On the Theoretical Limitations of Embedding-Based Retrieval

– Paper Presentation and Reproduction –

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Contents

Problem Statement and Related Work

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Problem

- Vector embeddings still follow the single-vector paradigm
- Retrieval failures: poor data, unrealistic queries, or embedding-space geometry?

Related Work

- IR evolution: parse vectors $\rightarrow$ dense embeddings
- Task complexity: QUEST (logical ops), BRIGHT (Leetcode reasoning)
- Empirical findings: lower dimensions $\Rightarrow$ more false positives; affects bias-variance tradeoff

Capacity of Vector Embeddings

Representational Capacity of Vector Embeddings

- Embedding representation:

$$\text{query}_i \xrightarrow{\text{emb. model}} u_i \in \mathbb{R}^d, \quad \|u_i\| = 1, i \in \{1, ..., m\}$$
$$\text{doc}_j \xrightarrow{\text{emb. model}} v_j \in \mathbb{R}^d, \quad \|v_j\| = 1, j \in \{1, ..., n\}$$

- cosine-sim$(u_i, v_j) = u_j^T v_j$ – dot product as matrix multiplication
- Query-relevance (qrel) matrix: $A = [\text{doc}_j \text{ relevant to query}_i]_{ij} \in \mathbb{R}^{m \times n}$
- **Q:** When is retrieval accurate?
- **A:** When all top-k results are returned.

Representational Capacity of Vector Embeddings

$$U := \begin{bmatrix} & | & \\ \cdots & u_i & \cdots \\ & | & \end{bmatrix}_i \in \mathbb{R}^{d\times m} \qquad V := \begin{bmatrix} & | & \\ \cdots & v_j & \cdots \\ & | & \end{bmatrix}_j \in \mathbb{R}^{d\times n}$$

- $\implies$ the similarity matrix

$$\mathbb{R}^{m\times n} \ni B := \left[u_i^T v_j\right]_{ij} = \begin{bmatrix} & \vdots & \\ — & u_i^T & — \\ & \vdots & \end{bmatrix} \begin{bmatrix} & | & \\ \cdots & v_j & \cdots \\ & | & \end{bmatrix} = U^T V$$

Representational Capacity of Vector Embeddings

- **Q:** When is retrieval accurate?
- **A:** When all top-k results are returned.

$$\Updownarrow$$

$$\forall i, j, k \quad A_{ij} > A_{ik} \implies B_{ij} > B_{ik}, \tag{rop}$$

i.e. the row-wise order is preserved.

Representational Capacity of Vector Embeddings

- **Q:** What embedding dimension preserves row-wise ordering?
- **A:** The minimal (embbeding) dimension d s.t. for $B \in \mathbb{R}^{m\times n}$

$$\exists U \in \mathbb{R}^{d\times m} \text{ and } V \in \mathbb{R}^{d\times n} \text{ s.t. } B = U^T V \qquad \text{(fact)}$$
$$\text{and (rop).}$$

- **Q:** Minimal d via linear algebra?
- **A:** $d_{\min} = \mathrm{rank} B$
- So we can summarize (fact) and (rop) as

$$\mathrm{rank}_{\mathrm{rop}} A := \min \left\{ \mathrm{rank} B \mid B \in \mathbb{R}^{m\times n}, \text{ s.t. } \forall i, j, k \quad A_{ij} > A_{ik} \implies B_{ij} > B_{ik} \right\},$$

the **row-wise order-preserving rank** of the qrel matrix A.

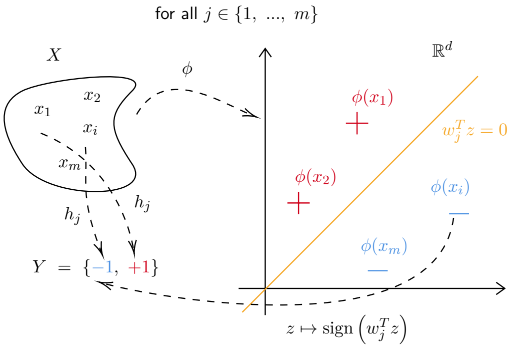
Representational Capacity of Vector Embeddings

Q: How to calculate $\text{rank}_{\text{rop}} A$?

