Large Language Models for Search

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11-711

Disclaimer:

All the discussions in this lecture are based on public information, plus educated guesses from the instructor

Outline

Overview of Modern Information Retrieval Systems

- An example search component updated by LLMs
- Glances of other components using LLMs

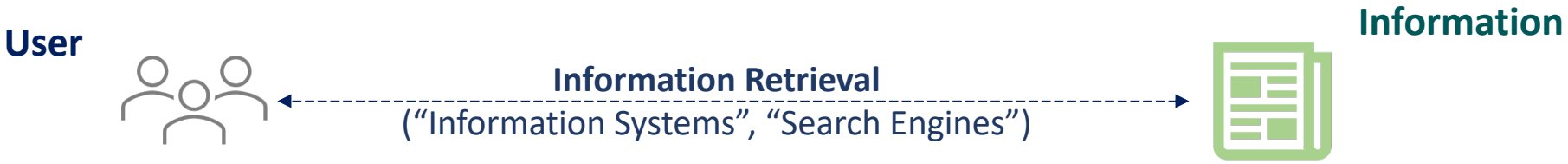
Dense Retrieval, a different way of search with LLMs

- End-to-end learned retrieval
- Notable extensions

Pretrain retrieval representations

Overview of Modern Information Retrieval Systems

Information Retrieval Systems



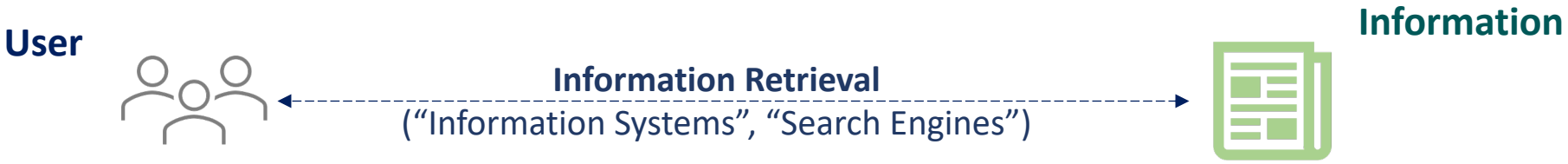
General Definition: Any system that finds information user needed

- Search Systems, QA Systems, Recommendation Systems, etc.

Specific Definition: Search engines that retrieve documents for user queries

- Explicit Query: User expressed information needs via texts, audios, or conversations
- Targeting Document: Satisfy user information needs by finding relevant documents

Information Retrieval Systems



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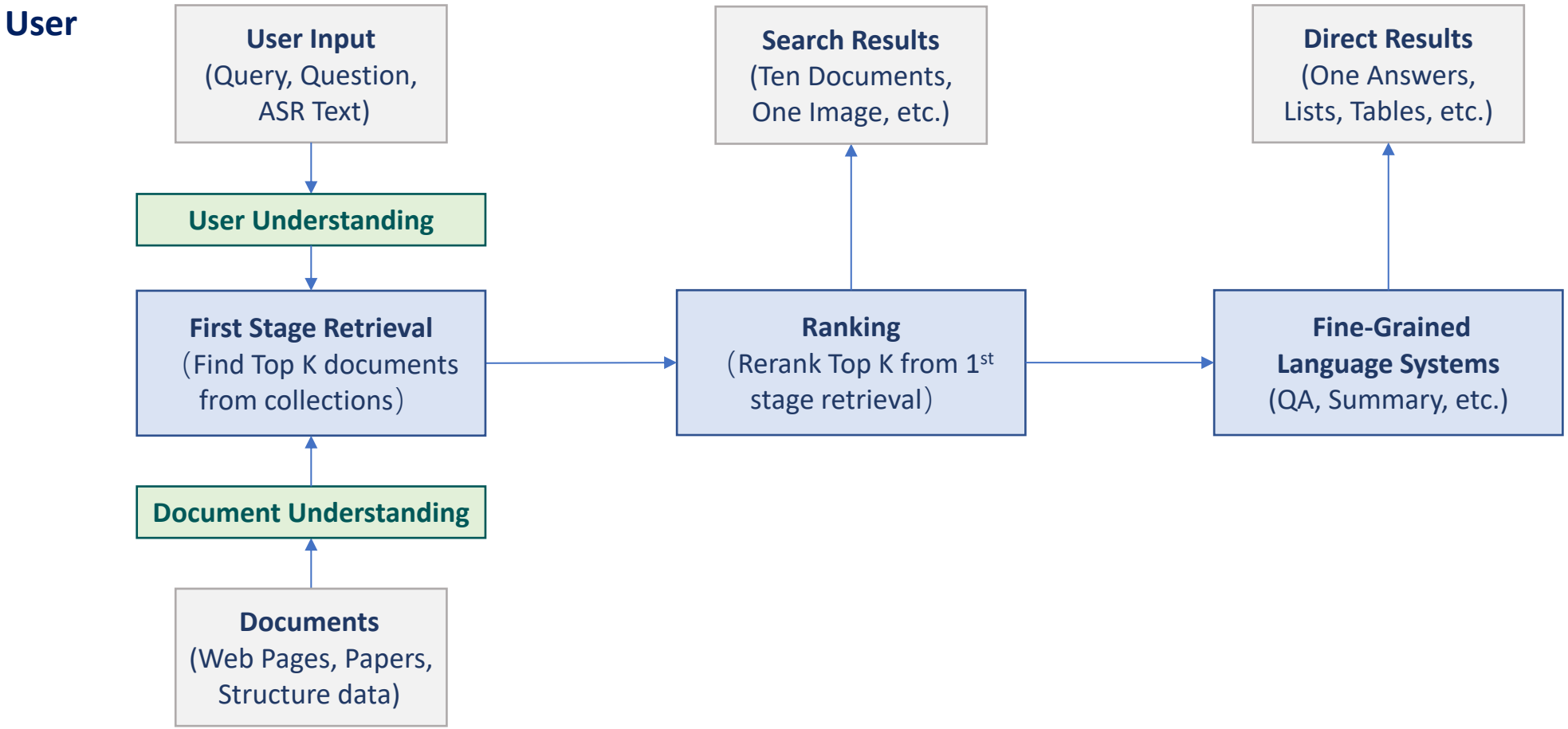
One of the most popular AI applications in past decades

The General Framework of Search Engines



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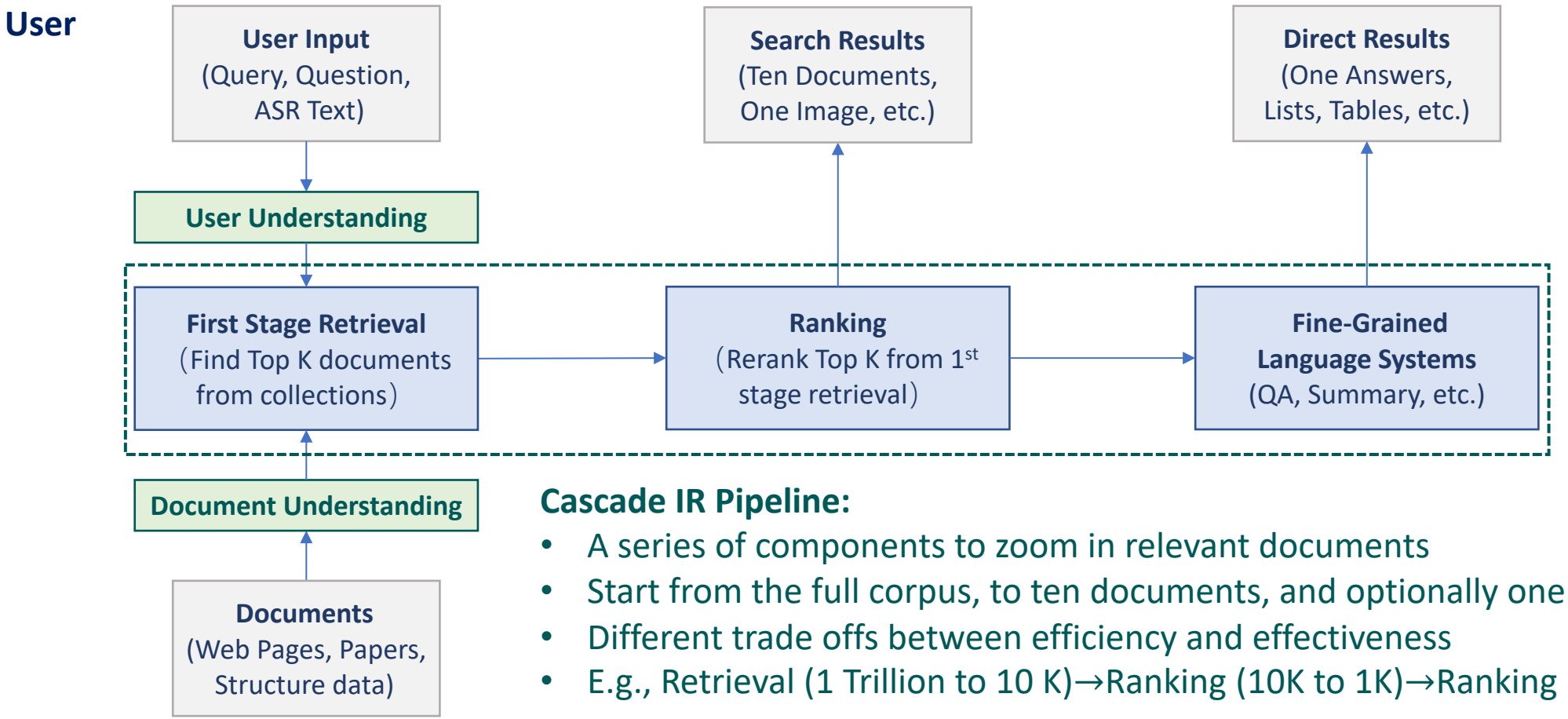

Cascade IR Pipeline:

- A series of components to zoom in relevant documents
- Start from the full corpus, to ten documents, and optionally one answer
- Different trade offs between efficiency and effectiveness
- E.g., Retrieval (1 Trillion to 10 K)→Ranking (10K to 1K)→Ranking (1K to 100)

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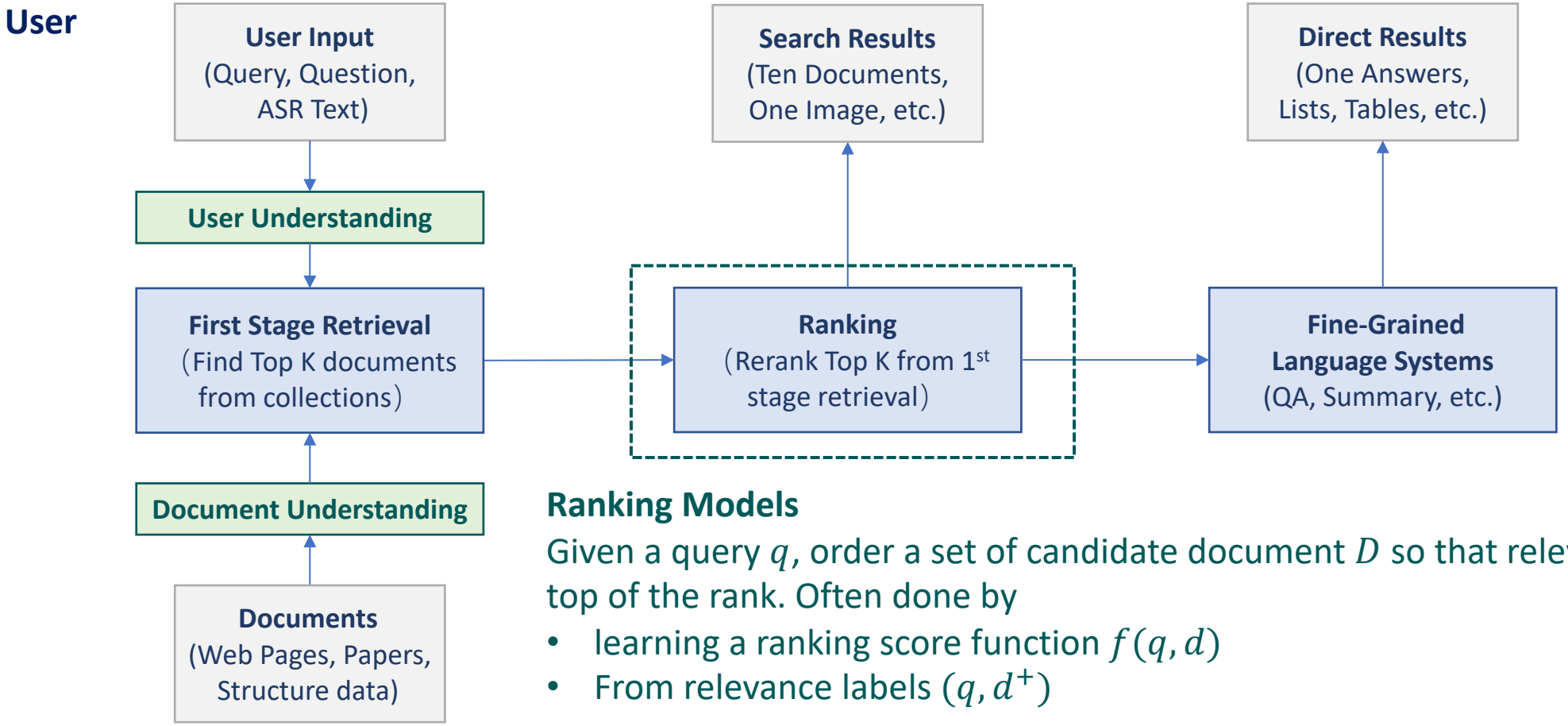
- End-to-end learned retrieval
- Notable extensions

Pretrain retrieval representations

Ranking Models



Ranking Models

Given a query q, order a set of candidate document D so that relevant document d^+ is on top of the rank. Often done by

- learning a ranking score function $f(q, d)$
- From relevance labels (q, d^+)

