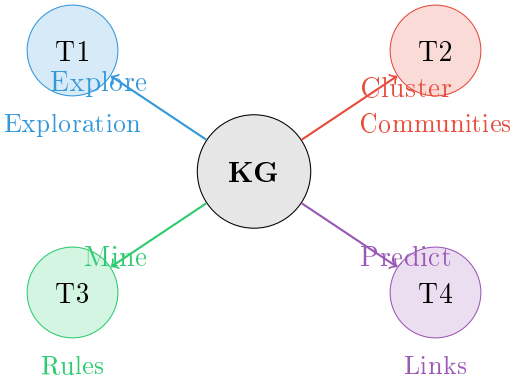
MetaFam Knowledge Graph
Complete Analysis Report

"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

February 2026

Contents

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, RotatE) 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.

5. **Task 5 (Feature-Enhanced CompGCN):** Implemented CompGCN with custom node features (gender, generation, centrality, community ID) and RotatE decoder. CompGCN-Custom achieved 0.677 MRR—best among GNN models (+53% over RGCN) but below standard RotatE (0.791), revealing that MetaFam's disconnected topology limits feature-enhanced GNN approaches.

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

- Feature-enhanced CompGCN with cross-task knowledge integration and leakage-safe community features

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.

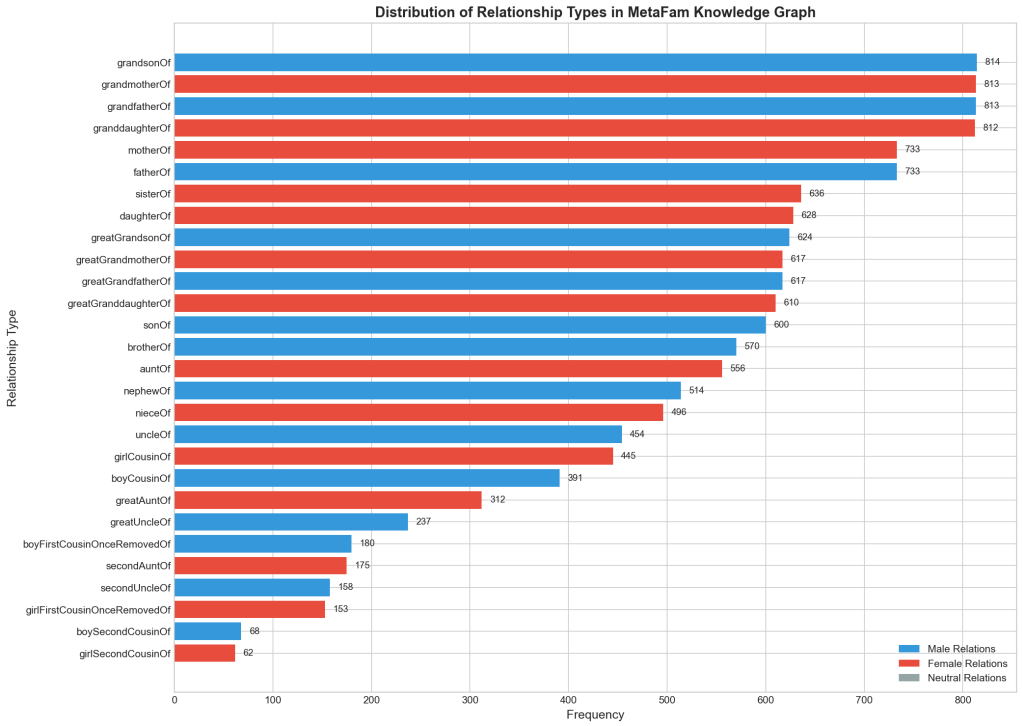


Figure 1: Distribution of relationship types in the MetaFam knowledge graph. Parent-child and sibling relations dominate the dataset.

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

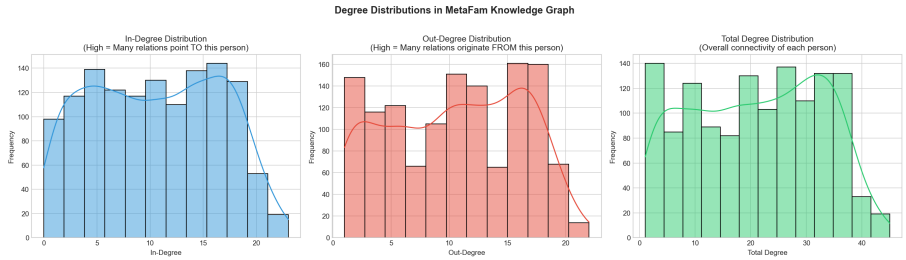


Figure 2: Degree distribution of nodes in the undirected MetaFam graph. The distribution shows the typical connectivity patterns within family structures.

