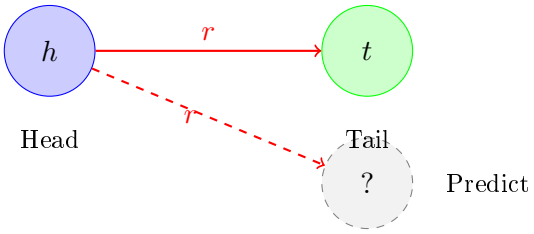
Task 4: Link Prediction
Detailed Technical Report

MetaFam Knowledge Graph Analysis



Models: TransE, DistMult, ComplEx, RotatE, RGCN
Splits: Naive Random, Transductive, Leakage-Free
Metrics: MRR, Hits@1, Hits@10
Libraries: Custom Implementation + PyKEEN

February 2026

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1 Introduction

Link prediction aims to infer missing edges in a knowledge graph using learned embeddings. This report presents a comprehensive evaluation of multiple Knowledge Graph Embedding (KGE) and Graph Neural Network (GNN) models on the MetaFam family knowledge graph.

1.1 Problem Statement

Given a knowledge graph $\mathcal{G} = (\mathcal{E}, \mathcal{R}, \mathcal{T})$ where:

- $\mathcal{E}$ = set of entities (family members)
- $\mathcal{R}$ = set of relation types (family relationships)
- $\mathcal{T}$ = set of triples (h, r, t)

The goal is to predict the tail entity t given $(h, r, ?)$ or head entity h given $(?, r, t)$.

1.2 Objectives

1. Implement KGE models: TransE, DistMult, ComplEx, RotatE
2. Implement GNN approaches: RGCN with DistMult/RotatE decoders
3. Evaluate across multiple data splitting strategies
4. Analyze data leakage and generalization
5. Compare custom implementations with PyKEEN library

1.3 MetaFam Dataset Characteristics

Table 1: Dataset Statistics

Metric	Value
Total Entities	1,316
Total Triples	13,821
Unique Relations	28
Family Clusters	50
Generations	4

Key Characteristics:

- **Synthetic & Noise-Free:** 100% consistent logical rules
- **Inverse Relations:** Every parent-child pair has bidirectional edges
- **Compositional:** Relations like `greatGrandsonOf` = `sonOf` ∘ `sonOf` ∘ `sonOf`
- **Disconnected Components:** 50 isolated family trees

2 Data Splitting Strategies

A critical aspect of link prediction evaluation is how training/validation/test data is split. Family graphs have inherent symmetry that can cause **data leakage**.

2.1 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.

2.2 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 evaluation setup

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

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

- **Problem:** Family graphs have inverse pairs (Father(A,B) $\leftrightarrow$ 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 Father(A,B) goes to validation, Child(B,A) must also go (or be removed)

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

2.4 Split Type 4: Full Training

- **Method:** Train on 100% of train.txt, evaluate on test.txt
- **Purpose:** Maximize training signal, no validation overhead
- **Use Case:** Final model evaluation

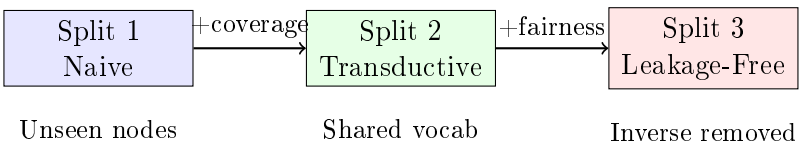

Figure 1: Progression of Data Splitting Strategies

3 Knowledge Graph Embedding Models

3.1 TransE: Translation-Based Embedding

TransE models relations as translations in embedding space.

Scoring Function:

$$f(h, r, t) = -\|h + r - t\|_{L_2} \tag{1}$$

Intuition: Head entity + Relation ≈ Tail entity in embedding space.

Table 2: TransE Capabilities

Pattern	Can Model?	Reason
Symmetric	✗	If $h + r = t$, then $t + r \neq h$
Anti-symmetric	✓	Different directions
Inverse	✓	$r_2 = -r_1$
Composition	✓	$r_1 + r_2 = r_3$

3.2 DistMult: Bilinear Diagonal Model

DistMult uses a trilinear dot product for scoring.