Ranking Models: Tree Models

Learning a ranking score function $f(q, d)$, with statistics machine learning models:

$$f(q, d) = \text{XGBoost}(\phi(q, d))$$

- $\phi(q, d)$: Ranking features, e.g.,
  - word overlaps between q and d
  - BM25 retrieval scores
  - Page rank of d
  - Freshness of d
- A learned combination of features that manually designed to capture q-d relevance

Ranking Models: Neural IR Models

Learning a ranking score function $f(q, d)$, with neural ranking models:

$$f(q, d) = \mathrm{NN}(\mathrm{M}_{qd})$$
$$\mathrm{M}_{qd}^{ij} = \mathrm{sim}(q^i, d^j)$$

- M_{qd}: The Translation matrix between q and d.
  - Each element is the embedding similarity between a query term q^i and a doc term d^j
- NN: A specifically designed network to pool term level similarities to q-d relevance
- Learning to model soft matches between q d terms, e.g., “pdf” and “reader”

Ranking Models: BERT Ranking

BERT models the relevance of (q, d) by simple classification [1]:

$$f(q, d) = \text{MLP}(\text{BERT}([\text{CLS}] \circ q \circ [\text{SEP}] \circ d)$$

- A MLP layer after the last layer's [CLS] representation to learn binary predictions: relevant/irrelevant

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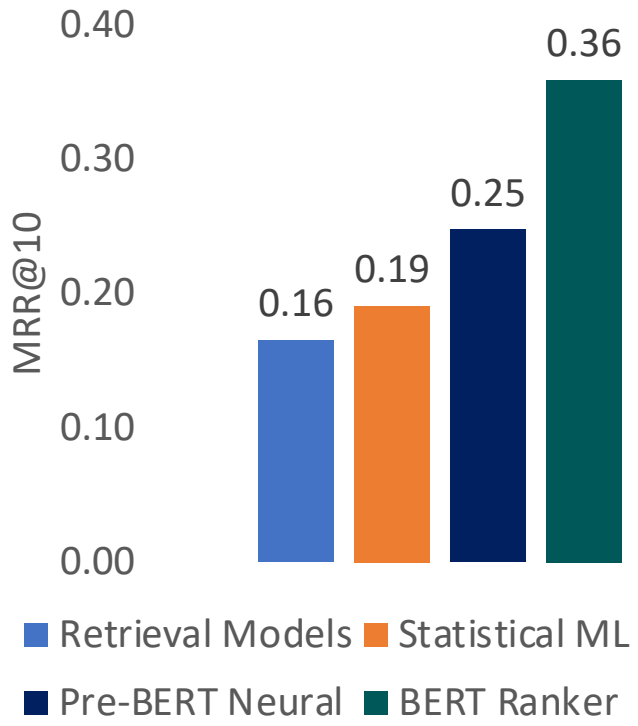

Figure 1: Ranking Performance on MS MARCO Passage Ranking Test [2]

Task: Rank answer passages for Bing questions from BM25 top 1000

- ~1M queries/labels from MS MARCO
- ~10M passages
- MRR: $\text{Mean}(\frac{1}{\text{Rank of d}^+})$

Significant gains from retrieval to neural ranker to BERT ranker

- Relevant doc moved from position 6 (1/0.16 MRR) to 4 to above 3

Also require far fewer supervisions

[1] Nogueira et al. "PASSAGE RE-RANKING WITH BERT." Arxiv 2019
[2] Qiao et al. "Understanding the Behaviors of BERT in Ranking". Arxiv 2019

Ranking Models: BERT Ranking

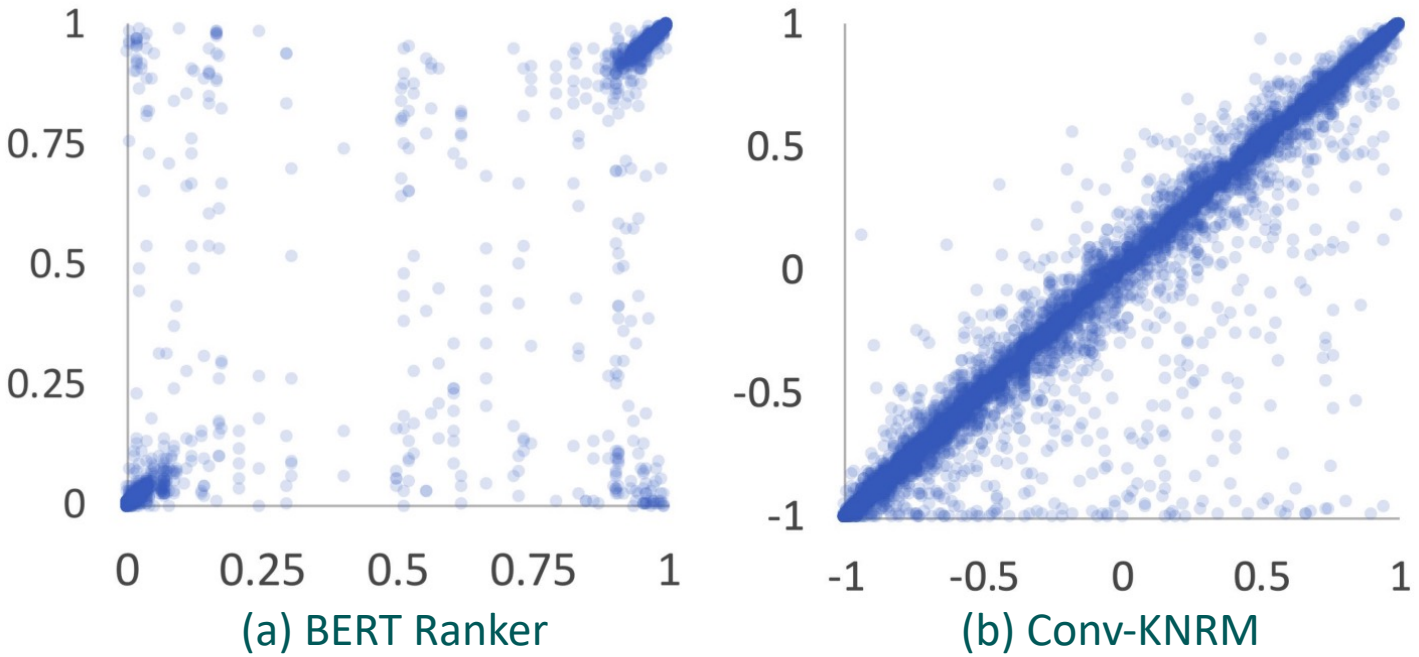

Figure 2: Ranking score of BERT and Pre-BERT Neural ranker (n-gram soft match) before (x) and after (y) removing a random document term [2]

BERT is more confident:

- Most ranking scores are close to 0 or 1

BERT is more global:

- Most document terms does not matter
- Some dramatically changed BERT's decision

ChatGPT for Ranking

Challenging to ask ChatGPT to generate a reasonable numerical ranking score for each document

One solution is to ask ChatGPT to rank a set of documents for a query

- E.g., input: q + p1, p2, p3, p4, ask ChatGPT to rank p1-p4

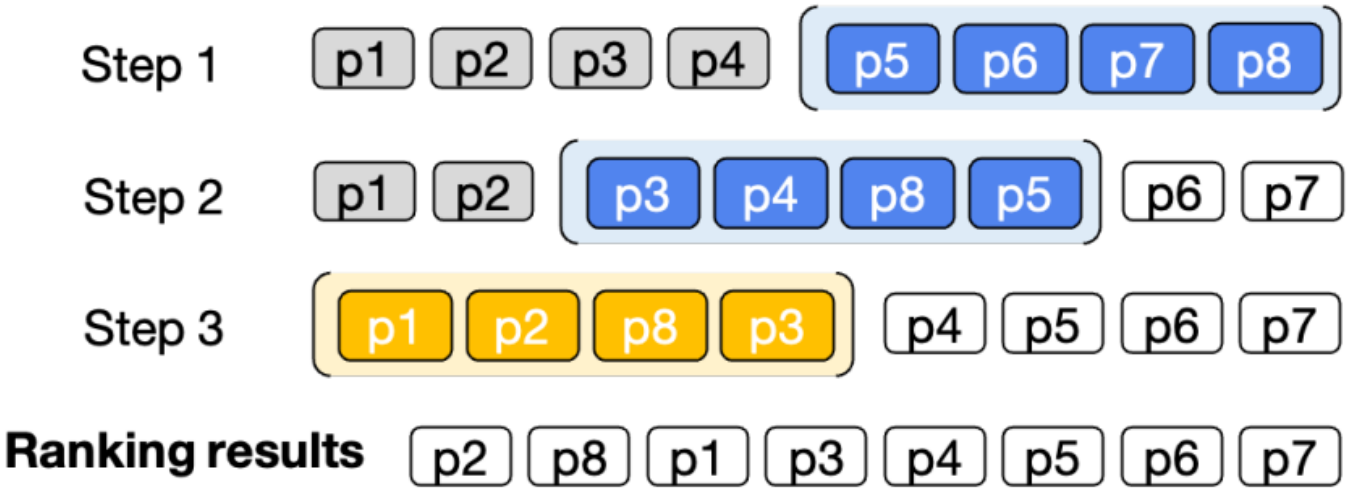

Figure 3: “Bubble Sorting” documents by prompting LLMs [3]

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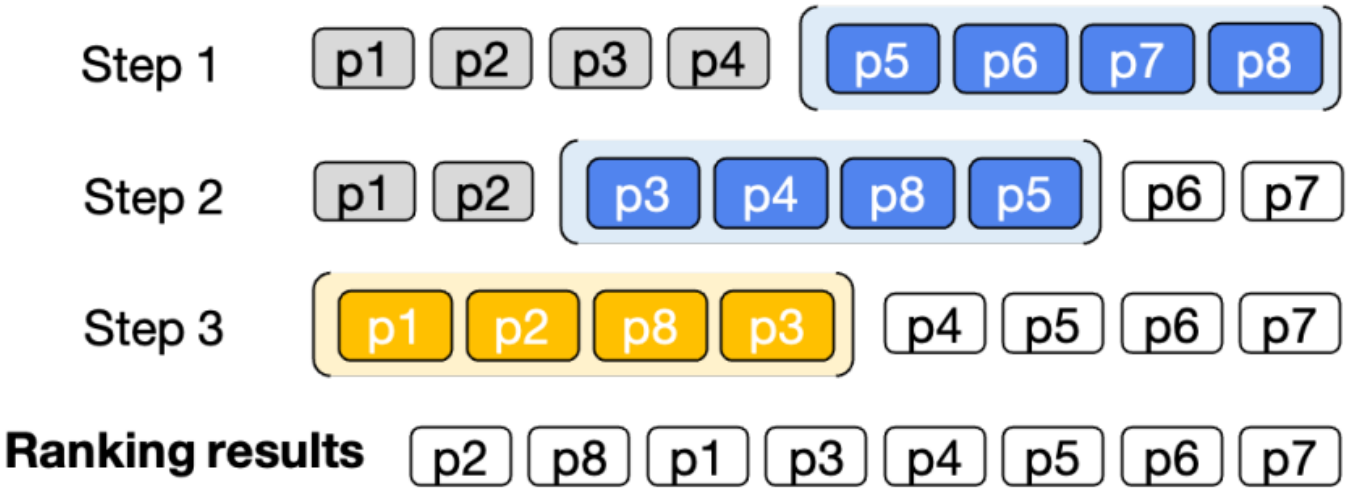
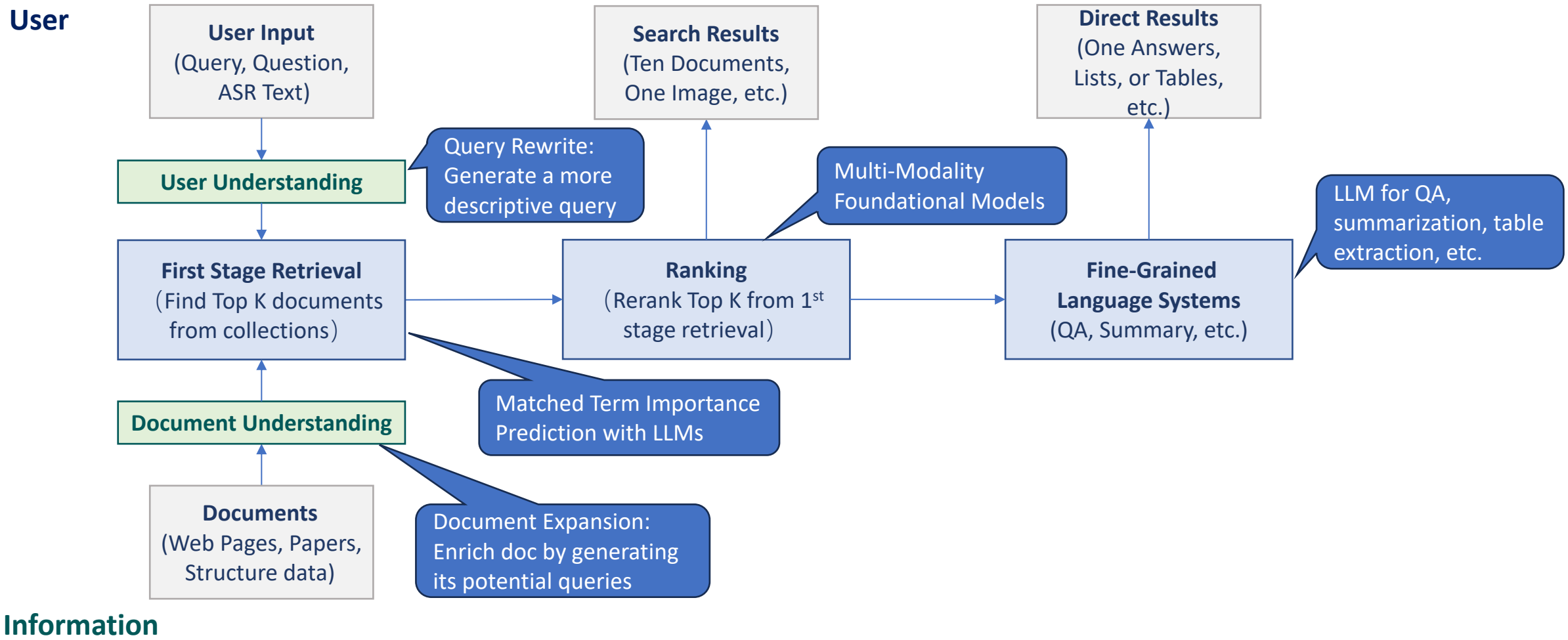