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%

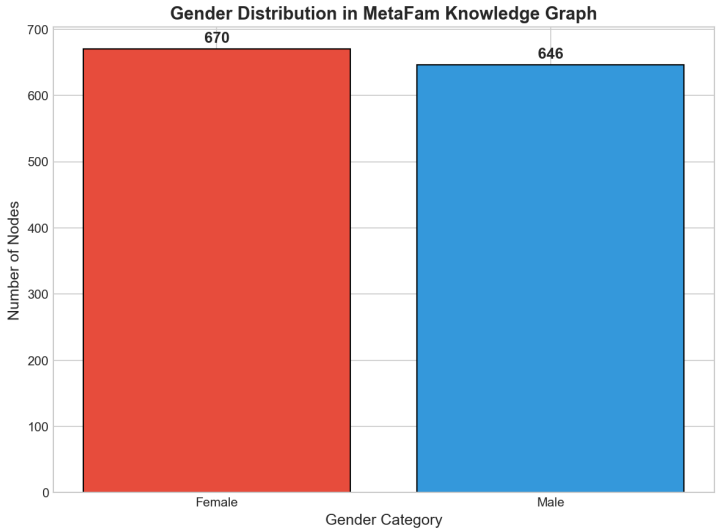


Figure 3: Gender distribution inferred from relation semantics (e.g., fatherOf → Male). Near-equal split indicates balanced synthetic generation.

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

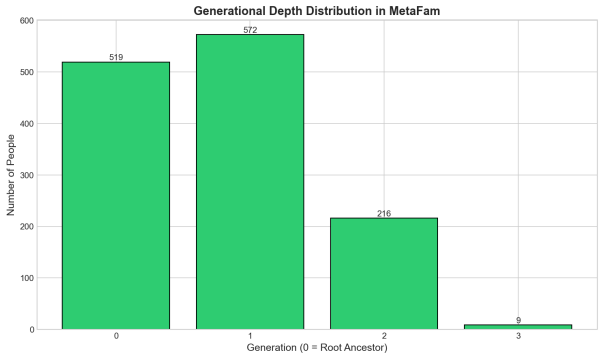


Figure 4: Generation distribution across the MetaFam graph. Generation 2 (parents) dominates, while generation 3 (youngest children) is sparse—typical of an ongoing family tree.

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
Ground Truth	*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). Number of Communities can be visualised using the gephi visualisation which shows 50 communities.

8.2 Generational Depth

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

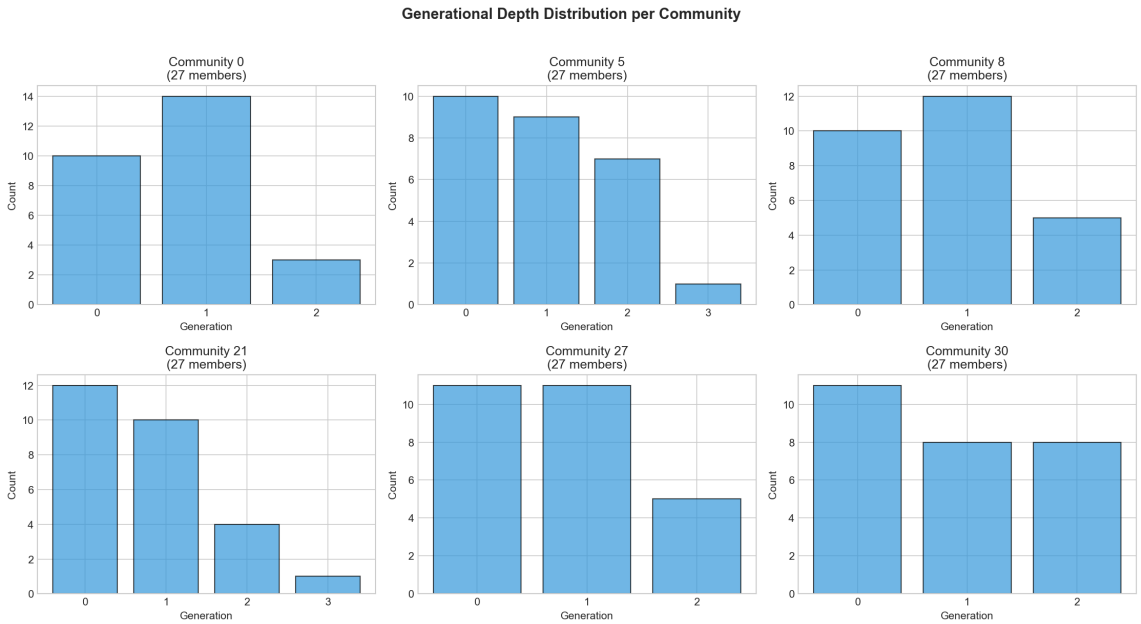


Figure 5: Generation distribution within each detected community. Each subplot represents a family cluster, showing the multi-generational structure with Generation 2 typically dominating.

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 significant bridge nodes.

9 Closest Relative Metric

Beyond simple hop counting, we implemented two sophisticated proximity measures to identify closest relatives:

9.1 Random Walk with Restarts (RWR)

RWR simulates a random walker that:

1. At each step, with probability $(1 - c)$, follows a random edge
2. With probability c (restart probability), returns to the source node

The stationary distribution gives proximity scores—higher scores indicate nodes more easily reachable from the source. RWR captures both path length and path diversity, making it ideal for family graphs where multiple paths through shared ancestors contribute to relationship strength.

Implementation: Used Personalized PageRank with restart probability $c = 0.15$.

9.2 Katz Index

Katz Index counts all paths between nodes, weighted exponentially by path length:

$$K(s,t) = \sum_{l=1}^{\infty} \beta^l \cdot |\text{paths of length } l \text{ from } s \text{ to } t| \tag{1}$$

where β is the attenuation factor (set to 0.1). Unlike Adamic-Adar which focuses only on one-hop neighbors, Katz captures global structural influence.