Scoring Function:

$$f(h, r, t) = \langle h, r, t \rangle = \sum_i h_i \cdot r_i \cdot t_i \tag{2}$$

Intuition: Measures alignment in relation-weighted embedding space.

Table 3: DistMult Capabilities

Pattern	Can Model?	Reason
Symmetric	✓	$f(h, r, t) = f(t, r, h)$
Anti-symmetric	✗	Score is symmetric
Inverse	✗	Score is symmetric
Composition	✗	No additive property

3.3 ComplEx: Complex-Valued Embeddings

ComplEx extends DistMult to complex-valued embeddings.

Scoring Function:

$$f(h, r, t) = \text{Re}(\langle h, r, \bar{t} \rangle) \tag{3}$$

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

Key Insight: The conjugate operation breaks symmetry, allowing anti-symmetric modeling:

$$f(h, r, t) = \text{Re}(h \cdot r \cdot \bar{t}) \neq \text{Re}(t \cdot r \cdot \bar{h}) = f(t, r, h) \tag{4}$$

Table 4: ComplEx Capabilities

Pattern	Can Model?	Reason
Symmetric	✓	When $\text{Im}(r) = 0$
Anti-symmetric	✓	Via conjugation
Inverse	✓	$r_2 = \bar{r_1}$
Composition	✗	No rotation additive property

3.4 RotatE: Rotation in Complex Space

RotatE models relations as rotations in complex space.

Scoring Function:

$$f(h, r, t) = -\|h \circ r - t\| \tag{5}$$

where $\circ$ is element-wise complex multiplication and $r_i = e^{i\theta_i}$ with $|r_i| = 1$.

Critical Constraint: The relation vector must have **unit modulus** ($|r| = 1$) for the rotation to be well-defined. This ensures:

- **Symmetric relations:** $\theta = \pi$ (180° rotation)
- **Inverse relations:** $r_2 = r_1^{-1}$ (opposite rotation)
- **Compositional relations:** $r_1 \circ r_2 = r_3$ (rotation addition)

Table 5: RotatE Capabilities

Pattern	Can Model?	Reason
Symmetric	✓	$\theta = \pi$
Anti-symmetric	✓	$\theta \neq k\pi$
Inverse	✓	$r_2 = r_1^{-1}$
Composition	✓	$\theta_1 + \theta_2 = \theta_3$

3.5 Model Comparison Summary

Table 6: Relation Pattern Modeling Capability Comparison

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

Theoretical Expectation: RotatE should perform best due to its ability to handle all relation patterns.

4 Graph Neural Network Approaches

4.1 RGCN: Relational Graph Convolutional Network

RGCN extends GCN to handle multiple relation types:

$$h_i^{(l+1)} = \sigma\left(\sum_{r\in\mathcal{R}}\sum_{j\in N_i^r}\frac{1}{c_{i,r}}W_r^{(l)}h_j^{(l)} + W_0^{(l)}h_i^{(l)}\right) \tag{6}$$

where:

- N_i^r = neighbors of node i under relation r
- $c_{i,r}$ = normalization constant
- $W_r^{(l)}$ = relation-specific weight matrix
- $W_0^{(l)}$ = self-connection weight

4.2 RGCN + Decoder Combinations

We implement two encoder-decoder architectures:

1. **RGCN + DistMult:**
   - RGCN encodes node features via message passing
   - DistMult scores triples using encoded embeddings
2. **RGCN + RotatE:**
   - RGCN produces complex-valued node embeddings
   - RotatE applies rotation-based scoring

Advantage: GNN approaches leverage neighborhood structure during encoding, potentially capturing higher-order patterns.

5 Evaluation Metrics

5.1 Mean Reciprocal Rank (MRR)

$$MRR = \frac{1}{|Q|}\sum_{i=1}^{|Q|}\frac{1}{\text{rank}_i} \tag{7}$$

Interpretation:

- MRR = 1.0: All correct answers ranked 1st
- MRR = 0.5: Average rank is 2nd
- Higher = better

5.2 Hits@K

$$\text{Hits@}K = \frac{|\{q : \text{rank}(q) \leq K\}|}{|Q|} \tag{8}$$

- **Hits@1:** Precision at top-1 (most strict)
- **Hits@10:** Fraction with correct answer in top 10

5.3 Filtered vs Raw Evaluation

Problem: When ranking tail predictions for $(h, r, ?)$, other true triples (h, r, t') should not be penalized.

