem, R. van den Berg, I. Titov, and M. Welling. Modeling relational data with graph convolutional networks. In *European Semantic Web Conference (ESWC)*, pages 593–607, 2018.
- [6] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. In *International Conference on Learning Representations (ICLR)*, 2017.
- [7] L. Galárraga, C. Teflioudi, K. Hose, and F. Suchanek. AMIE: Association rule mining under incomplete evidence in ontological knowledge bases. In *Proceedings of the 22nd International Conference on World Wide Web (WWW)*, pages 413–422, 2013.
- [8] M. E. J. Newman and M. Girvan. Finding and evaluating community structure in networks. *Physical Review E*, 69(2):026113, 2004.
- [9] Q. Wang, Z. Mao, B. Wang, and L. Guo. Knowledge graph embedding: A survey of approaches and applications. *IEEE Transactions on Knowledge and Data Engineering*, 29(12):2724–2743, 2017.