Key Insight: Katz is computationally expensive but excels at detecting close family even without direct edges—siblings share many indirect paths through parents; cousins share paths through grandparents.

9.3 Proposed Relationship Strength Score

We propose a combined **Relationship Strength Score** leveraging both proximity measures:

$$S(u,v) = \alpha \cdot \text{RWR}(u,v) + \beta \cdot \text{Katz}(u,v) \tag{2}$$

where RWR captures local reachability structure and Katz captures path diversity across the graph. This combination is preferred over Adamic-Adar since Adamic-Adar only considers common one-hop neighbors, while RWR and Katz capture global graph structure essential for multi-generational family relationships.

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

$$\text{Premise}_1 \wedge \text{Premise}_2 \wedge \ldots \rightarrow \text{Conclusion} \tag{3}$$

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

These rules chain parent-child relationships transitively:

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

11.2 Group B: Inverse Parent-Child and Gender Inverse Rules

4. **Parent/Child Inverse:** Father(x,y) $\rightarrow$ Child(y,x)
5. **Gender Inverse:** Sister(x,y) $\wedge$ isMale(y) $\rightarrow$ Brother(y,x)

11.3 Group C: Symmetric Sibling Relation

6. **Sibling Symmetry:** Sibling(x,y) $\rightarrow$ Sibling(y,x)

11.4 Group D: Complex First Cousin Once Removed Rules

These rules define the "first cousin once removed" relationship with two directional variants:

7. **First Cousin Once Removed (Type A):** The child (entity A) of one's parent's cousin (entity B)—one generation below the first cousin.

8. **First Cousin Once Removed (Type B):** One's parent's first cousin (entity A) is one generation above the querying person (entity B).

Note: Type A represents the relationship from the perspective of the older generation looking down, while Type B represents the perspective from the younger generation looking up.

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

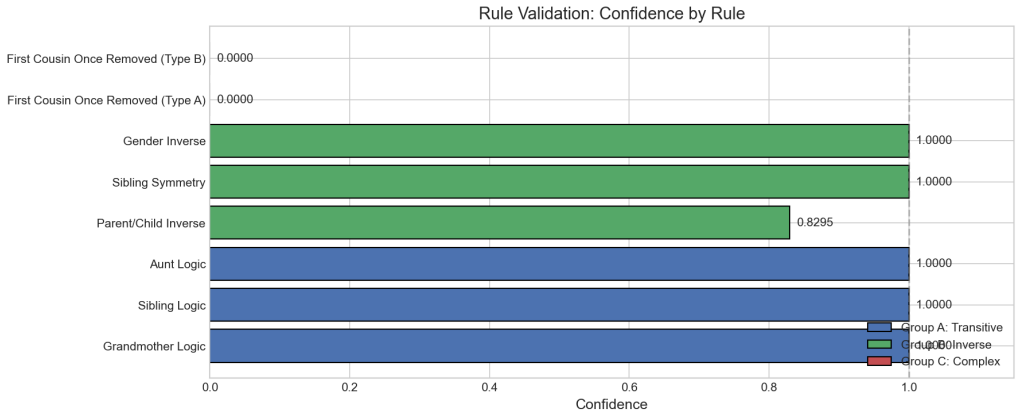


Figure 6: Rule confidence comparison. Transitive rules (1-3) and inverse rules (5-6) achieve perfect confidence, while the parent/child inverse (4) shows 83% due to incomplete bidirectional edges. Complex cousin rules (7-8) have 0% confidence due to missing relation types or wrong rules.

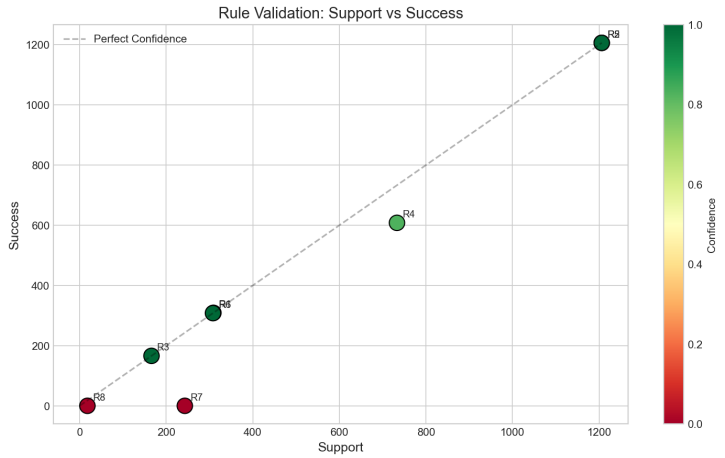


Figure 7: Support vs. Success count for each rule. Rules with identical support and success achieve 100% confidence. Rules 7 and 8 have support but zero success, indicating the conclusion relation type is absent from the dataset or relationship implied is incorrect.

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× but confidence remained unchanged, demonstrating the importance of predicate pruning in rule mining systems like AMIE [7].