Figure 3: "Bubble Sorting" documents by prompting LLMs [3]

- About 3-5% accuracy+ from GPT-4 over T5 ranker
- Can be distilled to smaller models
- As search mainly cares about top positions, no need to bubble sort all

LLMs in Many Places of Search Engines



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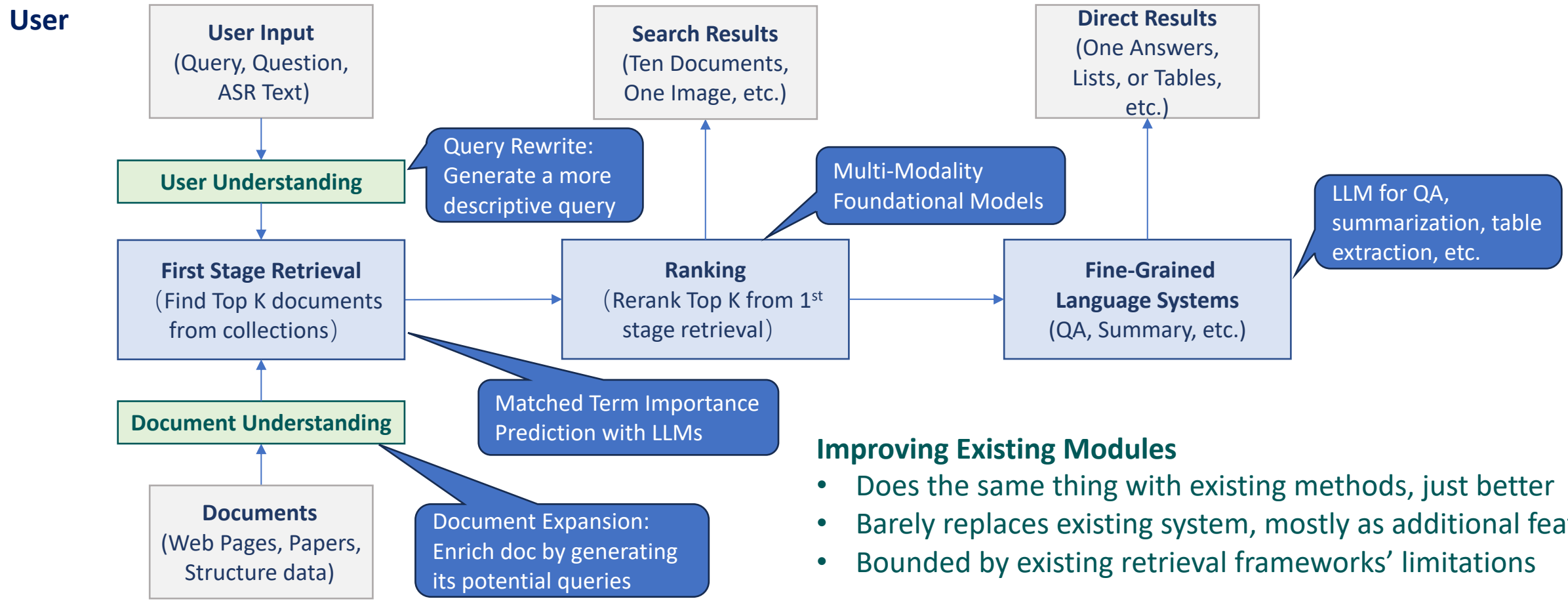

Improving Existing Modules

- Does the same thing with existing methods, just better
- Barely replaces existing system, mostly as additional features
- Bounded by existing retrieval frameworks' limitations

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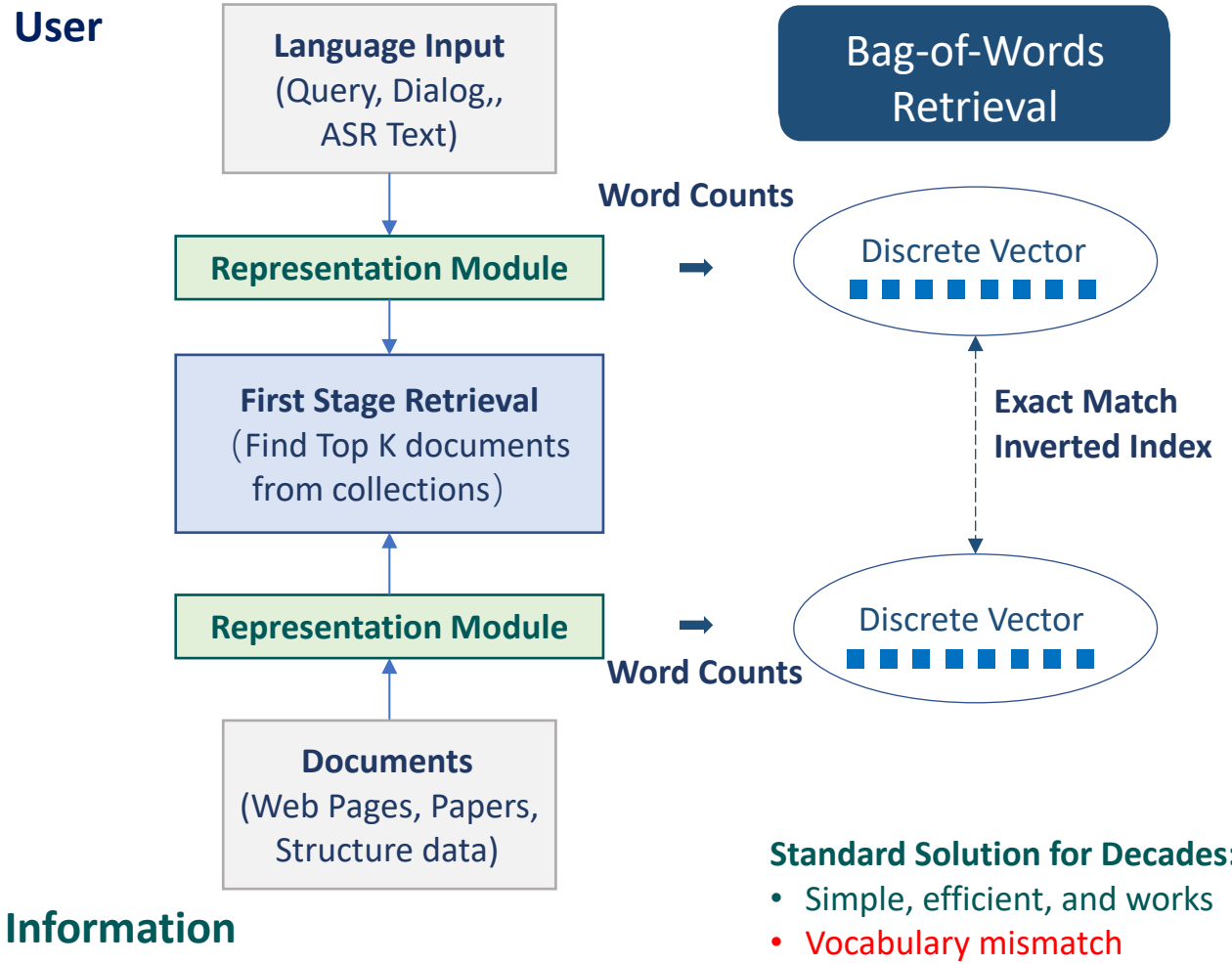
Biggest Pain Points in Previous Search Systems



Bag-of-Words first stage retrieval

- Retrieve documents that contain exact query terms

Intrinsic challenge: Vocabulary Mismatch

- Query and Relevant documents may not have term overlap

Standard Solution for Decades:

- Simple, efficient, and works
- Vocabulary mismatch

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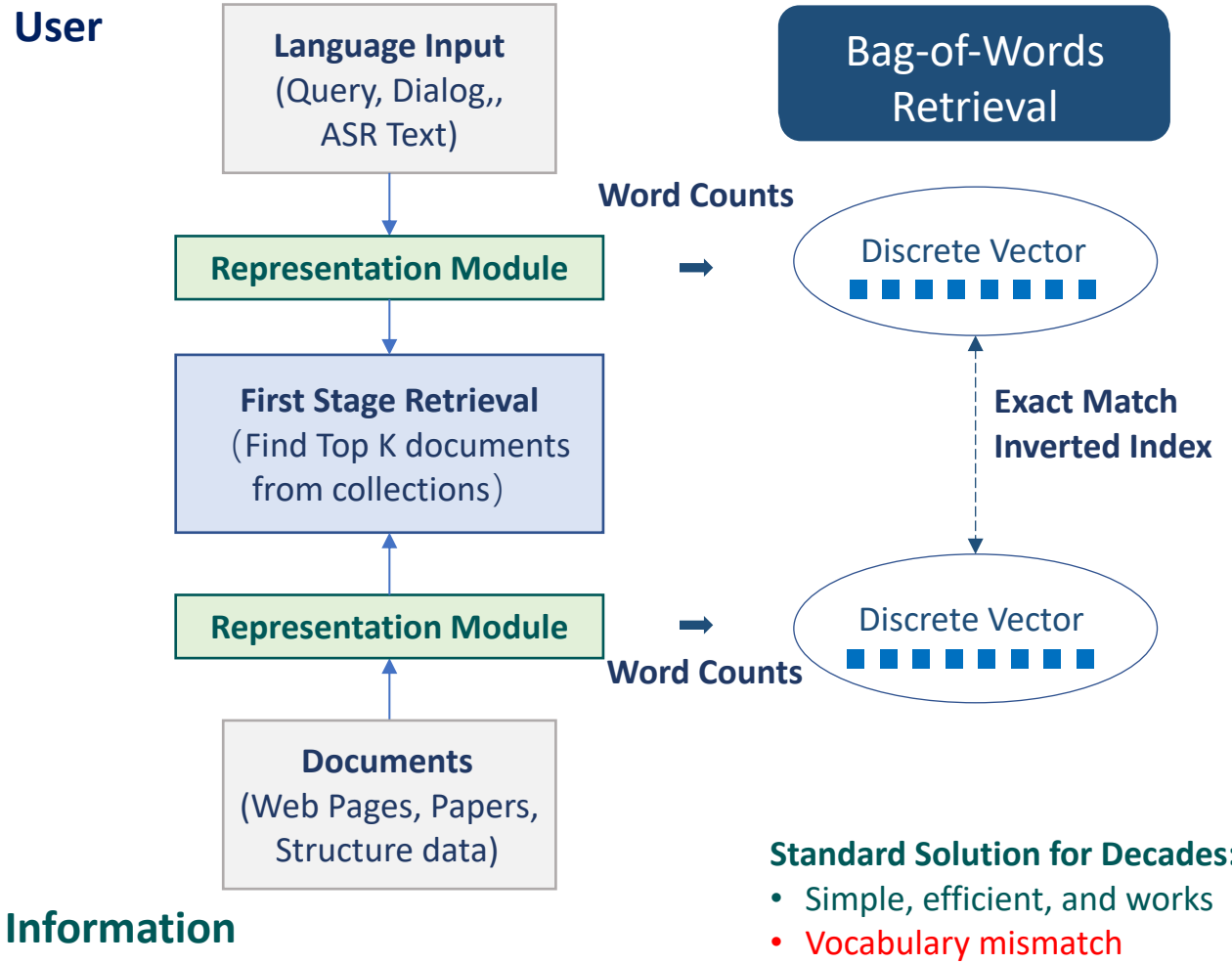

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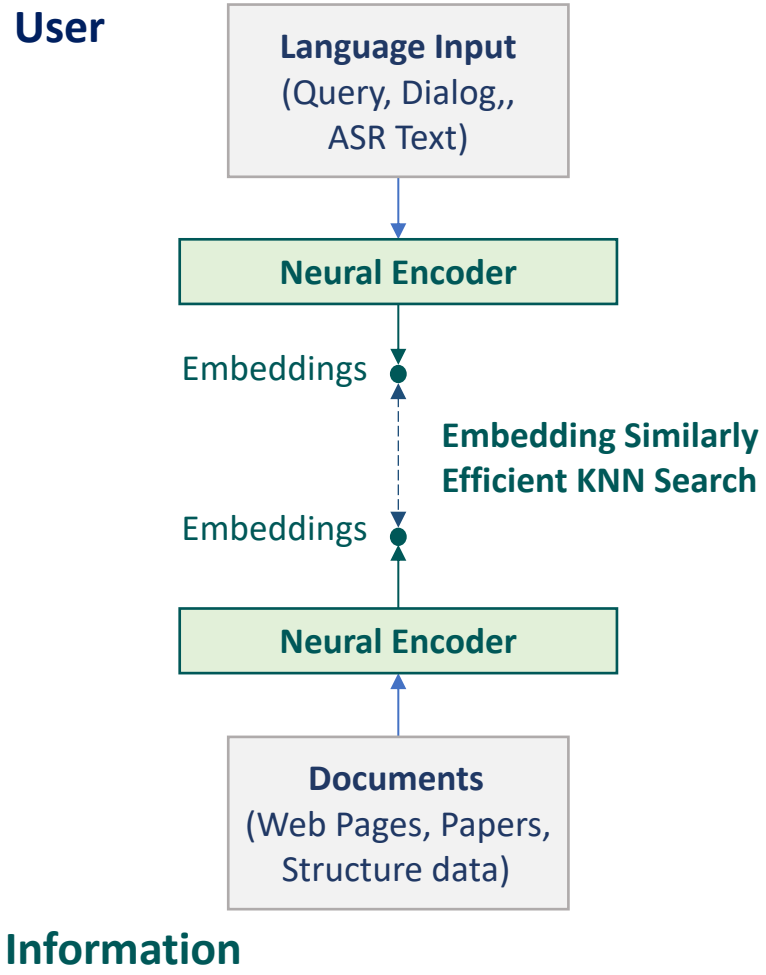
A huge pain point for IR systems