Idea: Quantify how hard it is to separate relevant from irrelevant documents.

Representational Capacity of Vector Embeddings

Learning theory



$$U := [w_j]_j \in \mathbb{R}^{d \times m}$$

$$V := [\phi(x_i)]_i \in \mathbb{R}^{d \times n}$$

$$A := [h_j(x_i)] \in \{\pm 1\}^{m \times n}$$

$$B := U^T V \in \mathbb{R}^{m \times n}$$

- How complex is a given binary classification problem?
- Complexity = min. dimension d s.t. sign$B = A$ and (fact):

$$\text{rank}_\pm A := \min\left\{\text{rank}B \mid B \in \mathbb{R}^{m \times n} \text{ s.t. } \text{sign}B = A\right\}$$ – sign-rank of A

Representational Capacity of Vector Embeddings

By Warren's theorem in real algebraic topology, ...

Lemma

Let $r < N/2$.
Then $\#(N \times N$ sign-matrices of sign-rank $\leq r)$ does not exceed $2^{O(rN \log N)}$.

Obersvation

$$\#(N \times N \text{ sign-matrices}) = 2^{N^2} > 2^{O(rN \log N)} \implies$$
$$\exists N \times N \text{ sign-matrices with sign-rank} > r \text{ for large } N.$$

So **there are sign-matrices with arbitrary large sign-rank**.

Representational Capacity of Vector Embeddings

The key result from the paper:

Theorem

Let $A \in \{0,1\}^{m \times n}$ be a binary matrix. Then $2A - \mathbf{1}_{m \times n} \in \{\pm 1\}^{m \times n}$, and we have

$$\mathit{rank}_{\pm}(2A - \mathbf{1}_{m\times n}) - 1 \leq \mathit{rank}_{\mathit{rop}} A \leq \mathit{rank}_{\pm}(2A - \mathbf{1}_{m\times n}).$$

Obersvations

- Sign-rank computation is NP-hard.
- Lemma: $\min d$ can be arbitrarily large compared to $\operatorname{rank} A$.
- Fixed $d \implies$ some qrel matrices are not representable.
- Order-preserving embedding in $d \Rightarrow$ bounded sign-rank (estimable via optimization).

Empirical Connection

Best-Case Optimization

- Theory: embedding capacity is geometric, not linguistic.

Free embedding optimization

- All $\binom{n}{2}$ queries over n documents – dense qrels
- For fixed dimension d, find largest representable n – critical-n
- Optimize query and document embeddings via gradient descent
- Perfect fit $\equiv$ 100% recall
- Contrastive loss: pull relevant docs closer than irrelevant ones

$$\mathcal{L}_{\text{InfoNCE}} = -\frac{1}{|Q|} \sum_{q \in Q} \sum_{\substack{d' \in D \\ d' \text{ relevant to } q}} \log \frac{\exp(\text{sim}(q, d')/\tau)}{\sum_{d \in D} \exp(\text{sim}(q, d)/\tau)}$$

Best Case Optimization

Implementation

- Original paper: training with JAX on H100 GPUs and TPU v5's
- Reproduced: training with PyTorch on a Kaggle P100 GPU
- Optimizer: Adam
- Training hyperparams:

```python
def train(
  num_of_docs: int,
  dimension: int,
  max_patience: int = 1000,
  temp: float = 0.1,
  learning_rate: float = 0.01,
  max_iters: int = 100000,
  min_delta: float = 0.00001
) -> float:
    ...
```

Best Case Optimization

PyTorch Model:

```python
class FreeEmbeddingsModel(torch.nn.Module):
  # ... init attributes ...
  def forward(self):
    """During training the embeddings must be normalized after optimization"""
    self.__qrel_matrix = self.__qrel_matrix.to(self.docs.device)

    queries_norm = self.queries
    docs_norm = self.docs

    logits = (queries_norm @ docs_norm.T) / self.__temp
    log_probs = torch.log_softmax(logits, dim=1)

    sum_pos_log_probs = (log_probs * self.__qrel_matrix).sum()
    M = self.__qrel_matrix.sum()
    total_loss = -sum_pos_log_probs / M
    return total_loss
```