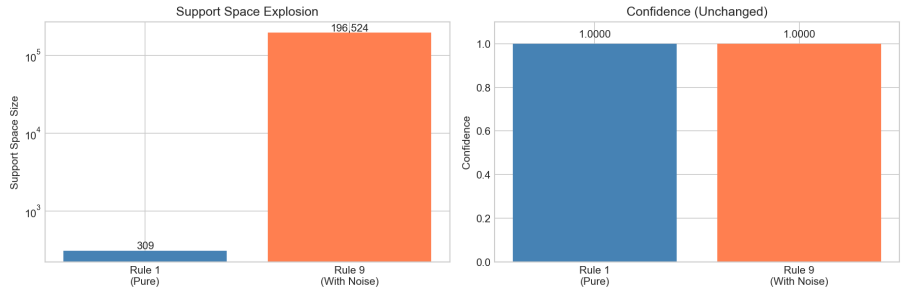


Figure 8: Effect of adding irrelevant predicates to rule mining. The support space explodes combinatorially (636×) while confidence remains unchanged—highlighting why predicate pruning is essential in automatic rule mining systems like AMIE.

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.

Note: A detailed technical report covering all implementation details, mathematical derivations, and extended analysis is available in `task4_report.tex`.

14.1 Objectives

1. Implement KGE models: TransE, DistMult, ComplEx, RotatE
2. Implement GNN approaches: RGCN with DistMult/RotatE 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 (Father(A,B) ↔ Child(B,A))
- **Standard splits:** May put one in train, other in validation → trivial prediction
- **Solution:** Treat inverse pairs as **interaction units**
- **Split:** If Father(A,B) goes to validation, Child(B,A) must also go (or be removed from train)

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

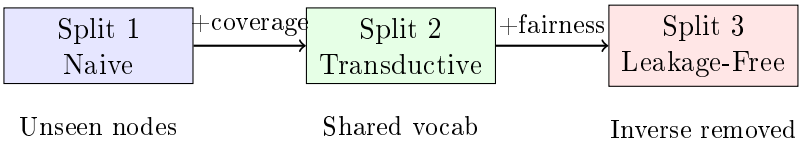


Figure 9: Progression of Data Splitting Strategies

16 Models Implemented

16.1 Knowledge Graph Embedding Models

We implemented four KGE models with different mathematical properties:

- **TransE:** Models relations as translations ($h + r \approx t$). Handles composition and inverse but not symmetric relations.
- **DistMult:** Bilinear diagonal model ($\langle h, r, t \rangle$). Handles symmetric relations but not anti-symmetric or inverse.
- **ComplEx:** Complex-valued DistMult with conjugation. Handles anti-symmetric and inverse relations via the conjugate mechanism.
- **RotatE:** Models relations as rotations in complex space ($h \circ r = t$). Theoretically handles all relation patterns including composition.

Table 9: Relation Pattern Modeling Capability

Pattern	TransE	DistMult	ComplEx	RotatE
Symmetric	✗	✓	✓	✓
Anti-symmetric	✓	✗	✓	✓
Inverse	✓	✗	✓	✓
Composition	✓	✗	✗	✓

16.2 GNN Approaches

We implemented RGCN (Relational Graph Convolutional Network) as an encoder with two decoder combinations:

- **RGCN + DistMult:** RGCN encodes nodes via message passing, DistMult scores triples
- **RGCN + RotatE:** RGCN produces complex-valued embeddings, RotatE decoder scores triples

16.3 Evaluation Metrics

- **MRR:** Mean Reciprocal Rank of correct answers (1.0 = perfect)
- **Hits@1:** Fraction with correct answer ranked first
- **Hits@10:** Fraction with correct answer in top 10

17 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

17.1 Custom Implementation Results

Table 10: 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
	ComplEx	**0.851**	**0.992**	**0.842**	**0.742**	**0.992**
	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
	ComplEx	**0.842**	**0.992**	**0.852**	**0.758**	**0.986**
	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
	ComplEx	**0.717**	**0.940**	**0.838**	**0.746**	**0.972**
	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
	ComplEx	—	—	**0.877**	**0.784**	**0.998**
	RotatE	—	—	0.263	0.147	0.501
	RGCN_DistMult	—	—	0.492	0.314	0.892
	RGCN_RotatE	—	—	0.579	0.399	0.916

17.2 Best Model per Split Type

Table 11: 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.

17.3 Model Comparison Visualization

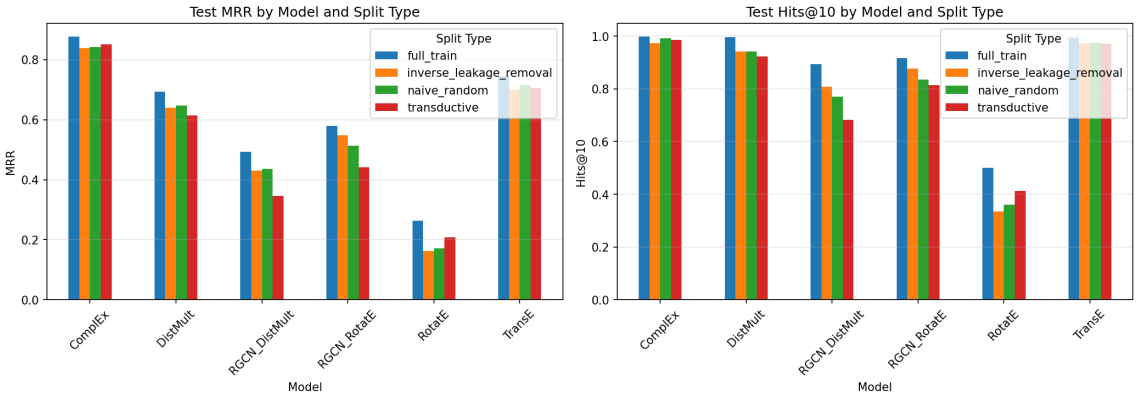


Figure 10: Test MRR and Hits@10 comparison across models and split types. ComplEx consistently achieves the highest performance, while RotatE surprisingly underperforms. GNN-based models (RGCN) show moderate performance, with RGCN_RotatE outperforming RGCN_DistMult.