- Discrete representations hard to optimize
- Bounds ranking performance
- Very ways to mitigate, making systems complicated

One solution: expand document with clicked queries

- Requires ton of user traffics
- Impossible for public domain
- Low coverage even in commercial search

Dense Retrieval: Matching with Fully Learned Embeddings



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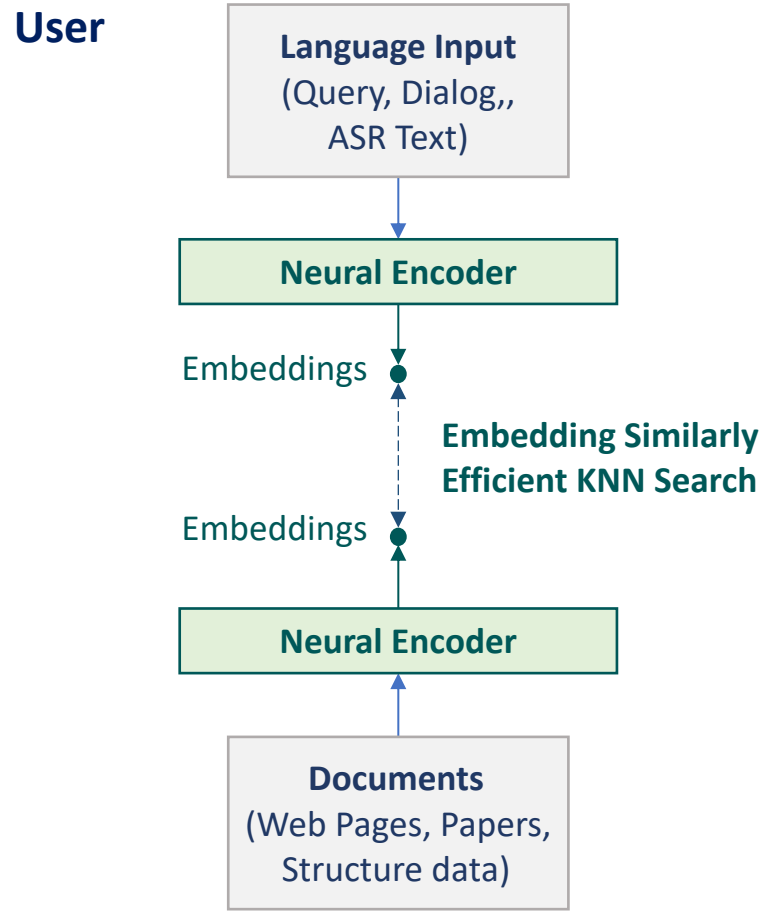

Matching with learned semantic representations instead of bag-of-words

A long-desired goal in IR, with lots of attempts for half a century

- Controlled vocabularies
- Ontologies
- Latent Semantic Index
- Topic Models
- Knowledge Graphs
- Shallow Neural Networks

No general success

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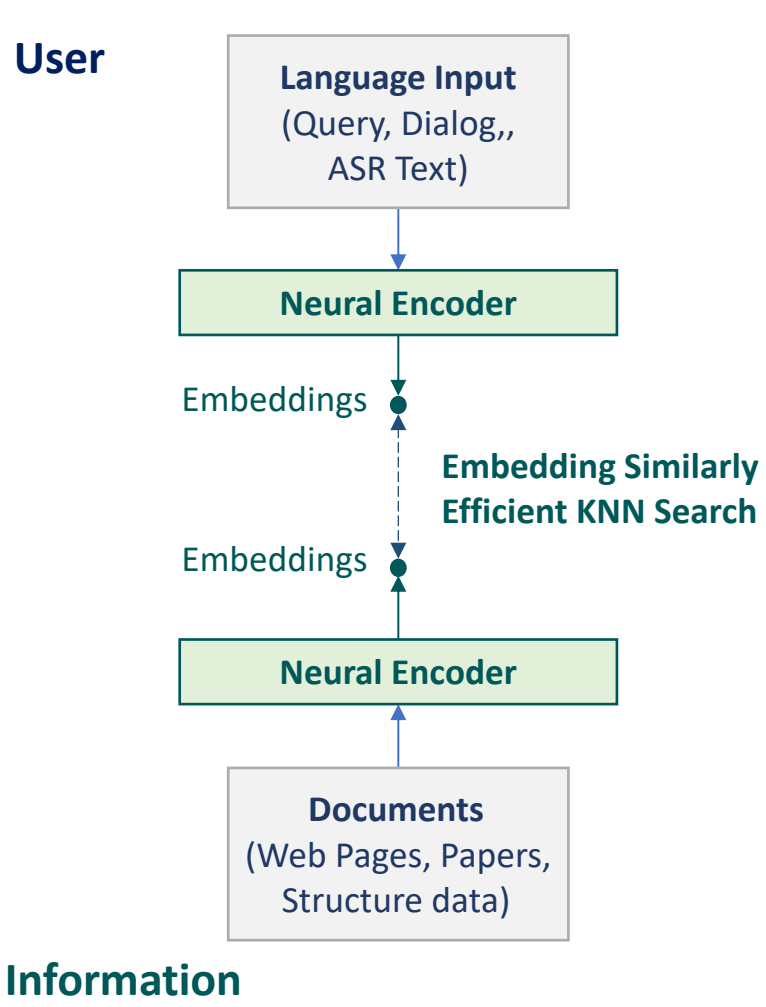

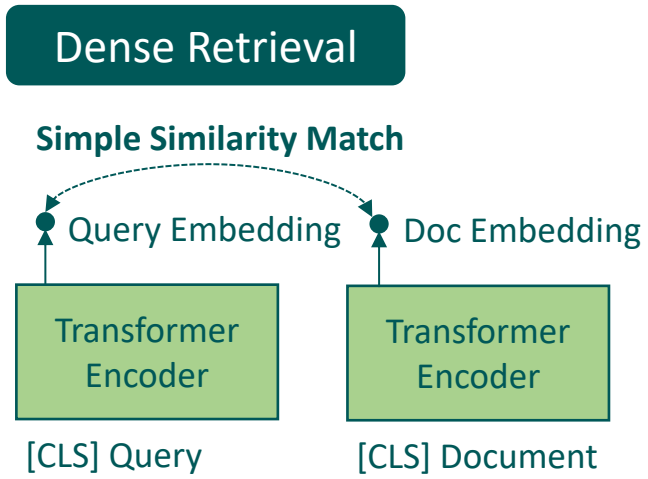

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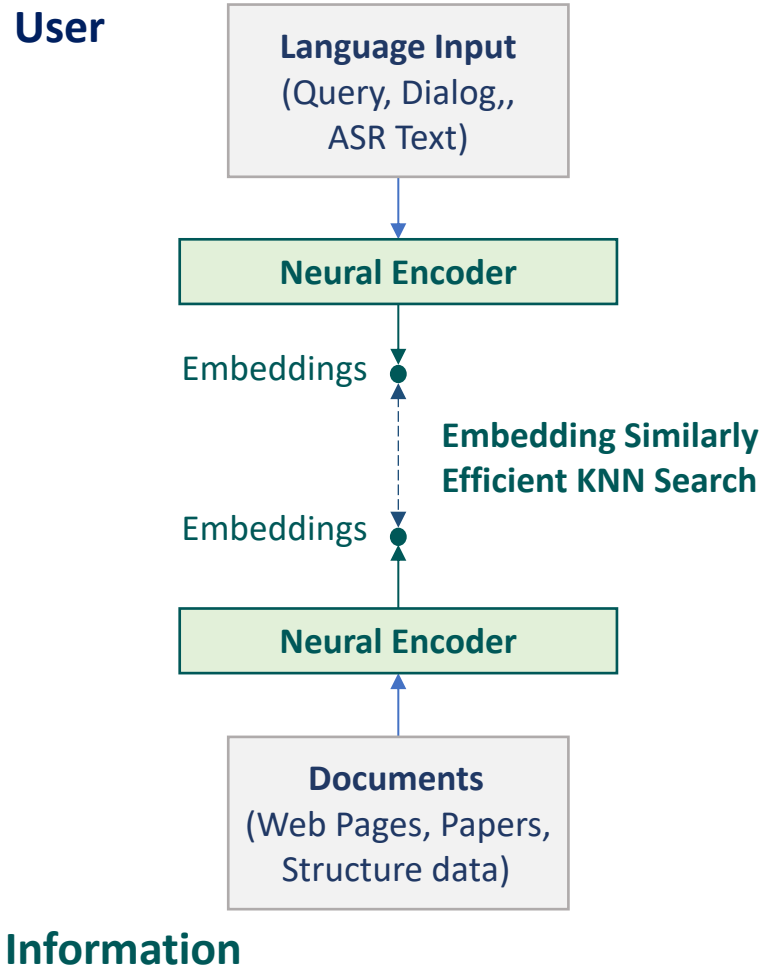

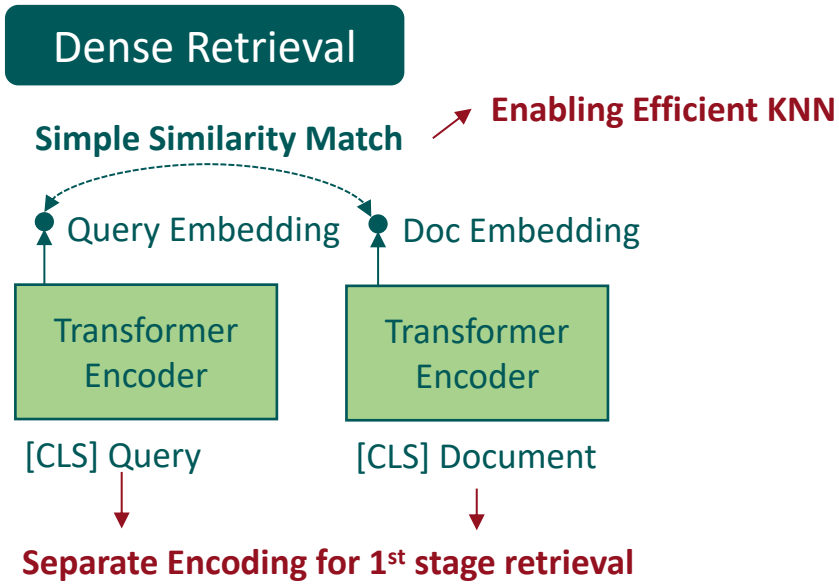

A representation-centric approach:

- All system capacity from encoders, only simple vector operations afterwards

Dense Retrieval: Formulation

A standard setup with BERT Encoders [4]

Retrieval Function: (Dual Encoder)

$$f(q, d) = \text{BERT}(q) \cdot \text{BERT}(d) = \text{MLP}\left(\overrightarrow{[\text{CLS}]}_q\right) \cdot \text{MLP}\left(\overrightarrow{[\text{CLS}]}_d\right)$$

Inference: (Approximate KNN Search)

$$D_q = \text{ANN}_{f(q,\circ)}$$

Finding K nearest neighbor in the corpus with approximate nearest neighbor search.

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Approximate nearest neighbor search (ANNS): Gain (sub-linear) efficiency by slightly scarifying KNN accuracy

- Partition-based methods: Split the space into regions and only search sub regions
  - E.g., hierarchical K-means trees
- Hash-based methods: Map data points by hashing functions and only search certain hash codes
  - E.g., Locality sensitive hash
- Graph-based methods: Connect data points by similarity edges and greedily traverse the graph
  - E.g., K-nearest neighborhood graph

Can achieve similar cost/efficiency as inverted index

Dense Retrieval: Training

Representation learning using standard query-relevant document pairs

Learning: (Contrastive Learning / Learning to Rank)

$$\theta^* = \text{argmin}_\theta \sum_{q} \sum_{d^+} \sum_{d^- \sim P_{D^-}} l(f(q, d^+), f(q, d^-))$$

Relevant q-d pairs (given)

Negative Sampling

Standard Ranking Loss

Dense Retrieval: Challenge

Standard random negatives too weak for retrieval

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Figure 4: Dense Retrieval Training Loss with Randomly Sampled Negatives on MSMARCO

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Standard Ranking Loss

Figure 4: Dense Retrieval Training Loss with Randomly Sampled Negatives on MSMARCO

A severe problem because of unique properties of retrieval

- Corpus size is **huge**: millions, billions, or trillions
- 99.99% are trivially irrelevant
- Retrieval is to distinguish a **small number** of hard negatives

Dense Retrieval: Training with Sparse Retrieval Negatives

Sampling negatives from top results of existing sparse retrieval systems

$$\theta^* = \text{argmin}_\theta \sum_q \sum_{d^+} \sum_{d^- \sim P_{D^-}} l(f(q, d^+), f(q, d^-))$$

- Negatives from existing inverted index (industry's sparse retrieval). (Bing Vector Search) [Waldburger 2019]
- Sampling from BM25 Top K. (DPR) [Karpukhin et al. 2020]
- Offline hard negative mining from production system (Facebook Embedding Search) [Huang et al. 2020]

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Pros:

- Bootstrap upon an existing system with meaningful negatives

Cons:

- Often negatives from sparse retrieval are still too trivial for dense retrieval
- Empirically, weaker generalization ability

Dense Retrieval: Training with Self Negatives

Sampling negatives globally from the entire corpus using the dense retriever itself (ANCE [5]).

$$\theta^* = \text{argmin}_\theta \sum_q \sum_{d^+} \sum_{d^- \sim \text{ANN}_{f(q,\circ)}} l(f(q, d^+), f(q, d^-))$$

- Sampling from the top retrieved results of the dense retrieval model
- Periodically refresh the dense retrieval index to keep negatives updated
- Start from sparse retrieval negatives to warm up

[5] Xiong et al. "Approximate nearest neighbor negative contrastive learning for dense text retrieval". ICLR 2021.