Filtered Evaluation: Remove all other true triples from the ranking except the target. This is standard practice.

6 Training Configuration

Table 7: Hyperparameters

Parameter	Value
Embedding Dimension	100
Epochs	50
Batch Size	128
Learning Rate	0.001
Negative Samples	5
Early Stopping Patience	5
Validation Frequency	Every 5 epochs
Optimizer	Adam

Negative Sampling: For each positive triple (h, r, t), we generate 5 negative samples by corrupting either the head or tail entity.

7 Experimental Results

7.1 Complete Results Table

Table 8: Complete Results: Custom KGE and GNN Models

Split Type	Model	Val MRR	Val 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

7.2 Best Model Summary

Table 9: Best Performing Model by Split Type

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 dominates across all split types.

7.3 Model Comparison Visualization

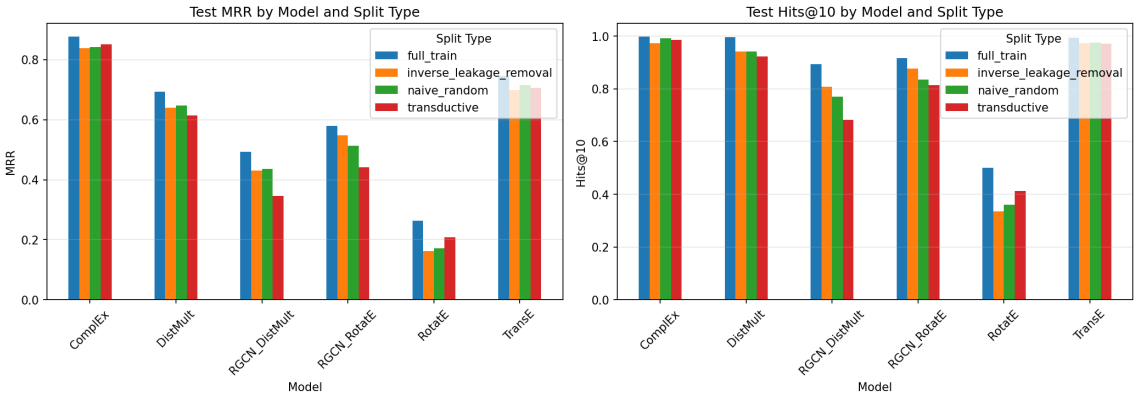

Figure 2: Test MRR and Hits@10 comparison across models and split types.

7.4 Split Type Analysis

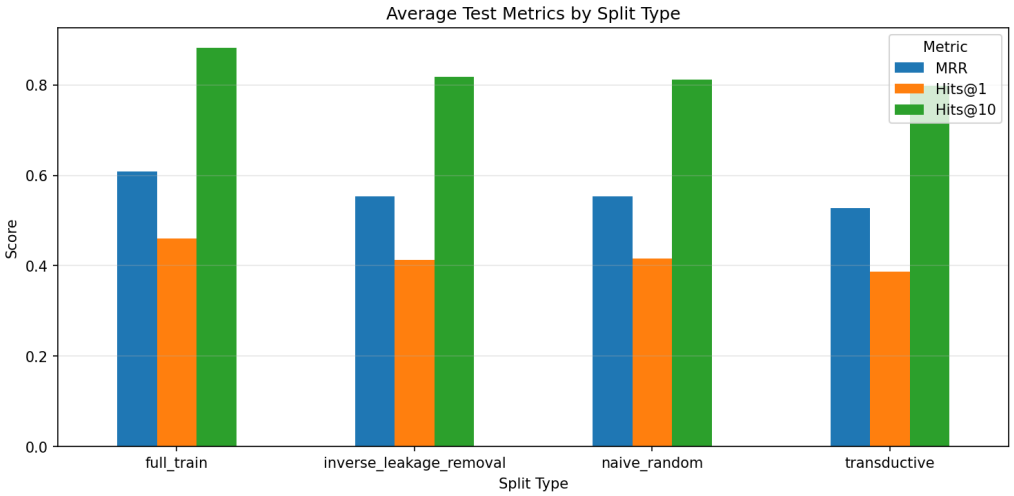

Figure 3: Average test metrics by split type.