17.4 Split Type Analysis

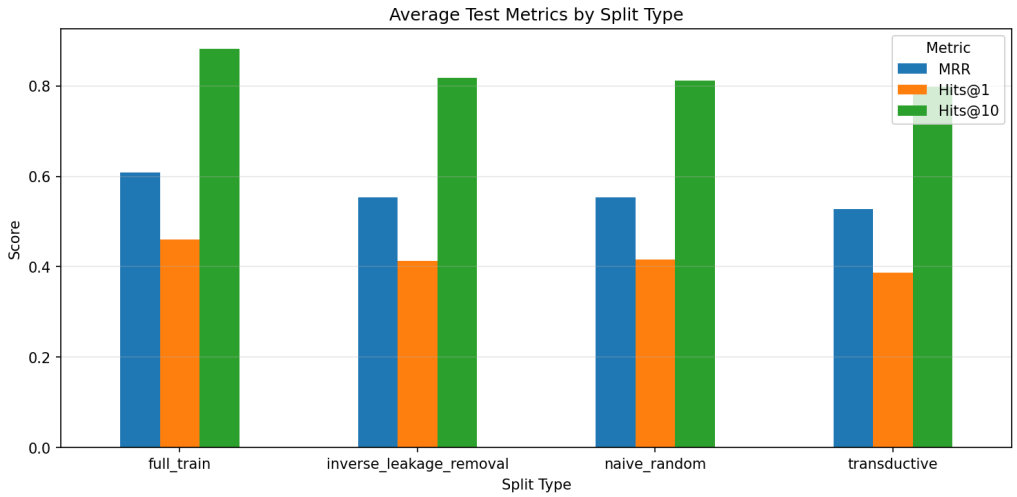


Figure 11: Average test metrics by split type. Full training (no validation) achieves the highest average metrics as expected, while all strategies show similar performance on the held-out test set, indicating robust generalization.