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- Sampling from the top retrieved results of the dense retrieval model
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Pros:

- Aligned training and testing distribution
- Strong performance in-domain and out-of-domain

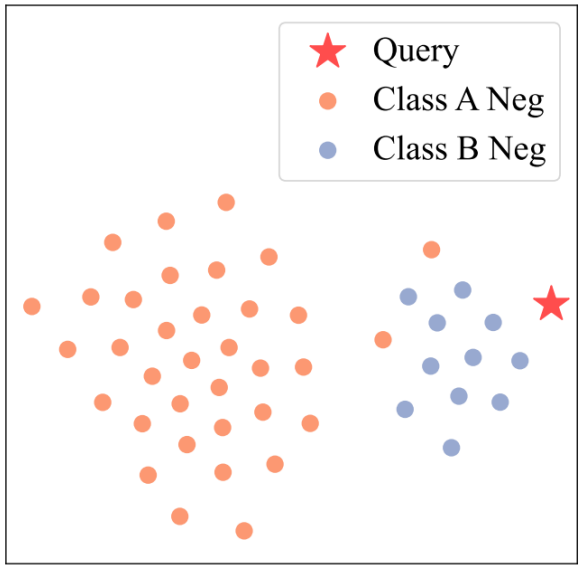
Cons:

- Overhead cost in refreshing the corpus index for negative sampling
- Instabilities from negative refreshes

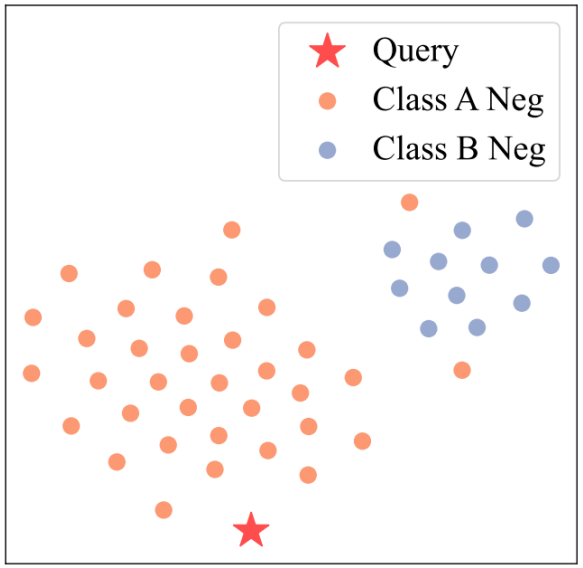
Dense Retrieval: Instabilities from Negative Sampling

Dense retriever swings between several groups of negatives [6]

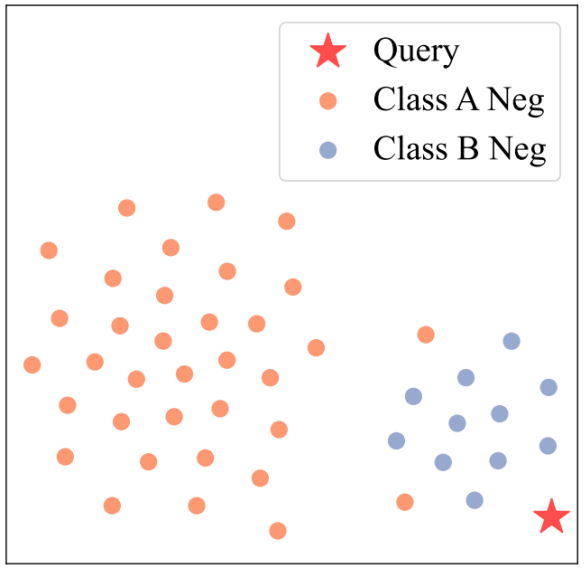
Query	Class A Negatives	Class B Negatives
most popular breed of rabbit	The Golden Retriever is one of the most **popular breeds** in the United States…	**Rabbit** habitats include meadows, woods, forests, grasslands, deserts and wetlands…



After Negative Refresh #1



After Negative Refresh #2



After Negative Refresh #3

Figure 5: T-SNE plots of a query and its two negative groups during ANCE training [6]

Dense Retrieval: Training with Smoothed Negatives

Smooth training by combining negatives from past samples and potential future samples (ANCE-Tele [7])

$$\theta^* = \text{argmin}_\theta \sum_q \sum_{d^+} \sum_{d^- \sim \text{Tele}_i} l(f(q, d^+), f(q, d^-))$$

$$\text{Tele}_i = \text{ANN}_{f_i(q,\circ)} + \text{Tele}_{i-1} + \text{ANN}_{f_i(d^+,\circ)}$$

Self-Negatives from current (i-th) training episode

Negatives from previous episode (Momentum)

Approximation of future negatives using neighbors of d^+ (Lookahead)

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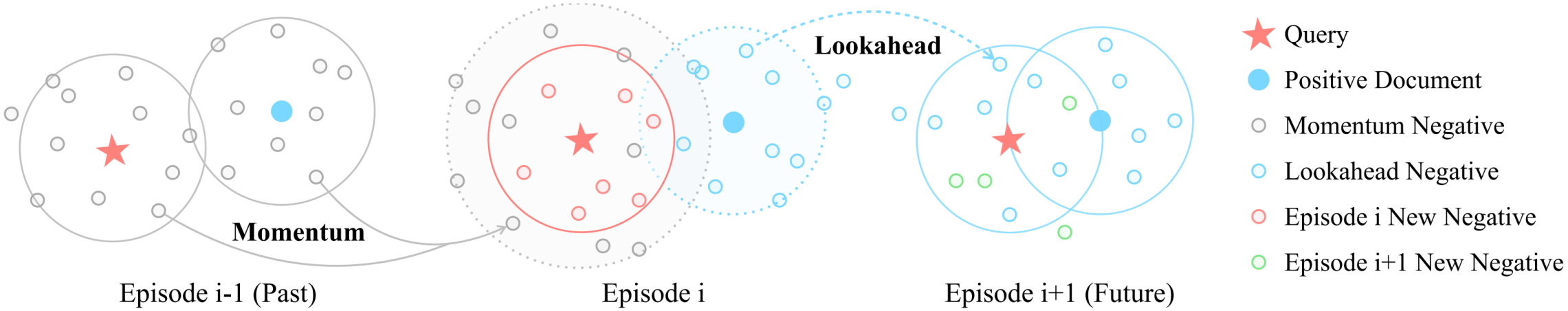


Figure 6: Smooth Negative Sampling with Momentum and Lookahead [6]

Dense Retrieval: Performances

Evaluation on supervised retrieval: MS MARCO Passage Task.

- Retrieve answer passages for Bing questions from a corpus of ~10M passages
- All dense retrievers start from RoBERTa base.

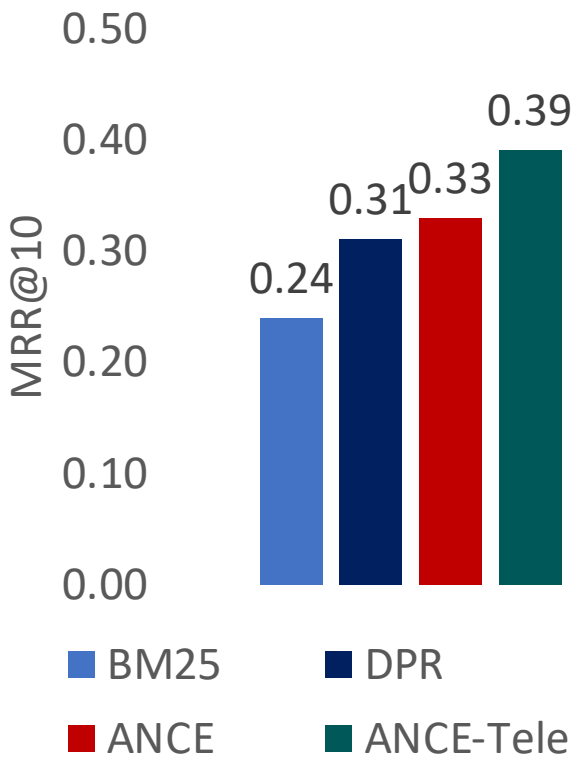


Figure 7: Supervised Retrieval Performances on MS MARCO.

BM25: Standard sparse bag-of-words based retrieval

DPR: Trained with BM25 negatives + random negatives

ANCE: Trained with self-negatives (warmed up by BM25 negative)

ANCE-Tele: Trained with momentum and lookahead global negatives

Dense Retrieval: Error Cases

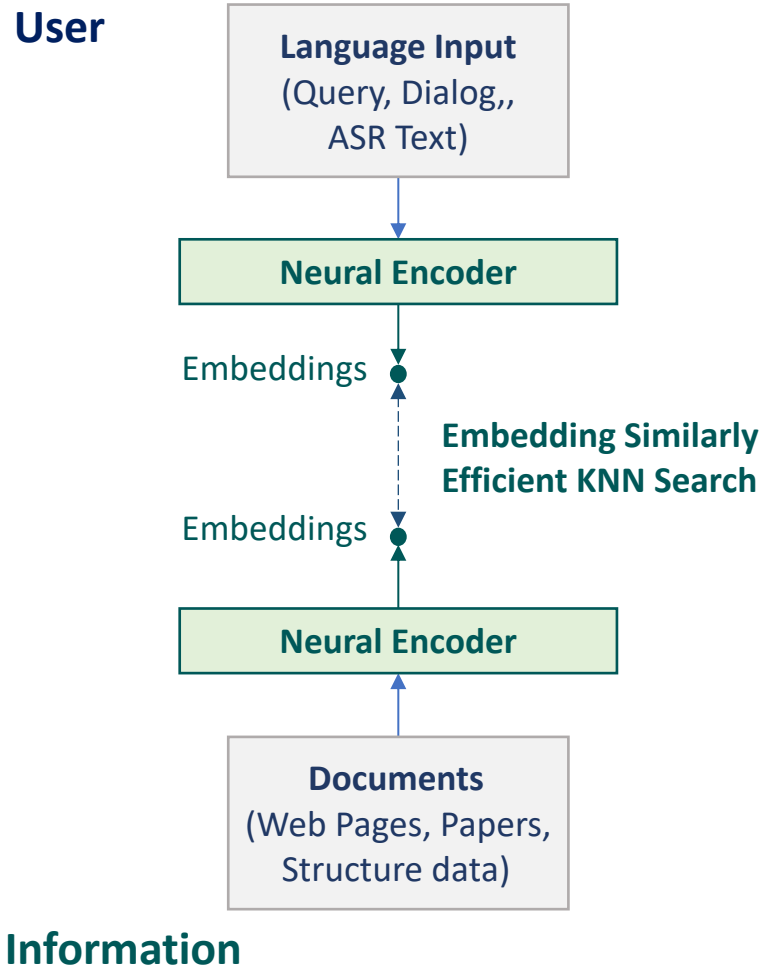
Retriever	Query	Bad Case	Relevant Document
BM25	What is the most popular food in Switzerland	Answers.com: Most popular traditional food dishes of Mexico	Wikipedia: Swiss cuisine
ANCE	How long to hold bow in yoga	Yahoo Answer: How long should you hold a yoga pose for	yogaoutlet.com: How to do bow pose in yoga

Table 1: Error Cases of BM25 and ANCE in TREC Deep Learning Track Document Retrieval 2019 [5]

Sparse retrieval and dense retrieval behave quite differently.

- BM25 and ANCE only agree on 20% of their top 100 rankings
- But both find relevant document in top 3

Dense Retrieval: Summary



A long-desired goal, finally achieved because of two advancements:

1. Representation power of LLMs (Major)
2. Retrieval-oriented fine-tuning (Last Mile)

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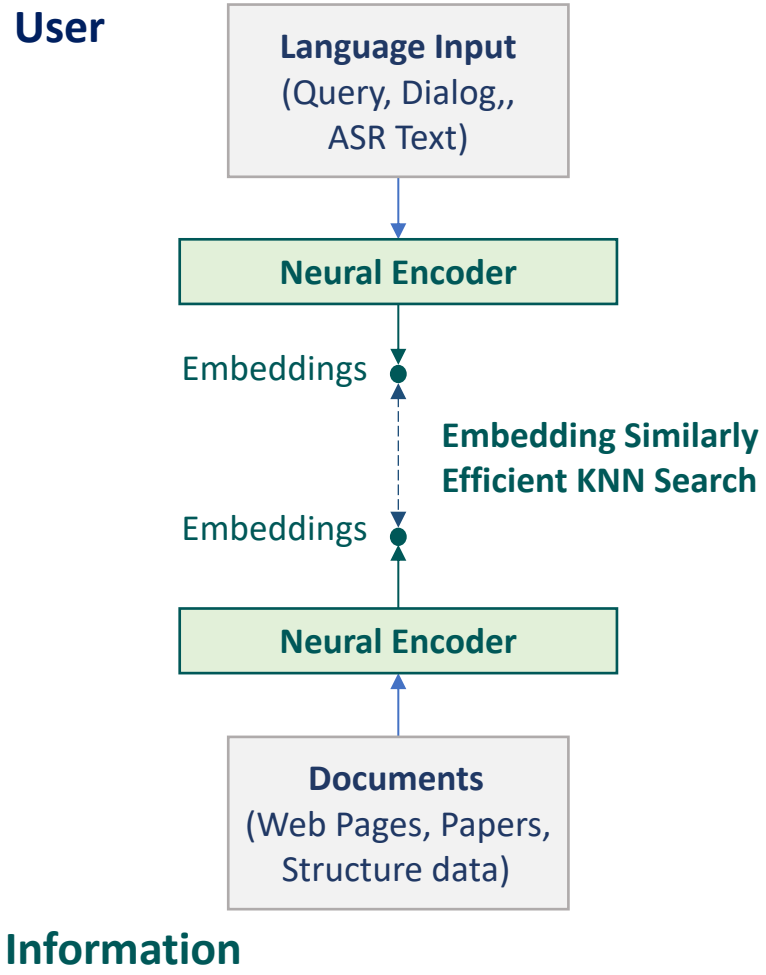