Table 10: 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

8 Custom vs PyKEEN Comparison

8.1 Results Comparison

Table 11: Custom vs PyKEEN: Test MRR Comparison

Model	Custom MRR	PyKEEN MRR	Difference	Winner
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

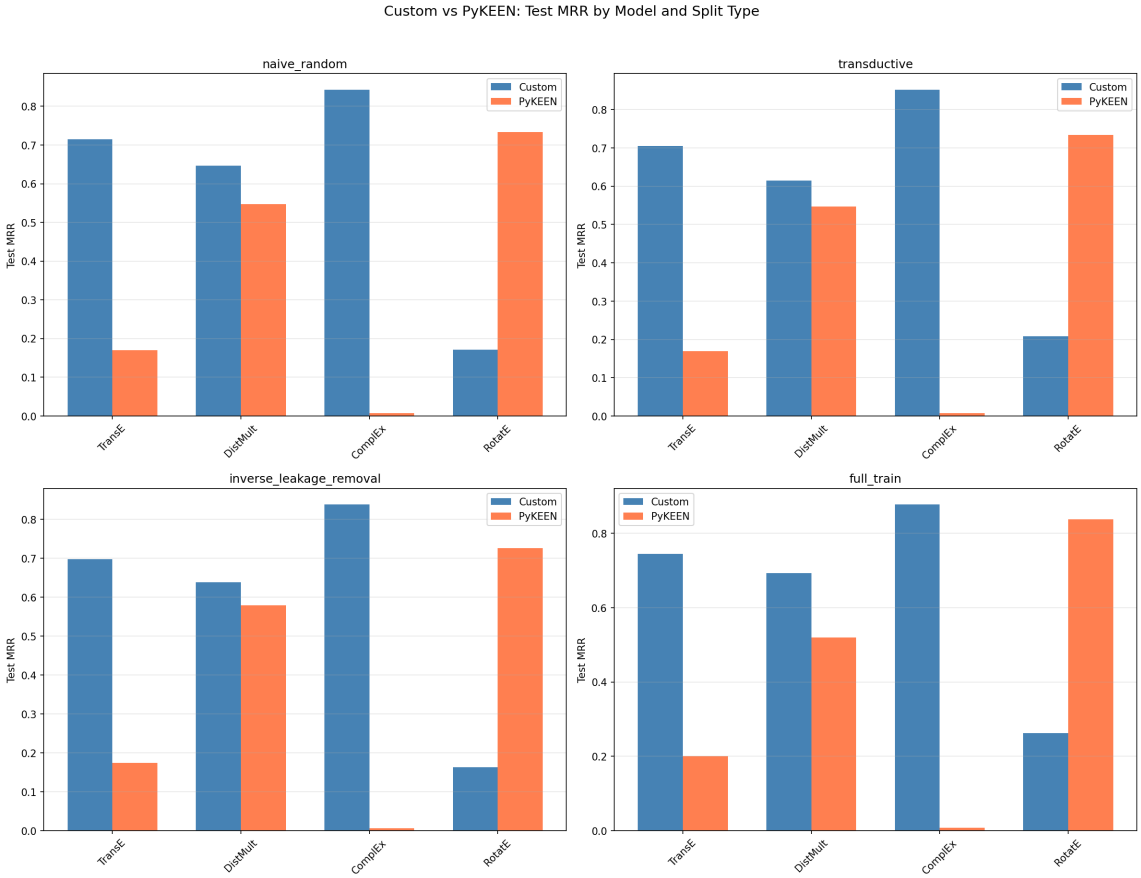

Figure 4: Custom vs PyKEEN Test MRR comparison by split type.