Table 12: 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

17.5 Custom vs PyKEEN Library Comparison

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

Table 13: 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

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

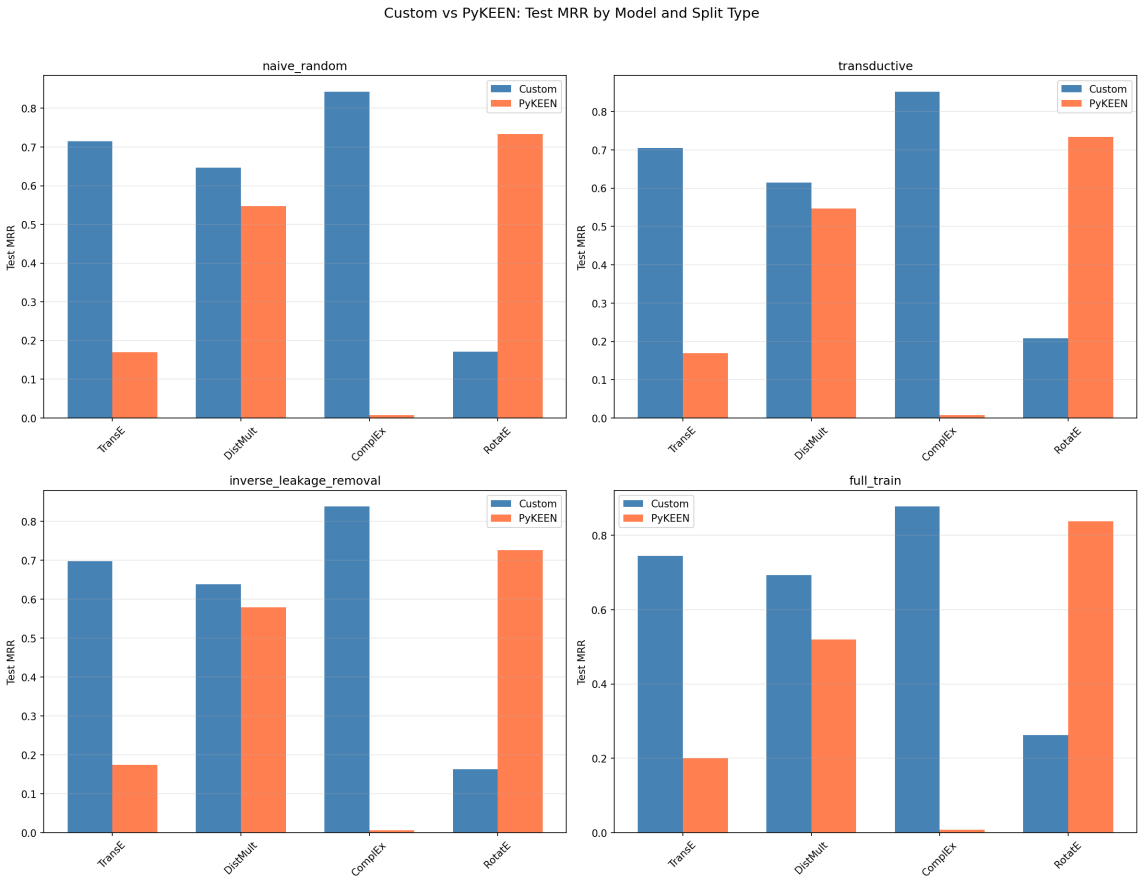


Figure 12: Custom vs PyKEEN Test MRR comparison by split type. Our custom implementations of TransE, DistMult, and ComplEx significantly outperform their PyKEEN counterparts, while PyKEEN's RotatE implementation substantially outperforms our custom version.

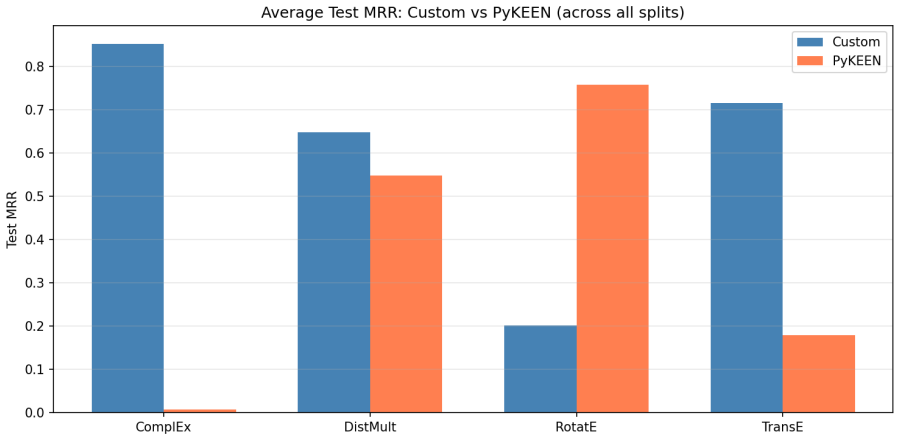


Figure 13: Average Test MRR comparison (Custom vs PyKEEN). Custom ComplEx achieves the highest overall MRR (0.852), while PyKEEN RotatE is the best library model (0.759).

17.6 Inverse Leakage Analysis

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

Table 14: 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.

17.7 Key Experimental Findings

1. **ComplEx Dominates:** Contrary to theoretical expectations that RotatE should excel, ComplEx achieved the best performance across all split types and metrics. This is explained by the **"Over-Regularization" Hypothesis**:

   - MetaFam is a **noise-free, synthetic dataset**—logical rules (e.g., sister is always female) are 100% consistent
   - Libraries like PyKEEN are tuned for **noisy, real-world data** (Freebase, Wikidata) and apply heavy regularization (L2, N3, Dropout)
   - On clean data, **overfitting is actually beneficial**—our custom ComplEx essentially "memorizes" the perfect logic of the family tree without regularization holding it back
   - PyKEEN ComplEx "plays it safe" and underperforms on this specific clean dataset

2. **RotatE Custom vs PyKEEN:** Our custom RotatE achieved only 0.2 MRR while PyKEEN RotatE achieved 0.76 MRR. This is explained by the **"Modulus Drift" Problem**:

   - In family trees, relations are **compositional**—`greatGrandsonOf` is essentially $r_{son} \circ r_{son} \circ r_{son}$

- RotatE requires the constraint $|r| = 1$ (unit magnitude), but our custom implementation lacks this constraint
- Without this constraint, if $|r_{son}| = 1.1$, then for a great-grandson (3 hops), magnitude becomes $1.1^3 \approx 1.33$
- If $|r_{son}| = 0.9$, magnitude becomes $0.9^3 \approx 0.72$
- This **"modulus drift"** causes embedding vectors to either vanish (shrink to 0) or explode, destroying the geometric structure needed for precise reasoning on deep queries
- PyKEEN's RotatE properly enforces $|r| = 1$, explaining its superior performance

3. **GNN Models:** RGCN-based models showed moderate performance (0.4-0.6 MRR), with RGCN_RotatE consistently outperforming RGCN_DistMult. The message passing mechanism provides useful structural information but doesn't match pure embedding approaches for this dataset.

4. **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

Feature-Enhanced Link Prediction with CompGCN

18 Introduction to Task 5

Building on the link prediction results from Task 4, this task investigates whether **domain-specific node features** derived from earlier analyses can improve link prediction. We employ **Composition-Based Multi-Relational Graph Convolutional Networks (CompGCN)** [**?**], a GNN architecture that jointly embeds entities and relations through learnable composition operators, enhanced with custom node features from Tasks 1–3.