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A "Painkiller" solution

- Eliminate a major bottleneck of existing search solutions
- A fundamental solution for an intrinsic challenge of status quo

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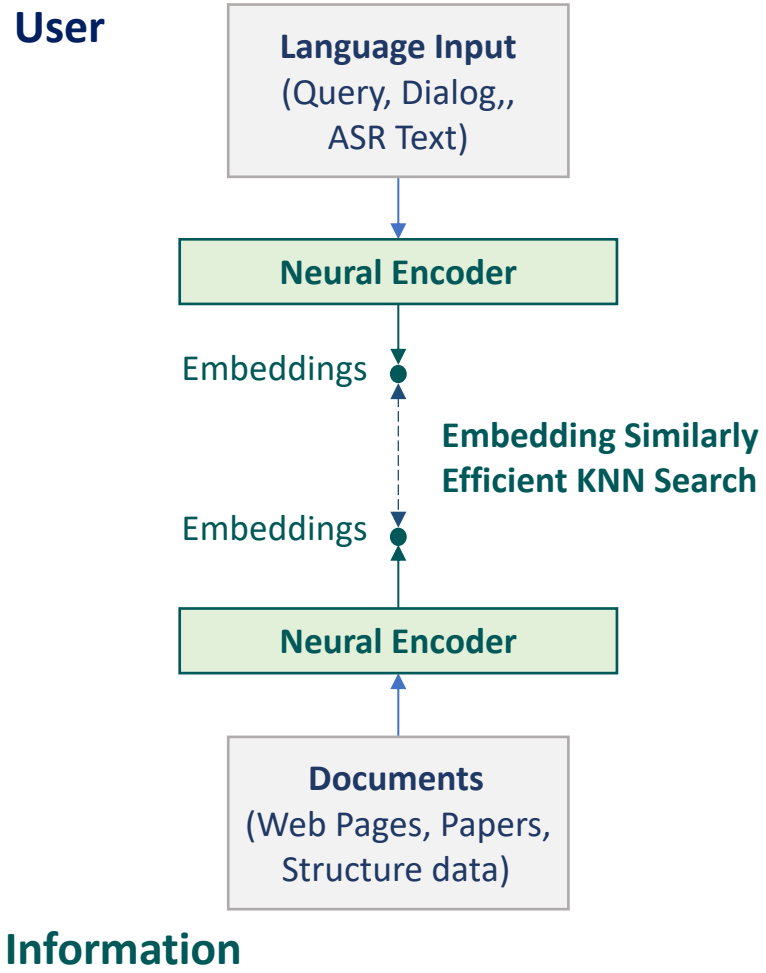

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A "Painkiller" solution

- Eliminate a major bottleneck of existing search solutions
- A fundamental solution for an intrinsic challenge of status quo

Enabled lots of potentials

- Democratize state-of-the-art search
- Ride the generalization power of LLMs
- Unify many modalities and scenarios in one embedding space

Many vector-based search startups and heavy investments

Outline

Overview of Modern Information Retrieval Systems

- An example search component updated by LLMs
- Glances of other components using LLMs

Dense Retrieval, a different way of search with LLMs

- End-to-end learned retrieval
- **Notable extensions**

Pretrain retrieval representations

Dense Retrieval Extensions: Stronger Foundation Models

Sentence T5 Encoder-Decoder: bringing in benefits of T5

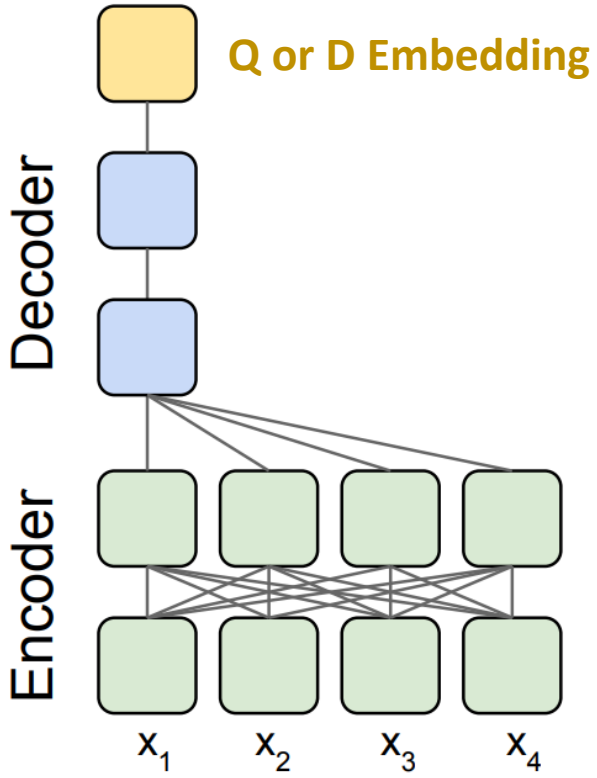


Figure 8: Architecture of SentenceT5 Encoder-Decoder [7].

Benefits:

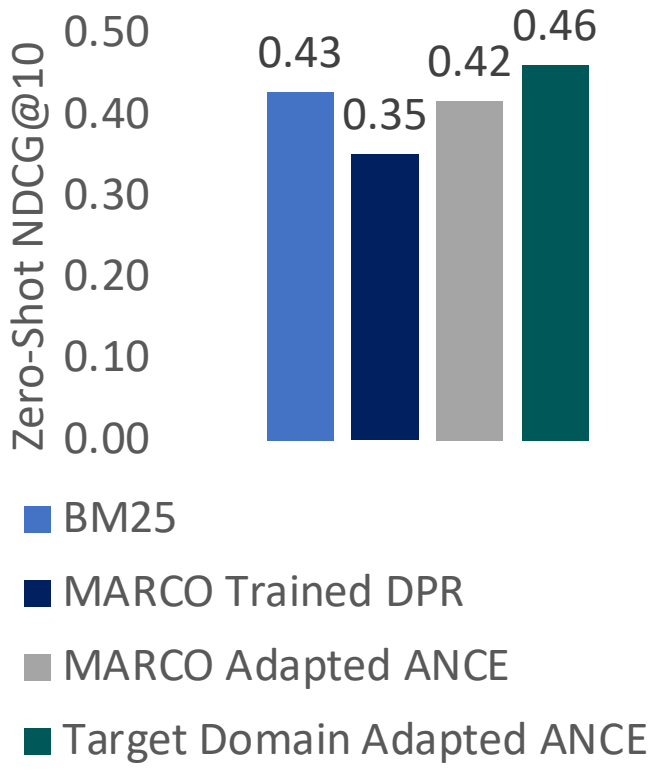
- Better pretrained model (T5 > RoBERTa)
- Easy to introduce prompts/instructions, especially task specific ones in multi-task setting
- Current go-to solution at T5's scales

[7] Ni et al. "Sentence-T5: Scalable Sentence Encoders from Pre-trained Text-to-Text Models". ACL 2022.

Dense Retrieval Extensions: Robust Zero-Shot

Various techniques to make web-trained dense retrievers generalizable to other search domains

- Lots of real-world needs (e.g., OpenAI embedding API, AWS Open Search, Azure Search)
- Most successful techniques are to continuously pretrain underlying LLM in target corpus



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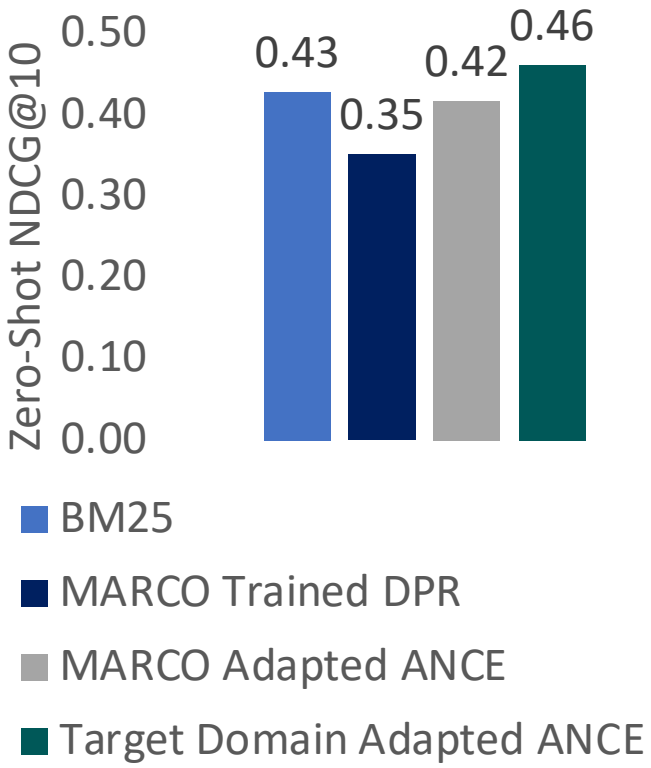


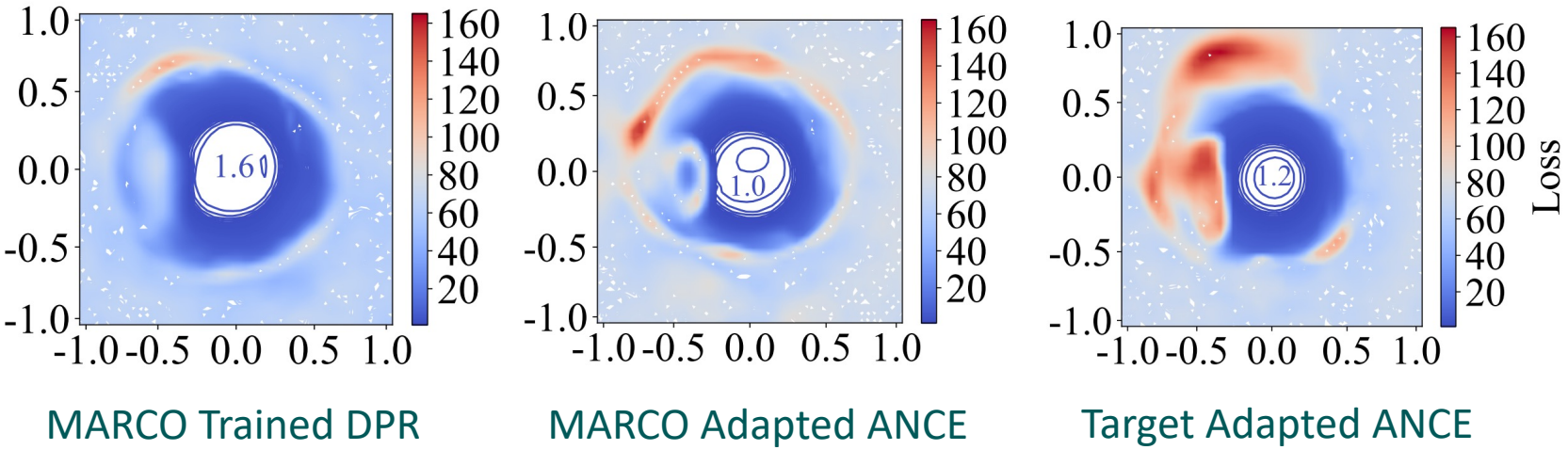
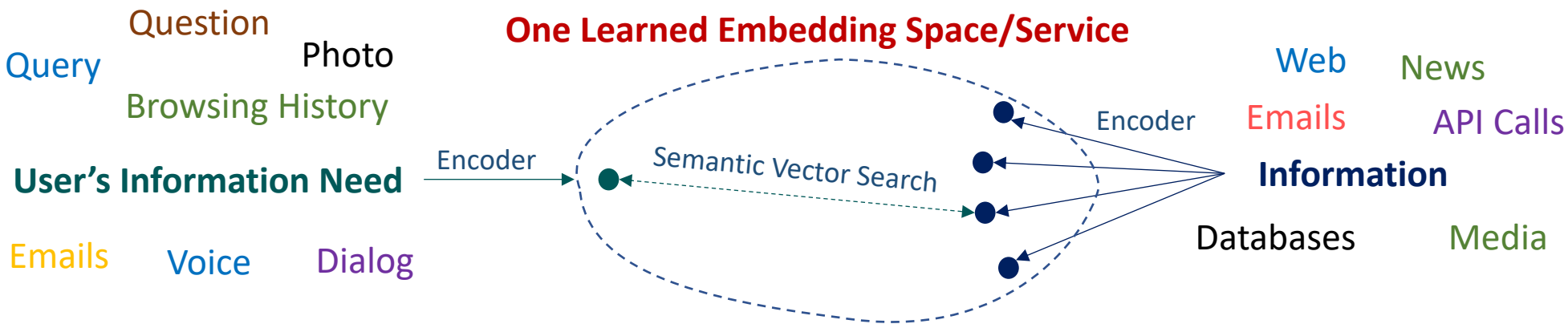


Figure 9: Loss landscape of dense retrieval models on MARCO development set.

