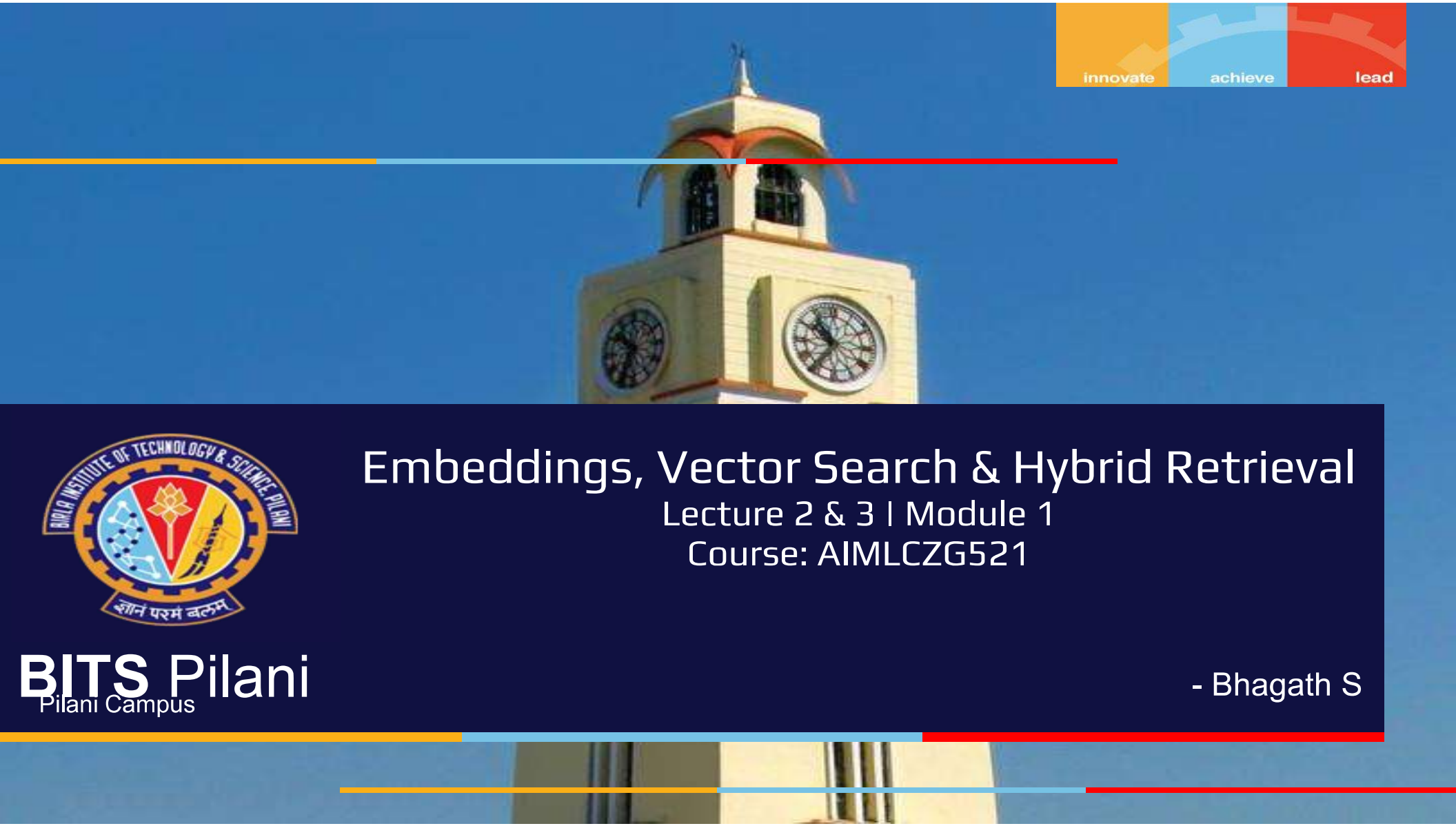


innovate achieve lead

Embeddings, Vector Search & Hybrid Retrieval

Lecture 2 & 3 | Module 1

Course: AIMLCZG521

- Bhagath S

BITS Pilani

Pilani Campus

What We'll Learn Today

Part 1: Foundations

- Encoder models & embedding generation
- Transformer architecture for embeddings
- Vector similarity mathematics
- Embedding model landscape

Part 2: Vector Databases

- ANN search algorithms (HNSW, IVF, PQ)
- Index structure mathematics
- Database solutions & tradeoffs
- Cost engineering

Part 3: Sparse Retrieval

- TF-IDF fundamentals
- BM25 algorithm & mathematics
- Hybrid search rationale

Part 4: Hybrid Systems

- Reciprocal Rank Fusion (RRF)

Prerequisites Review

Basic transformer architecture
(self-attention, feedforward layers),
matrix operations.