Best Case Optimization

Results

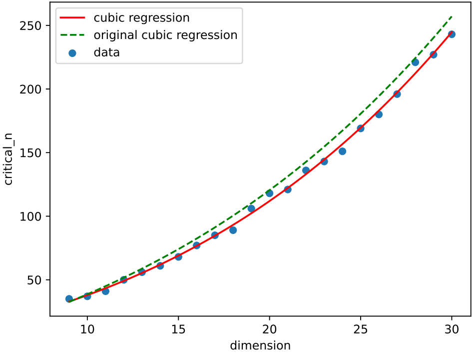


Figure: Free embedding optimization results (reproduced up to dim. 30; paper reports dim. 45)

$$y_{\text{o}} = 0.0037d^3 + 0.0520d^2 + 4.0309d - 10.5322$$

$$y_{\text{r}} = 0.003866d^3 + 0.06175d^2 + 2.84d - 0.4842$$

$$R_o^2 = 0.999 \qquad R_r^2 = 0.997$$

$$\text{RSSE} = 58.287 \qquad \text{RMSE} = 8.243$$

Emb. dimension d	**Critical** n
512	5.37×10^5
768	1.79×10^6
1024	4.22×10^6
4096	2.67×10^8

Table: Extrapolated values based on the reproduced regression.

Real-World Datasets

$$\rho = \frac{|E|}{\frac{|V|(|V|-1)}{2}}$$

$$s_i = \sum_{j \in N(i)} w_{ij}$$

$$\bar{s} = \frac{1}{|V|} \sum_{i \in V} s_i$$

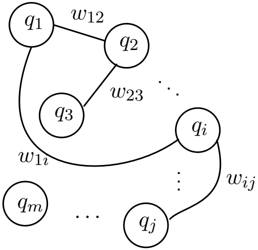


Figure: Query-query Jaccard-weighted graph with graph density and average strength metrics.

- Test on real-world datasets
- Existing benchmarks are too sparse

Dataset Name	Graph Density	Average Query Strength
NQ	0	0
HotPotQA	0.000037	0.1104
SciFact	0.001449	0.4222
FollowIR Core17	0.025641	0.5912

Table: Dataset statistics on standard benchmark models.

Real-World Datasets – LIMIT

LIMIT dataset's original construction:

- **Document structure:** X likes $attr_1, \ldots, attr_m$
- **Query structure:** Who likes $attr_i$?
- **Relevance pattern:** $\binom{n}{2} \times n$
  - 46 documents, $\sim \binom{46}{2} \approx 1000$ queries
- Names from public datasets
- Attributes generated via Gemini 2.5 Pro + BM25 filtering
- Small and large-scale versions (up to 50k docs)
- **Dataset statistics:** 0.085481 density, 28.4653 average query strength

Real-World Datasets - Benchmark on LIMIT

Models from the paper:

Model	Parameters	MRL
Snowflake Arctic L	0.3B	✓
E5-Mistral 7B	7B	✗
GritLM 7B	7B	✗
Qwen3 Embed	8B	✓
Promptriever Llama3 8B	8B	✗
Gemini Embed	unknown	✓

Table: Traditional SoTA embedding models.

Other models:

- BM25
- GTE-ModernColBERT

Inference device: A100 GPU

Real-World Datasets - Benchmark on LIMIT

Models from the reproduction:

Model	Parameters	MRL
Snowflake Arctic L	0.3B	✓
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Qwen3 Embed	8B	✓
~~Promptriever Llama3 8B~~	~~8B~~	~~✗~~
~~Gemini Embed~~	~~unknown~~	~~✓~~
Qwen3 Embed	0.6B	✓

Table: Traditional SoTA embedding models

.