Dense Retrieval Extensions: Universal Retrieval

Map queries and documents in variant formats and modalities into one central embedding space

- Enable cross scenario and cross modality information access
- One unified entry for search



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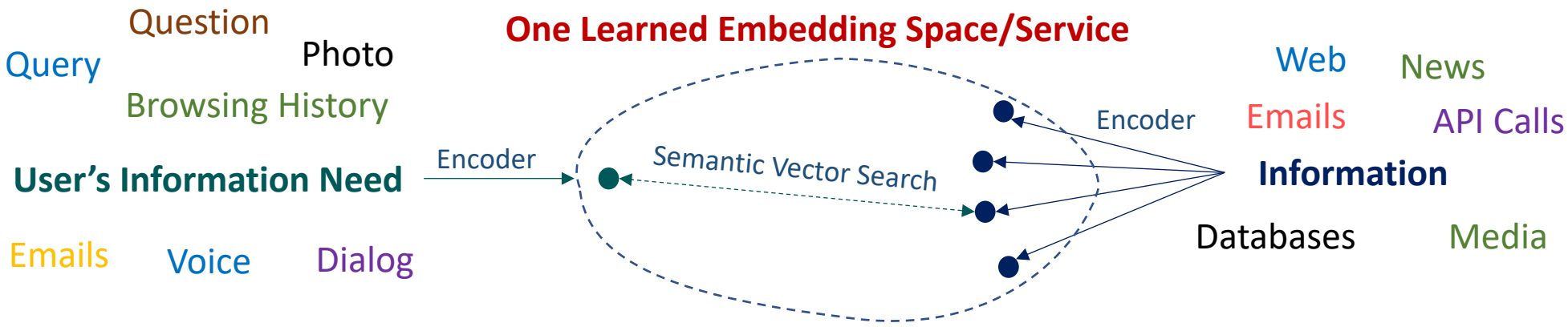

Current Solution: Ride the universal representation capability of foundational models

- Linearize structured data with prompts, e.g., Table BERT, and use text model
- Leverage multi-modality foundational models, e.g., CLIP for image-text
- Continuous pretrain LM on other data formats, e.g., code, molecular SMILE

Outline

Overview of Modern Information Retrieval Systems

- An example search component updated by LLMs
- Glances of other components using LLMs

Dense Retrieval, a different way of search with LLMs

- End-to-end learned retrieval
- Notable extensions

Pretrain retrieval representations

Anisotropy/Non-Uniformity

Zero-shot performance of pretrained embeddings on semantic text similarity (STS) tasks

- STS Task: producing a similarity score for a given pair of sentences
- Metric: by Pearson correlation with human rating (e.g., 5 being exact same meaning/paraphrase)

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Model	STS12	STS13	STS14	STS15	STS16	STSb
Avg. GloVe embeddings	55.14	70.66	59.73	68.25	63.66	58.02
Avg. BERT embeddings	38.78	57.98	57.98	63.15	61.06	46.35
BERT CLS-vector	20.16	30.01	20.09	36.88	38.08	16.50

Table 3: BERT embedding similarity performances on STS tasks [10]

Much worse performance than GloVe Embeddings.

- [CLS] is near random.
- Mean-pooling over tokens is better but still much worse than word embeddings

Anisotropy/Non-Uniformity

The sequence embedding space of many pretrained LLMs are highly non-uniform

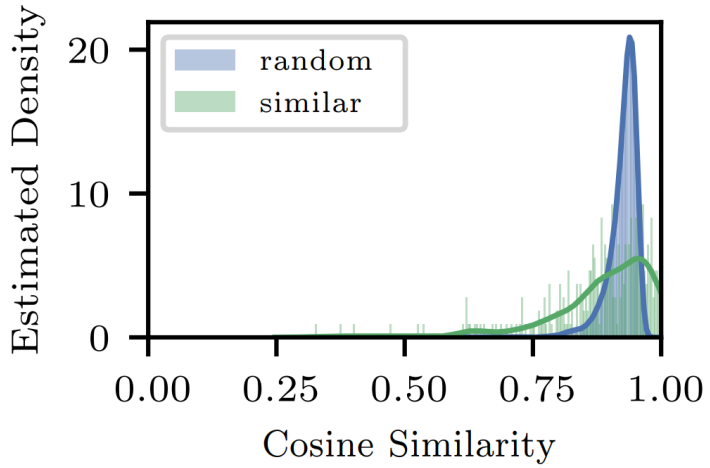

Figure 11: Similarity of RoBERTa $\overrightarrow{[\mathrm{CLS}]}$ on semantically similar and random pairs from STS-S [11]

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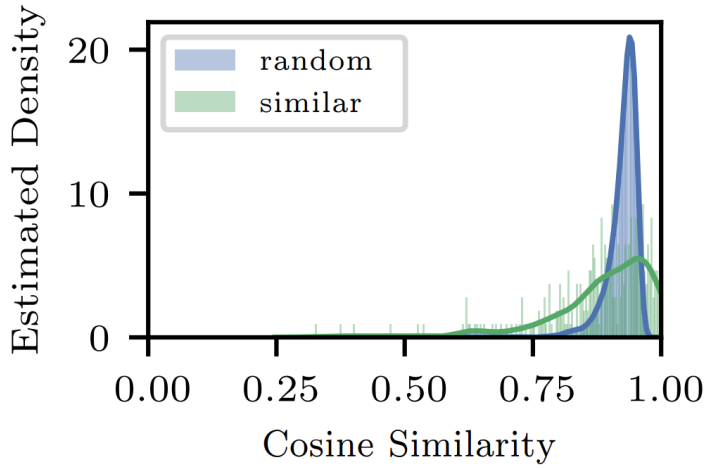

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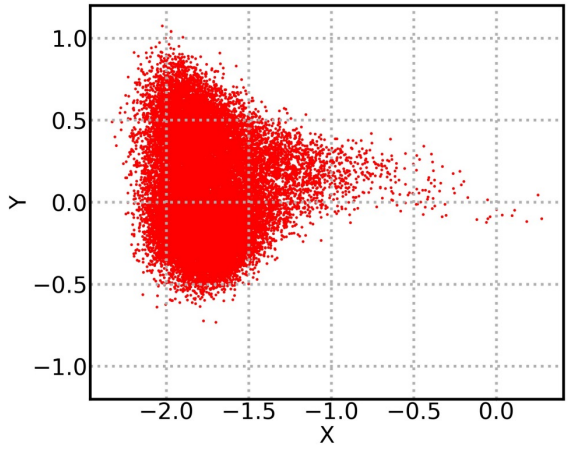

Figure 12: SVD 2-D mapping of word embeddings from Transformer trained on EN→DE [12]

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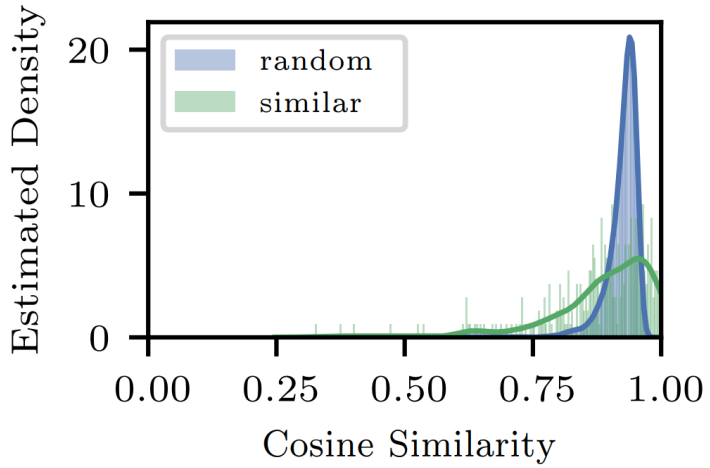

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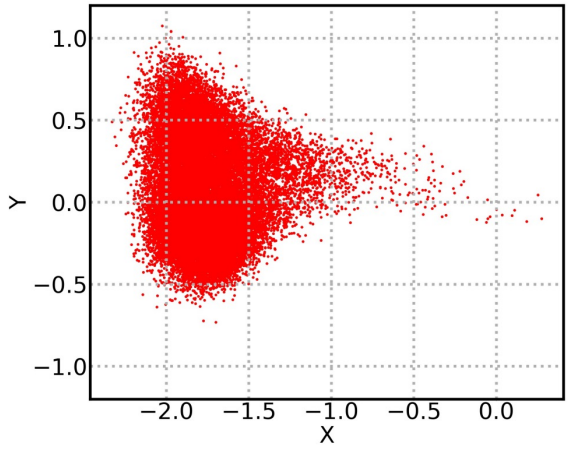


Figure 12: SVD 2-D mapping of word embeddings from Transformer trained on EN→DE [12]

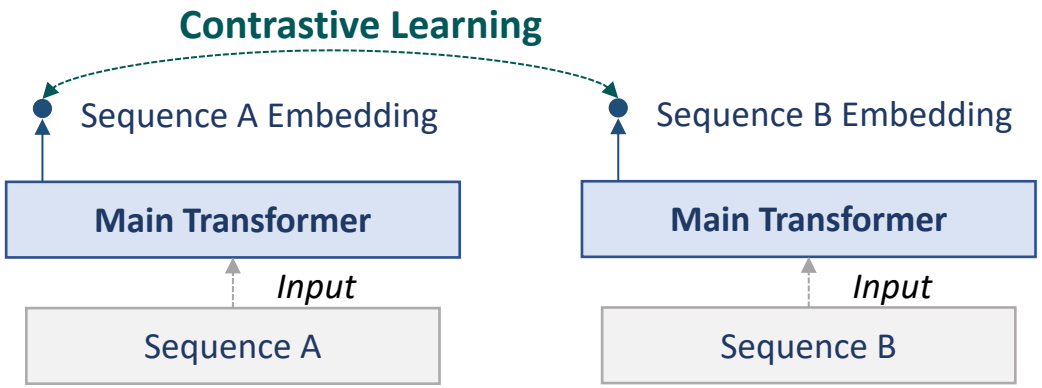
Most rare tokens are pushed to a narrow cone in the space, and [CLS] is a rare token in learning

- Every training signal pushes all negatives away from the positive
- Rare tokens (without much or any positive pulls) are pushed away from all positives, into a narrow cone

Solution: Sequence Contrastive Learning

Pretraining sequence representations with Sequence Contrastive Learning (SCL) [11]

Adding pretraining task: $L_{\mathrm{SCL}} = \mathrm{E}(\frac{\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{+}))}{\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{+}))+\sum_{s-}\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{-}))})$



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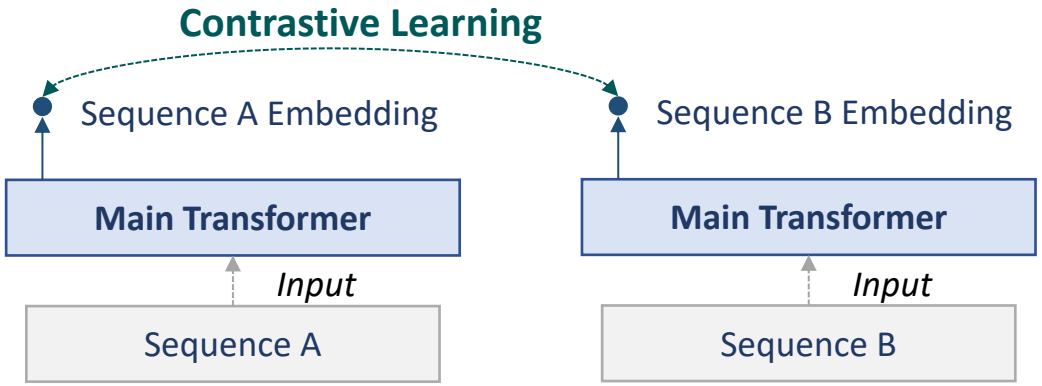
Embeddings of positive contrast sequence pairs

Embeddings of negative sequence pairs



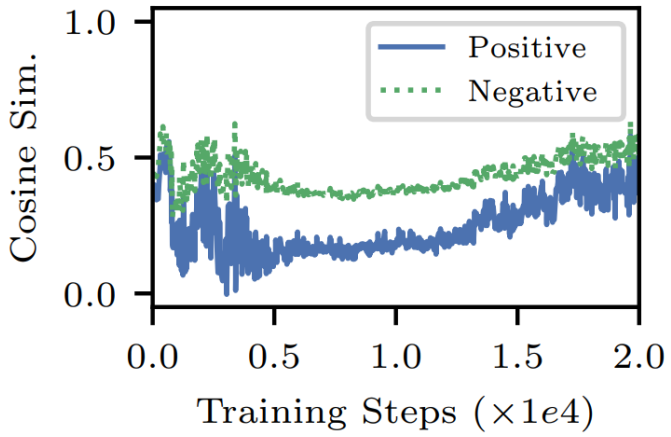
Construction of positive contrast sequence pairs:

- *Data augmentation*: cropping [11], random replacement, back translation, different dropout (SimCSE), etc.
- *Unsupervised pairs*: co-occurrence in doc (co-doc), etc.
- *Supervisions*: Web QA pairs, search query-clicked docs…

Solution: Sequence Contrastive Learning

Recalibration of the embedding space, e.g., using cropped sequence pairs (90% overlap)

Training Pair Similarity
(Without SCL)



Failed without SCL
(Although 90% overlap!)