We'll build everything else from scratch.

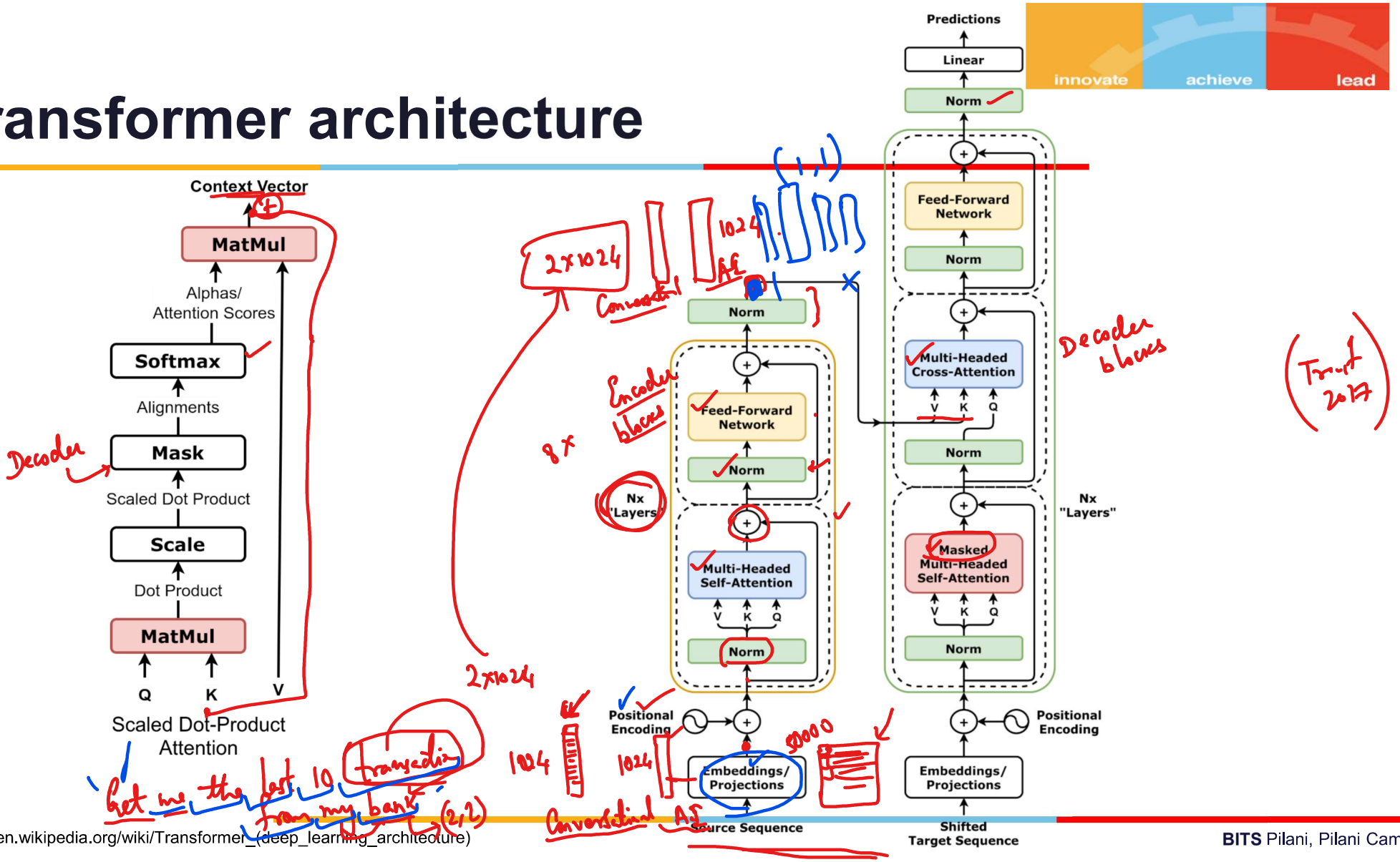
Learning Objectives

By the end of this lecture, you will be able to:

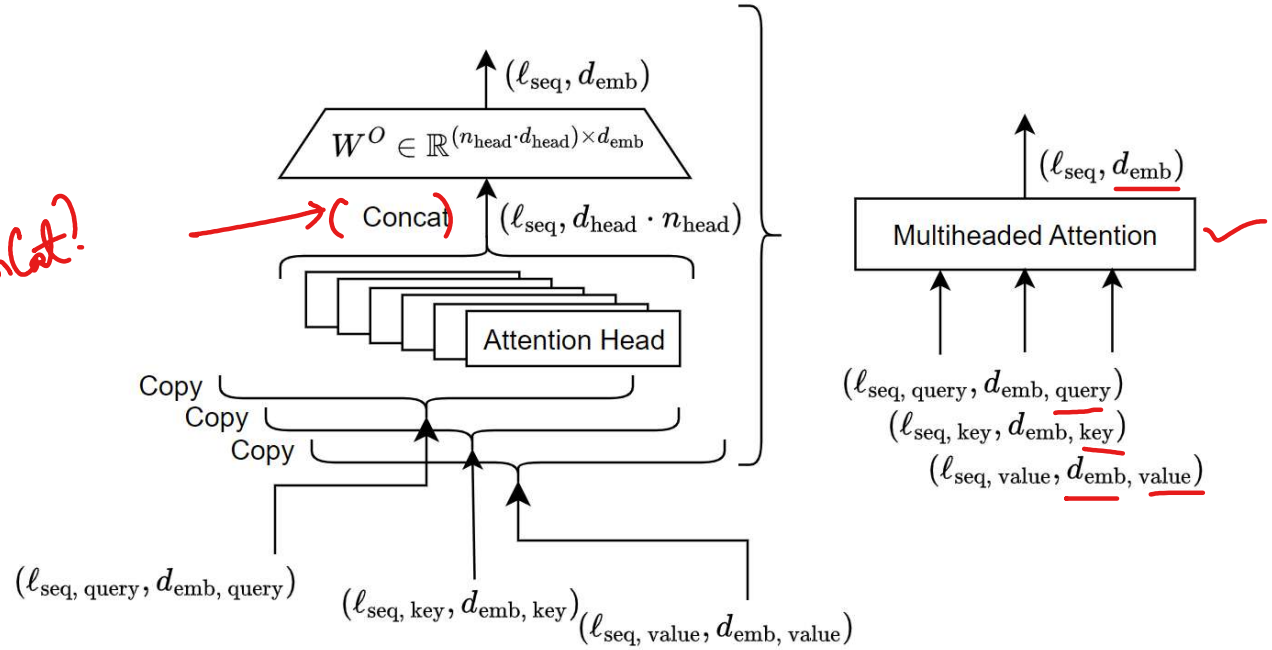
- ✓ **Explain** how transformer encoder models create contextual embeddings through self-attention and pooling strategies
- ✓ **Calculate and compare** vector similarity using cosine similarity, L2 distance, and dot product metrics
- ✓ **Evaluate and select** appropriate ANN indexing strategies (HNSW, IVF, PQ) based on dataset size, memory constraints, and accuracy requirements
- ✓ **Implement** BM25 scoring from scratch, understanding term frequency saturation and document length normalization
- ✓ **Design** hybrid retrieval systems that combine dense and sparse methods using Reciprocal Rank Fusion (RRF)

https://en.wikipedia.org/wiki/Transformer_(deep_learning_architecture)

Transformer architecture

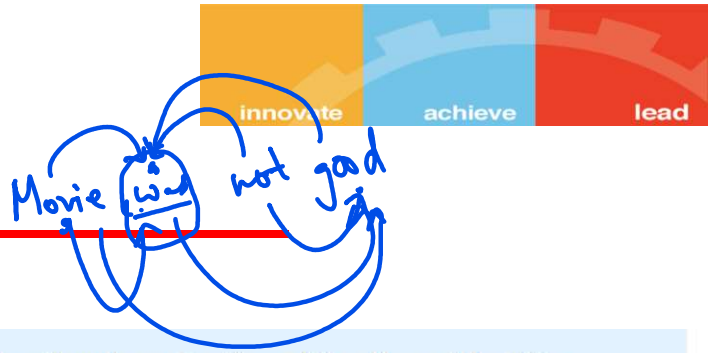


Multi-headed Attention



https://en.wikipedia.org/wiki/Transformer_(deep_learning_architecture)

What are Encoder Models?