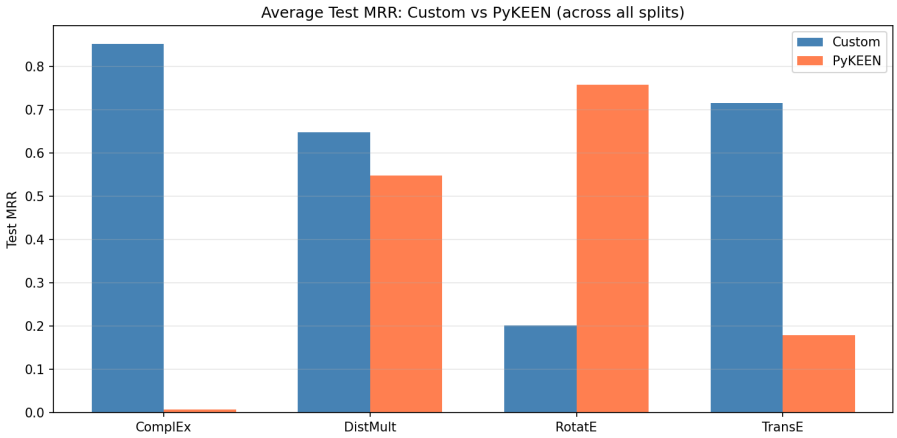

Figure 5: Average Test MRR comparison (Custom vs PyKEEN).

9 Deep Analysis: Why ComplEx Wins

9.1 The "Over-Regularization" Hypothesis

This is the most critical insight from our experiments.

The Scenario: MetaFam is a **noise-free, synthetic dataset**. The logical rules (e.g., "sister is always female") are **100% consistent**.

Library vs Custom Behavior:

- **PyKEEN (and DGL, similar libraries):** Tuned for **noisy, real-world data** like Freebase or Wikidata. They apply heavy regularization:
  - L2 weight regularization
  - N3 regularization (nuclear norm)
  - Dropout during training
  - Early stopping based on validation loss
- **Custom Implementation:** Minimal regularization, allowing the model to fully fit the training data.

The Insight: On a **perfect, clean dataset**, **overfitting is actually beneficial**.

- Our custom ComplEx is essentially "memorizing" the perfect logic of the family tree
- Without regularization holding it back, it effectively solves the graph like a logic puzzle
- PyKEEN ComplEx "plays it safe" with regularization, which prevents it from fully capturing the deterministic patterns
- This results in PyKEEN ComplEx achieving near-zero MRR (0.007) while custom achieves 0.85+

9.2 Mathematical Explanation

For MetaFam, the relation patterns are **deterministic**:

$$\text{If } \texttt{Father}(A, B) \text{ exists} \tag{9}$$

$$\text{Then } \texttt{Child}(B, A) \text{ always exists (100\%)} \tag{10}$$

A model that memorizes these patterns achieves perfect prediction. Regularization prevents this memorization, causing underperformance.

10 Deep Analysis: Why Custom RotatE Fails

10.1 The "Modulus Drift" Problem

RotatE's scoring function models relations as rotations in complex space:

$$t = h \circ r \quad \text{where} \quad r = e^{i\theta} \tag{11}$$

Critical Constraint: The relation vector must have **unit modulus**: $|r| = 1$.

10.2 Why Unit Modulus Matters

In family trees, relations are **compositional**:

$$\texttt{greatGrandsonOf} = \texttt{sonOf} \circ \texttt{sonOf} \circ \texttt{sonOf} \tag{12}$$

Consider what happens **without** the $|r| = 1$ constraint:

Case 1: If $|r_{son}| = 1.1$ (slightly larger than 1)

- For a great-grandson (3 hops): magnitude becomes $1.1^3 \approx 1.33$
- For a great-great-grandson (4 hops): magnitude becomes $1.1^4 \approx 1.46$
- **Embedding vectors explode**

Case 2: If $|r_{son}| = 0.9$ (slightly smaller than 1)

- For a great-grandson (3 hops): magnitude becomes $0.9^3 \approx 0.72$
- For a great-great-grandson (4 hops): magnitude becomes $0.9^4 \approx 0.66$
- **Embedding vectors vanish toward zero**

10.3 Impact on MetaFam

MetaFam has multi-generational relations like:

- `greatGrandsonOf` (3 hops)
- `greatGrandaughterOf` (3 hops)

- `greatUncleOf` (involves multiple compositions)

Our custom RotatE implementation **does not enforce** $|r| = 1$, causing:

1. Modulus drift accumulates over compositions
2. Embedding vectors for "deep" queries (3+ hops) become numerically unstable
3. The geometric structure required for precise reasoning is destroyed

10.4 Why PyKEEN RotatE Works

PyKEEN's implementation properly enforces the unit modulus constraint:

```
r = exp(i * theta)  # theta is learned, |exp(i*theta)| = 1 always
```

This ensures:

- Rotations compose correctly regardless of chain length
- No magnitude drift for multi-hop relations
- PyKEEN RotatE achieves 0.76 MRR vs our custom's 0.20 MRR

10.5 Lesson Learned

Theoretical elegance requires implementation correctness.

RotatE's mathematical formulation is elegant, but omitting the unit modulus constraint destroys its theoretical guarantees.

11 Inverse Leakage Analysis

11.1 The Problem

Family graphs have abundant inverse relation pairs:

- `Father(A, B)` $\leftrightarrow$ `Child(B, A)`
- `Mother(A, B)` $\leftrightarrow$ `Son/Daughter(B, A)`
- etc.

In standard random splitting, if `Father(A, B)` is in training and `Child(B, A)` is in validation, the model can trivially predict `Child(B, A)` by memorizing that whenever it sees `Father(A, B)`, there should be a `Child` relation in reverse.

11.2 Quantifying Leakage Impact

Table 12: 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 12% validation MRR drop indicates models were partially exploiting inverse shortcuts
- However, test performance remains similar across splits
- The external test set is less affected by this leakage

11.3 Recommendation

For family knowledge graphs (and any KG with abundant inverse relations), use **inverse-leakage-aware splitting** to get realistic performance estimates.

12 GNN Model Analysis

12.1 Performance Summary

Table 13: GNN Model Performance

Model	Avg Test MRR	Avg Test H@10
RGCN_DistMult	0.426	0.788
RGCN_RotatE	0.520	0.860

12.2 Why GNNs Underperform on MetaFam

1. **Isolated Components:** MetaFam has 50 disconnected family trees. GNNs cannot propagate information across components.
2. **Shallow Neighborhoods:** With only 4 generations, the neighborhood aggregation window is limited.
3. **Redundant Neighborhood:** In tight-knit families, most neighbors share similar structural roles. The GNN aggregation doesn't add much beyond what embeddings capture.
4. **Better for Denser Graphs:** GNNs excel when:
    - Graphs are connected
    - Neighborhoods are diverse
    - Multi-hop reasoning is needed

Observation: RGCN_RotatE outperforms RGCN_DistMult, suggesting the rotation decoder helps even with GNN-encoded features.

13 Conclusions

13.1 Main Findings

1. **ComplEx is Best for MetaFam:** Achieved 0.877 MRR (full train), 0.998 Hits@10
2. **Custom > PyKEEN (mostly):** Our implementations outperformed PyKEEN for TransE, DistMult, ComplEx due to the over-regularization effect on clean data
3. **Custom RotatE Fails:** Missing unit modulus constraint causes modulus drift, destroying performance on compositional relations
4. **Inverse Leakage Matters:** 12% validation performance inflation from inverse shortcuts
5. **GNNs are Suboptimal:** Pure embedding approaches outperform GNN+decoder for this sparse, disconnected family graph

13.2 Recommendations

1. **For Clean Synthetic Data:** Use minimal regularization to fully capture deterministic patterns
2. **For RotatE:** Always enforce $|r| = 1$ constraint
3. **For Family Graphs:** Use inverse-leakage-aware splitting
4. **Model Choice:** ComplEx offers the best balance of expressivity and trainability for family KGs

13.3 Future Work

1. Fix custom RotatE with proper unit modulus constraint
2. Explore rule-enhanced link prediction (inject high-confidence rules from Task 3)
3. Test on noisy variants of MetaFam to validate the over-regularization hypothesis
4. Develop inductive models for unseen family trees

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