Training Pair Similarity
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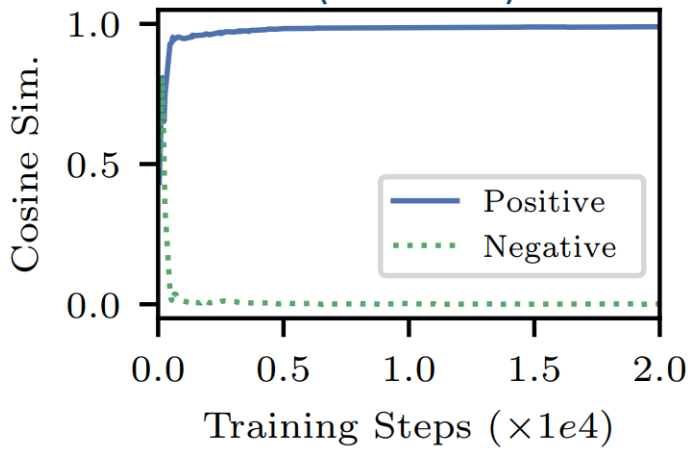

Easy-to-Learn Task
(90% overlap, after all)

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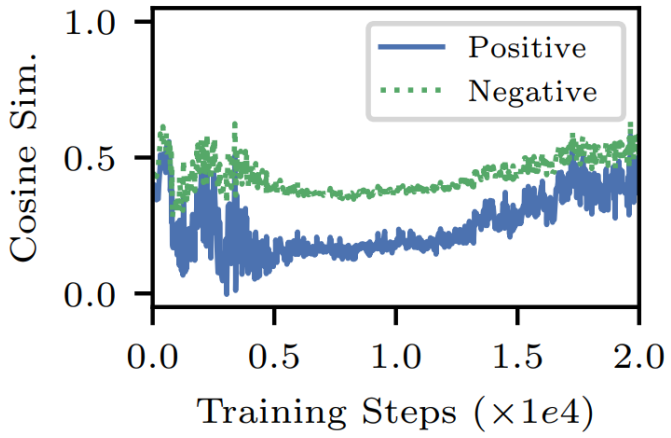

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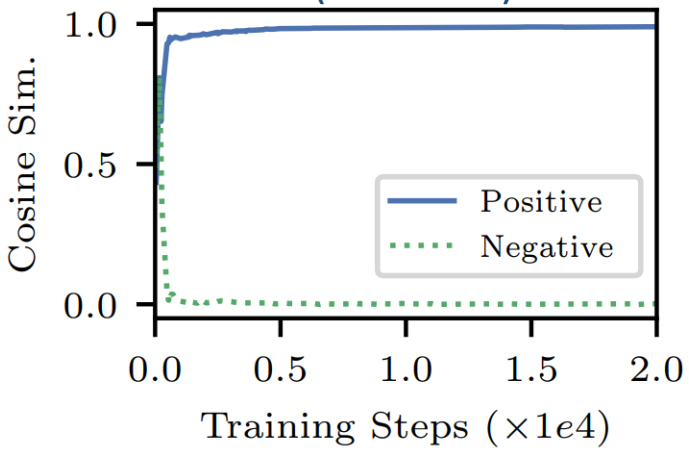
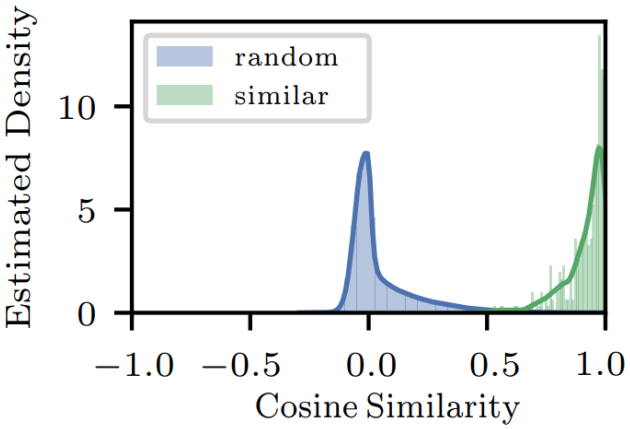


Easy-to-Learn Task
(90% overlap, after all)

STS-B Similarity
(With SCL)



Effective Calibration
& Good Zero-Shot Ability

Decent zero-shot performance on many sequence similarity tasks and non-random performance on retrieval

Deeper Look into Contrastive Learning

Two forces in contrastive learning: Alignment and Uniformity [13]

$$L_{\mathrm{SCL}} = \mathrm{E}\left(\frac{\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{+}))}{\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{+}))+\sum_{s-}\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{-}))}\right)$$

$$\sim \underbrace{\cos(\boldsymbol{s},\boldsymbol{s}^{+})}_{\text{Align positive pairs together}} + \underbrace{\log(\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{+})) + \sum_{s-}\exp(\cos(\boldsymbol{s},\boldsymbol{s}^{-})))}_{\text{Uniformly spread random pairs in the space}}$$

- Proof in Wang et al. [12] that, if exist, perfectly aligned/uniform encoders minimize the two terms
- Note: here negatives are sampled uniformly, not from a long tail distribution

Deeper Look into Contrastive Learning

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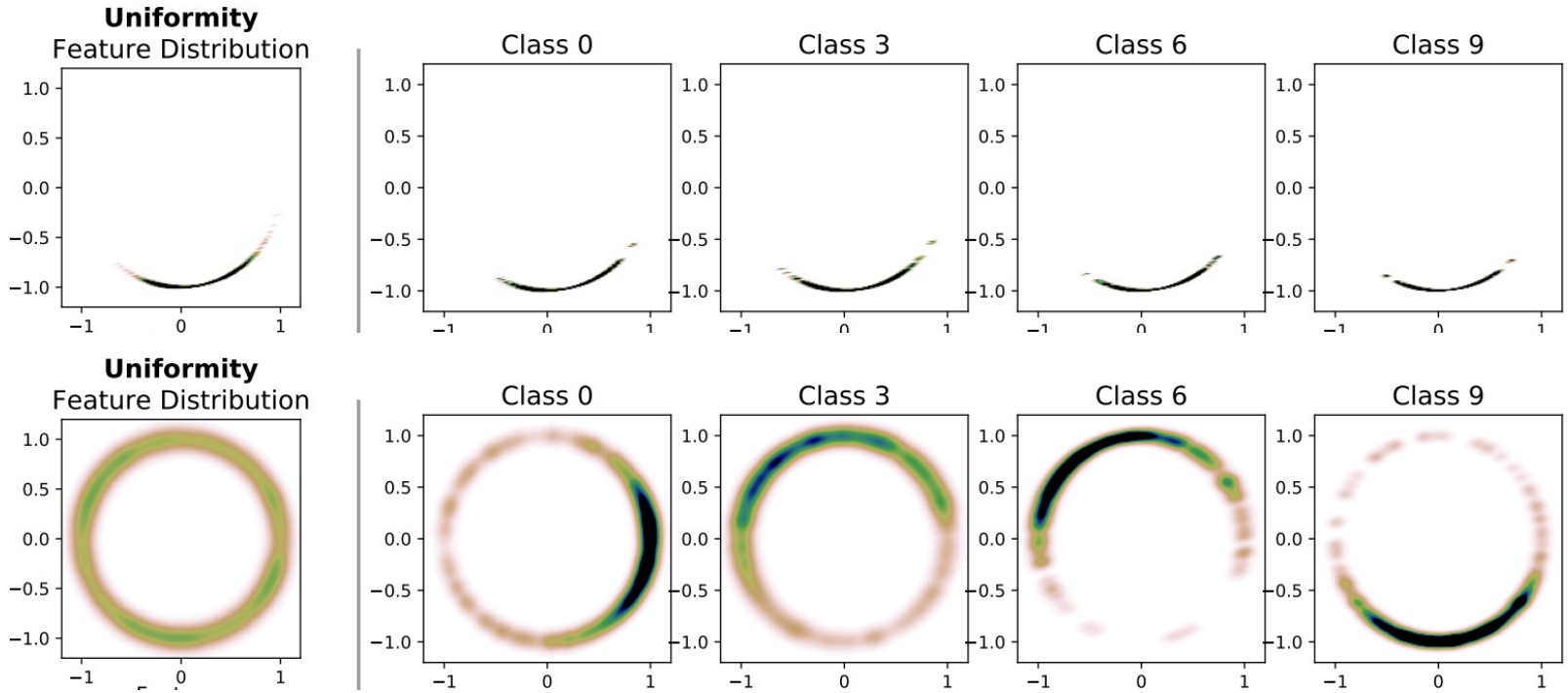

Figure 13: Uniformity of image features in CIFAR-10 from random network (top) and unsupervised contrastive learning (bottom) [12]

Alignments

What information does unsupervised contrastive pairs bring in to align the embedding space?

Method	Sequence A	Sequence B
SimCSE	The Steelers enjoy a large, widespread fanbase nicknamed Steeler Nation.	The Steelers enjoy a large, widespread fanbase nicknamed Steeler Nation.
Inverse Cloze Task (ICT)	The Steelers enjoy a large, widespread fanbase nicknamed Steeler Nation.	They currently play their home games at Acrisure Stadium on Pittsburgh's North Side in the North Shore neighborhood,
Cropping Augmentation	The Steelers enjoy a large, widespread fanbase nicknamed ___	____ enjoy a large, widespread fanbase nicknamed Steeler Nation.
Co-document	The Steelers enjoy a large, widespread fanbase nicknamed Steeler Nation.	In the NFL's "modern era" (since the AFL–NFL merger in 1970) the Steelers have posted the best record in the league.

Very limited semantic signals in the alignment for search relevance

- Either strong term overlaps or loosely correlated

Solution: Weak Supervision from Web Graph

Leverage Anchor Texts and the document they point to pseudo query-relevant document pairs

Method	Sequence A	Sequence B
Anchor-Document	Vegetarian Society of Ireland	The Vegetarian Society of Ireland is a registered charity. Our aim is to increase awareness of vegetarianism in relation to health,
Actual Argument Retrieval Data	Becoming a vegetarian is an environmentally friendly thing to do.	Health general weight philosophy ethics You don't have to be vegetarian to be green. Many special environments have been created by

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Web graph and anchor information is widely used in many web and search applications

- Determine the importance of a web page (Page Rank)
- Enrich the representation of a document , using 3rd party information (Document Expansion)
- Serve as pseudo queries for feature-based ranking models

[14] Nie et al. "Unsupervised Dense Retrieval Training with Web Anchors". SIGIR 2023.

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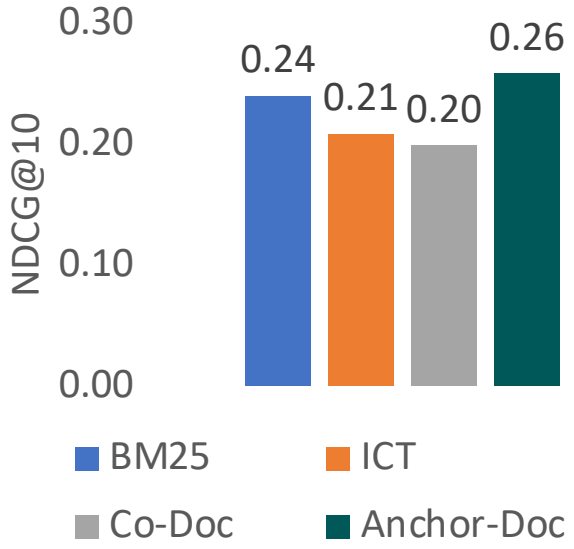

Figure 14: MARCO NDCG@10 of BM25 and dense retrievers trained by different unsupervised signals

Anchor-Doc the only unsupervised signal source outperforms BM25

- Data cleaning required to filter out functional anchors, e.g., "homepage"

A widely useful information in standard web search

- Page Rank, Document Expansion, etc.

Still a weakly supervised method, rather than a pretraining method

- Behavior closer to weak supervision/transfer learning, not pretraining

Pretraining and Retrieval: Recap

We are still not seeing the emergent power of LLMs in embedding-based retrieval

- The fact we need these solutions/mitigations shows there is something missing

Auto-regressive LM + scaling up solved a lot of problems, but not everything

- Web search is perhaps the biggest money-making AI application, yet not fully covered by GPT-X

“Bitter lesson”, more compute and large-scale trump specific designs, is deemed to happen

- But that may not be achieved all by current language models

BEIR Tasks

Zero-Shot Retrieval: Transfer from MARCO to BEIR Benchmark.

- A fused benchmark of 18 public tasks, with diverse domains and tasks

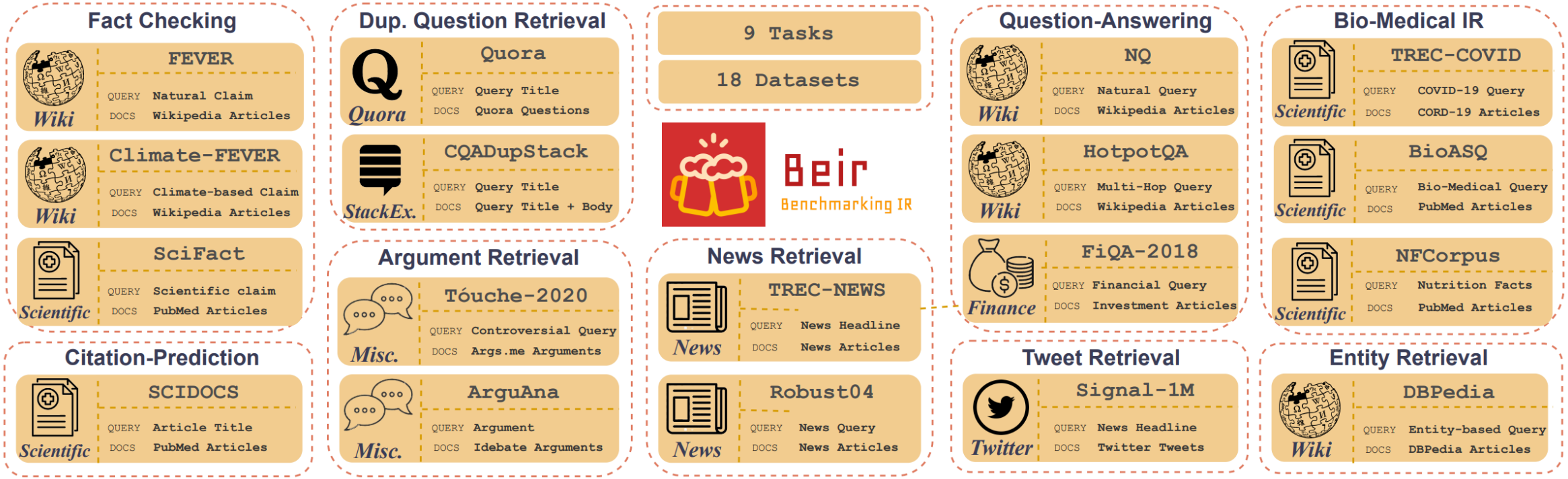

Figure 15: Tasks included in BEIR [6]