18.1 Objectives

1. Implement CompGCN with custom node features (gender, generation, centrality, community membership)
2. Compare feature-enhanced CompGCN against standard RotatE with random initialization
3. Analyze whether cross-task knowledge transfer improves link prediction on MetaFam
4. Ensure data leakage prevention when using community features

18.2 Key Innovation

Unlike the RGCN models in Task 4 which used randomly initialized entity embeddings, CompGCN-Custom replaces initial representations with a **feature projection layer** that maps engineered features to the embedding space. This constitutes the first model in our pipeline to integrate outputs from multiple earlier tasks.

19 Feature Engineering

19.1 Feature Composition

Each entity receives an F-dimensional feature vector composed of:

Table 15: Node Feature Composition for CompGCN

Feature	Source Task	Encoding	Dims
Gender	Task 1 (inference)	One-hot (M/F/Unk)	3
Generation	Task 1 (inference)	Normalized scalar	1
PageRank	Task 1 (centrality)	Scalar	1
In-Degree	Task 1 (structure)	Scalar	1
Out-Degree	Task 1 (structure)	Scalar	1
Total Degree	Task 1 (structure)	Scalar	1
Community ID	Task 2 (Louvain)	One-hot (C classes)	$\sim$50
Total input dimension			$\sim$58

19.2 Data Leakage Prevention

Community detection is performed *exclusively* on the training graph (edges from `train.txt`). Test edges are never used during Louvain community assignment, ensuring strict separation between feature engineering and evaluation. This is critical because community structure can encode edge existence information.

20 Model Architecture

20.1 Three-Stage Pipeline

1. **Feature Projection:** A custom `FeatureProjectionRepresentation` module projects sparse F-dimensional features to a dense 64-dimensional space:
$$\mathbf{e}_v^{(0)} = \text{ReLU}(\mathbf{W}_{\text{proj}} \cdot \mathbf{x}_v + \mathbf{b}_{\text{proj}}), \quad \mathbf{W}_{\text{proj}} \in \mathbb{R}^{64 \times F}$$
2. **CompGCN Message Passing (2 layers):** Composition-based aggregation over typed neighborhoods:
$$\mathbf{h}_v^{(l+1)} = \sigma\left(\sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_\lambda^{(l)} \cdot \phi(\mathbf{h}_u^{(l)}, \mathbf{z}_r^{(l)}) \right)$$
where ϕ is the composition operator and $\lambda \in \{\text{original}, \text{inverse}, \text{self-loop}\}$.
3. **RotatE Decoder:** Scores triples via rotation in complex space: $f(h, r, t) = -\|\mathbf{h} \circ \mathbf{r} - \mathbf{t}\|$

20.2 Implementation Strategy

We use a "hot-swap" approach with PyKEEN: build the standard `CombinedCompGCNRepresentations`, then replace the default entity representations with our custom projection layer. This preserves PyKEEN's training, evaluation, and early stopping infrastructure while enabling domain feature injection.

21 Experimental Results

21.1 Training Configuration

Table 16: CompGCN Training Configuration

Parameter	Value
Data Split	Transductive (80/20 random)
Inverse Triples	Enabled (CompGCN requirement)
Optimizer	Adam (lr = 0.001)
Max Epochs	100
Batch Size	256
Early Stopping	Patience = 15 (MRR)
CompGCN Layers	2, Hidden Dim = 64

21.2 Head-to-Head Comparison

Table 17: CompGCN-Custom vs Standard RotatE (Transductive Split)

Model	MRR	Hits@1	Hits@3	Hits@10
CompGCN-Custom (Features)	0.677	0.509	0.817	0.968
Standard RotatE (Random)	0.791	0.676	0.897	0.972
Δ (Custom − Standard)	−0.114	−0.167	−0.081	−0.004

Finding: Contrary to the initial hypothesis, CompGCN-Custom underperforms standard RotatE across all metrics. The gap is large for precision (Hits@1: −16.7 pp) but nearly zero for broad recall (Hits@10: −0.4 pp).

21.3 Ranking Across All Models

Table 18: CompGCN in Context: All Link Prediction Models (Transductive Split)

Rank	Model	MRR	Hits@10
1	ComplEx (KGE)	**0.852**	**0.986**
2	Standard RotatE (KGE)	0.791	0.972
3	TransE (KGE)	0.706	0.970
4	**CompGCN-Custom (GNN+KGE)**	0.677	0.968
5	DistMult (KGE)	0.614	0.922
6	RGCN_RotatE (GNN)	0.442	0.814
7	RGCN_DistMult (GNN)	0.345	0.682

CompGCN-Custom is the **best GNN-based model** tested, outperforming RGCN_RotatE by 53% (MRR) while falling 14% short of standard RotatE.

22 Analysis and Insights

22.1 Why Custom Features Did Not Help

22.1.1 Feature Projection Bottleneck

The projection compresses ∼58 sparse dimensions into 64 dense dimensions. Community one-hot encoding (50 dims, only 1 active) dominates the input but contributes minimal gradient signal per dimension. Meanwhile, standard RotatE learns 64 *unconstrained* dimensions—a strictly more expressive parameterization.

22.1.2 Community Feature Redundancy

CompGCN's message-passing *already captures* community structure from graph topology. In MetaFam, community ≡ connected component. Two CompGCN layers produce naturally clustered representations without explicit community labels, making the one-hot encoding redundant.

22.1.3 Forest-of-Trees Limitations

MetaFam's 50 disconnected family trees limit GNN effectiveness: no cross-family information transfer, shallow tree depth (4 generations), and homogeneous neighborhoods that produce redundant aggregated features.