Other models:

- BM25
- GTE-ModernColBERT

Inference devices:

- Kaggle T4 GPUs with 4-bit quantization using *bnb-my-repo*.
- GeForce GTX 1650

Real-World Datasets - Benchmark on LIMIT

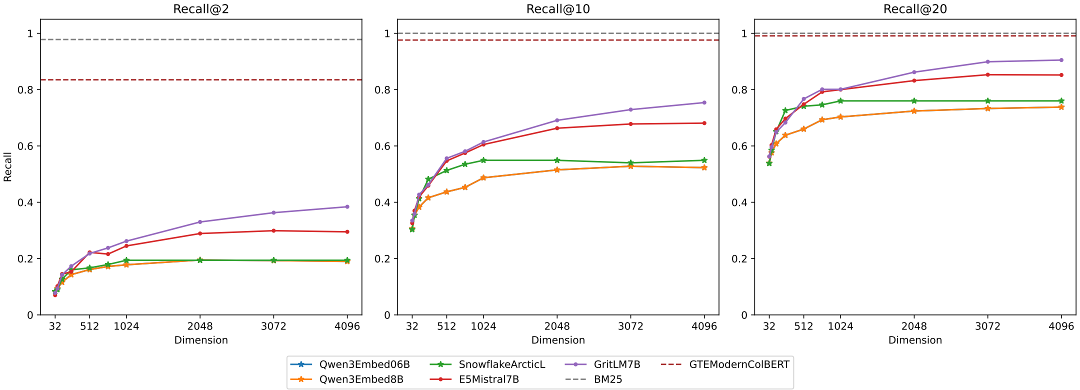


Figure: Expected results (for selected models) on LIMIT-small.

Real-World Datasets - Benchmark on LIMIT

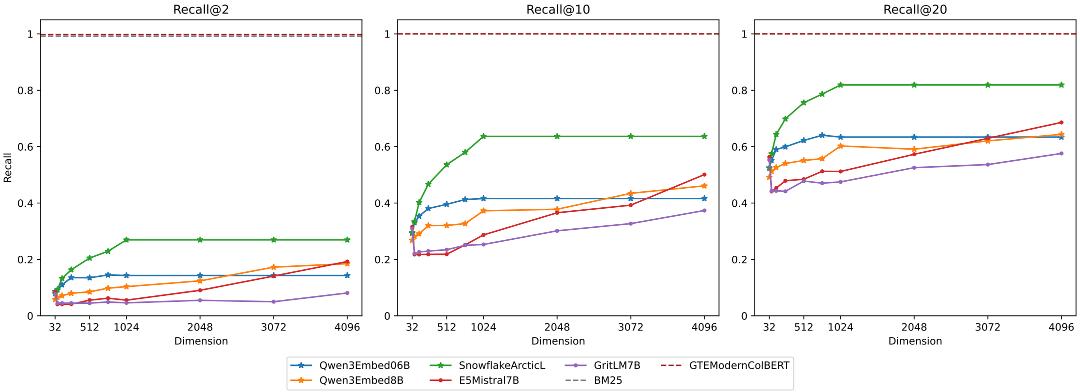
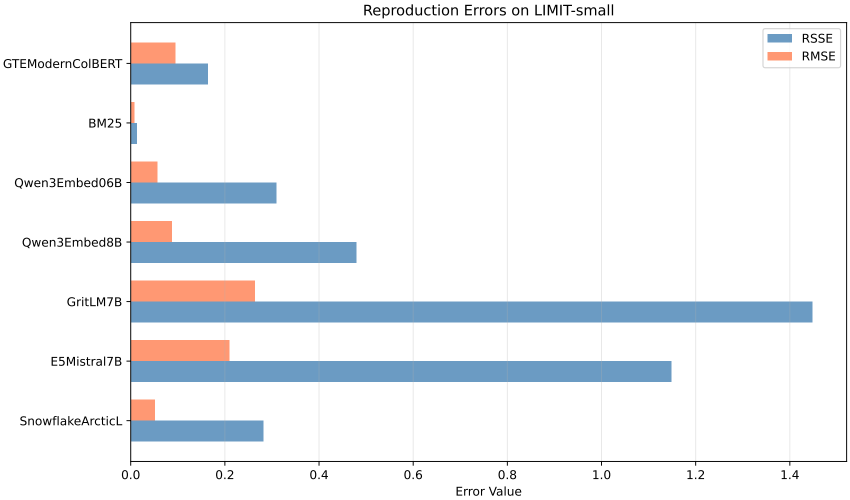


Figure: Reproduced results on LIMIT-small.