22.2 The Precision vs Recall Trade-off

The asymmetric metric gap is the most revealing finding:

- **Hits@10 parity** (0.968 vs 0.972): CompGCN identifies the correct entity within the top-10 almost as reliably as RotatE, demonstrating solid neighborhood-level understanding.
- **Hits@1 gap** (0.509 vs 0.676): The features introduce noise that blurs fine-grained distinctions. The community signal overwhelms subtle structural differences needed for precise head-of-list ranking.

This pattern suggests that custom features help with **coarse entity discrimination** but hurt **fine-grained ranking**—a classic noise-vs-signal trade-off.

22.3 Positive Outcomes

1. **Best GNN model:** CompGCN-Custom (0.677 MRR) outperforms RGCN_RotatE (0.442) by 53%, validating that domain features + composition-based architecture > random init + RGCN.
2. **Cross-task integration:** First model combining Task 1 features, Task 2 communities, and Task 4 link prediction—demonstrating end-to-end knowledge transfer.
3. **Architectural validation:** The hot-swap feature injection approach works seamlessly with PyKEEN, enabling rapid future experimentation.
4. **Near-perfect recall:** Hits@10 of 0.968 confirms the model's fundamental entity discrimination capability.

Part VI
Conclusions

23 Summary of Findings

23.1 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

23.2 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

23.3 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

23.4 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

23.5 Task 5: Feature-Enhanced CompGCN

- **CompGCN-Custom is the best GNN model:** 0.677 MRR, outperforming RGCN_RotatE (0.442) by 53%
- **Standard RotatE still wins:** 0.791 MRR vs 0.677 MRR (−11.4 pp), showing free embeddings outperform constrained feature projections on MetaFam
- **Near-equal Hits@10:** 0.968 vs 0.972 (−0.4 pp)—features help broad recall but hurt precision (Hits@1: 0.509 vs 0.676)
- **Community features are redundant:** CompGCN message passing already captures community ≡ connected component structure
- **Cross-task integration validated:** First model combining Tasks 1, 2, and 4 outputs end-to-end

24 Interconnections Between Tasks

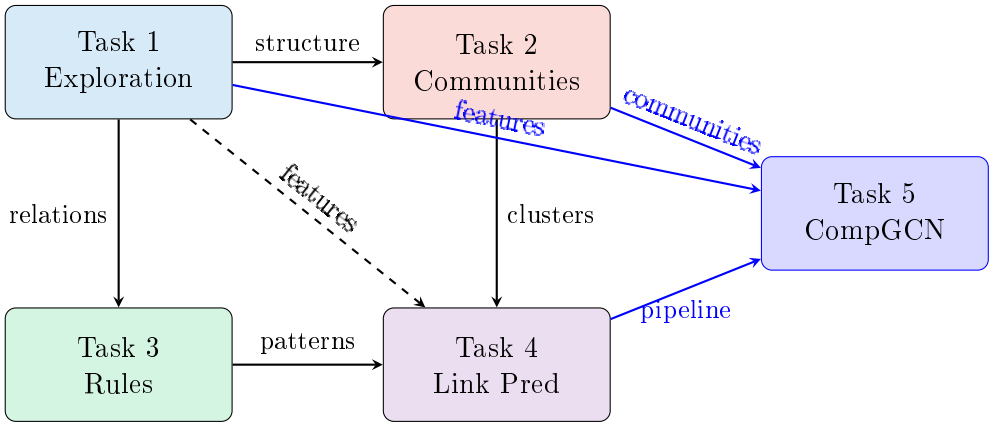


Figure 14: Task Dependencies and Information Flow. Task 5 (blue) integrates outputs from Tasks 1, 2, and 4.

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
5. **Tasks 1+2 → Task 5:** Node features (gender, generation, centrality) and community IDs are injected as CompGCN initial representations
6. **Task 4 → Task 5:** Link prediction framework (splits, evaluation, RotatE decoder) is reused and extended with GNN-based entity representation

25 Technical Recommendations

25.1 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**

25.2 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. **ComplEx** is the best model for clean, synthetic family KGs
4. Consider **GNN+decoder** when neighborhood structure is informative, but prefer **CompGCN over RGCN** for multi-relational graphs
5. **Feature injection** helps GNN recall but can hurt precision—use learned embeddings rather than sparse one-hot features for community encoding

26 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
5. **Learned community embeddings:** Replace one-hot encoding with low-dimensional community embeddings to improve CompGCN feature quality
6. **Feature ablation:** Systematically isolate which node features benefit GNN link prediction vs introduce noise
7. **Connected KG evaluation:** Test CompGCN-Custom on denser graphs where cross-community message passing is possible

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
|   +-- 05_CompGCN_Custom.ipynb  # Task 5: CompGCN + features
+-- 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
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 20: Link Prediction Metrics

Metric	Formula	Range
MRR	$\frac{1}{\lvert Q\rvert}\sum\frac{1}{\text{rank}_i}$	[0, 1]
Hits@1	$\frac{\lvert\text{rank}\leq 1\rvert}{\lvert Q\rvert}$	[0, 1]
Hits@10	$\frac{\lvert\text{rank}\leq 10\rvert}{\lvert Q\rvert}$	[0, 1]

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