Real-World Datasets - Benchmark on LIMIT



Real-World Datasets - Qrel patterns

- Dense qrel patterns in LIMIT make retrieval more difficult.
- Intuitively, sparser patterns should be easier for models to learn.
- **Q:** Can we show this empirically?

Real-World Datasets - Qrel patterns

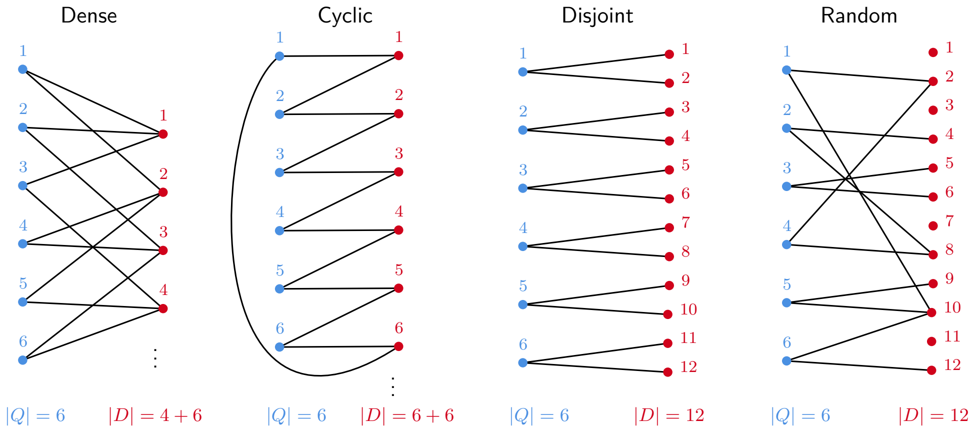


Figure: Different qrel patterns with 6 queries, 12 docs, $k = 2$ relevant doc/query.

Real-World Datasets - Qrel patterns

Experimental setup:

- Evaluated on previously introduced qrel patterns and LIMIT models
- Two settings:
  - **Paper:** $1000 \approx \binom{46}{2}$ queries, 50000 docs $(46 + 49954)$; A100 GPU
  - **Reproduction:** $23 \approx \binom{8}{2}$ queries, 2000 docs $(8 + 1992)$; P100 & GeForce GTX 1650 GPU
- $k = 2$ relevant documents per query (both settings)

Real-World Datasets - Qrel patterns

Results:

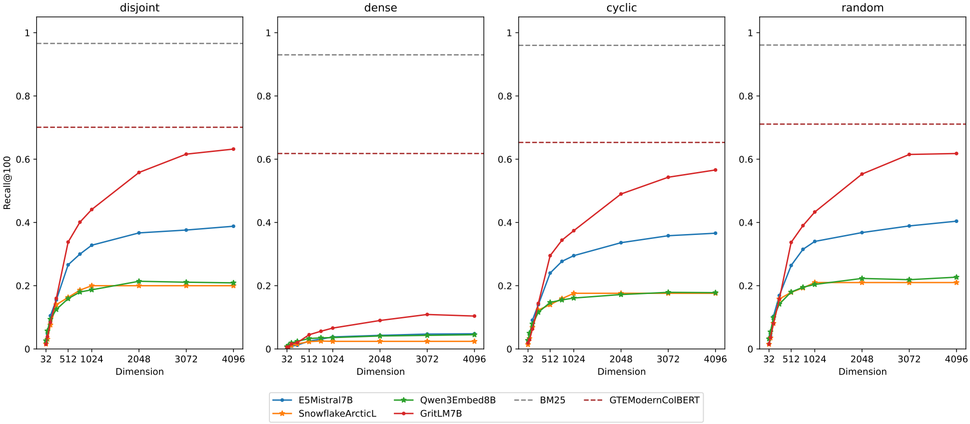


Figure: Expected results from the paper.

Real-World Datasets - Qrel patterns

Results

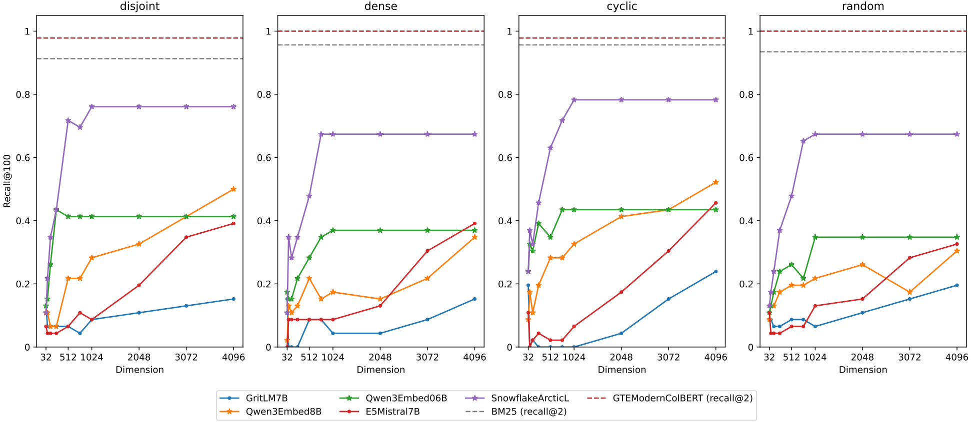


Figure: Reproduced results (quantized larger models).

Real-World Datasets - BEIR vs LIMIT

- BEIR – Benchmarking Information Retrieval – benchmark datasets
- Models perform well $\iff$ overfit on BEIR
- **Q:** Are BEIR and LIMIT connected?

Real-World Datasets - BEIR vs LIMIT

- **A: No**, the sample correlations are not statistically significant.

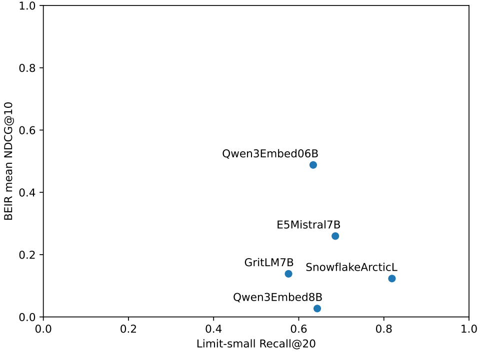


Figure: SciFact and NFCorpus datasets from BEIR vs Limit-small (on quantized models): $r = -0.162$, p-value $= 0.793 \gg 0.05$.

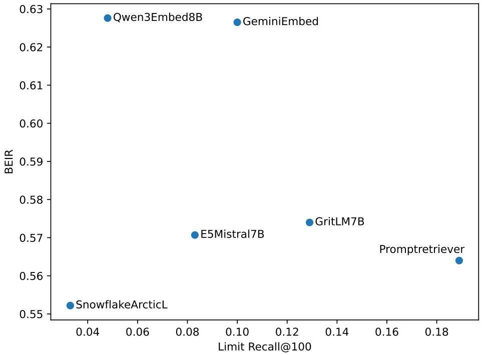


Figure: BEIR vs Limit from the paper: $r = -0.208$, p-value $= 0.691 \gg 0.05$.

Conclusion

Key Takeaways

- Single-embedding retrieval is limited by embedding space geometry.
- **Ways to overcome this**:
  - Higher-dimensional embeddings or traditional statistical methods (BM25, TF–IDF).
  - Multi-embedding models (e.g., ModernColBERT) to preserve token-level information.

References

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