Bidirectional Transformers for Understanding

Core Capability: Encoder models can see the **entire input sequence** at once (bidirectional context), making them ideal for:

- Understanding meaning (semantic representation)
- Classification tasks (sentiment, intent)
- Creating embeddings for similarity search

BERT (2018)

Training: Masked Language Modeling (MLM)

```
"The [MASK] brown fox [MASK] over the lazy dog" →
Predict: "quick", "jumps"
```

Key insight: Random tokens replaced with [MASK], model predicts independently. Missing tokens can't be used for generation.

GPT (2018)

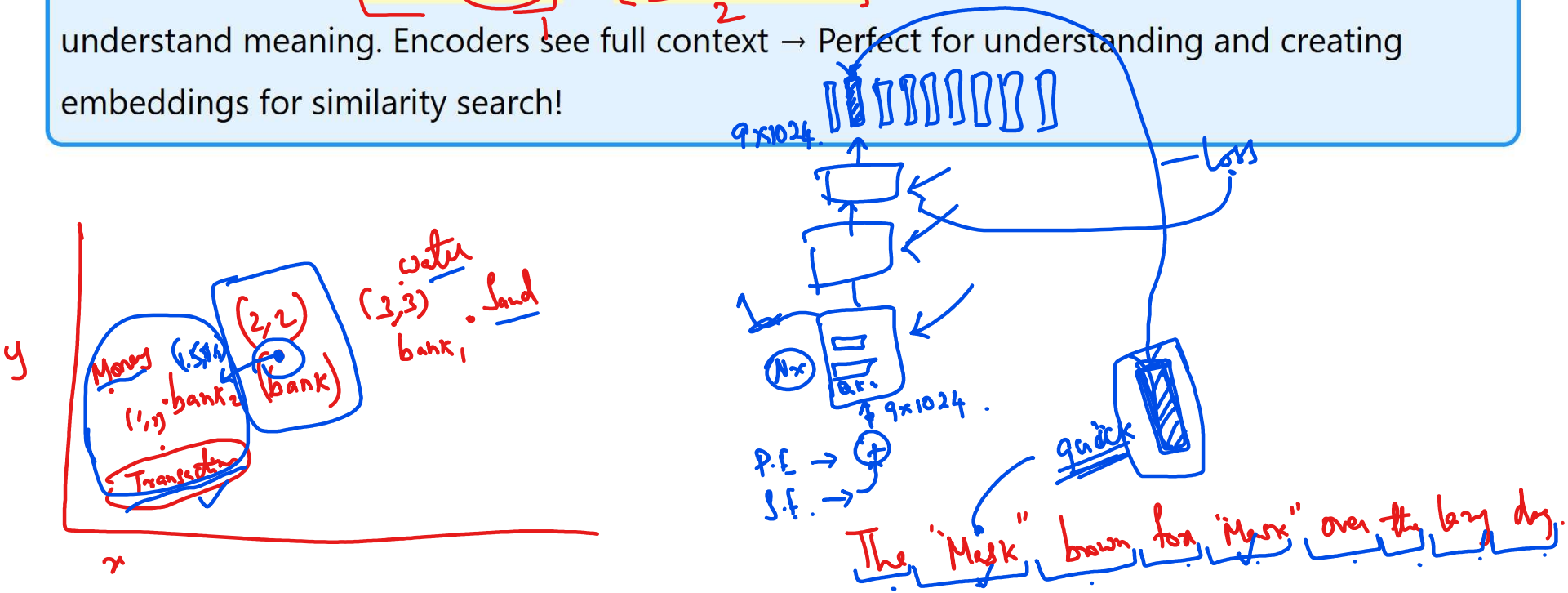
Training: Autoregressive (Causal LM)

```
"<s> A B C D" → Predict each token auto-regressively
```

Key insight: Tokens predicted left-to-right. Can condition on leftward context, so it can be used for generation.

Why Encoders for Embeddings?

The word "bank" in "river bank" vs "bank account" needs to see words on **BOTH sides** to understand meaning. Encoders see full context → Perfect for understanding and creating embeddings for similarity search!



Encoder vs Decoder

Encoder

Input Processing

(e.g., text, tokens)

Bi-directional

Attends to entire sequence
Context from both directions

Self-attention

Parallel processing
Position-aware encoding

Encoders see **full context** → Perfect for understanding, classification, and creating embeddings for similarity search!

Decoder

Output Generation

(probabilities)

Uni-directional

Causal masking
Left-to-right generation

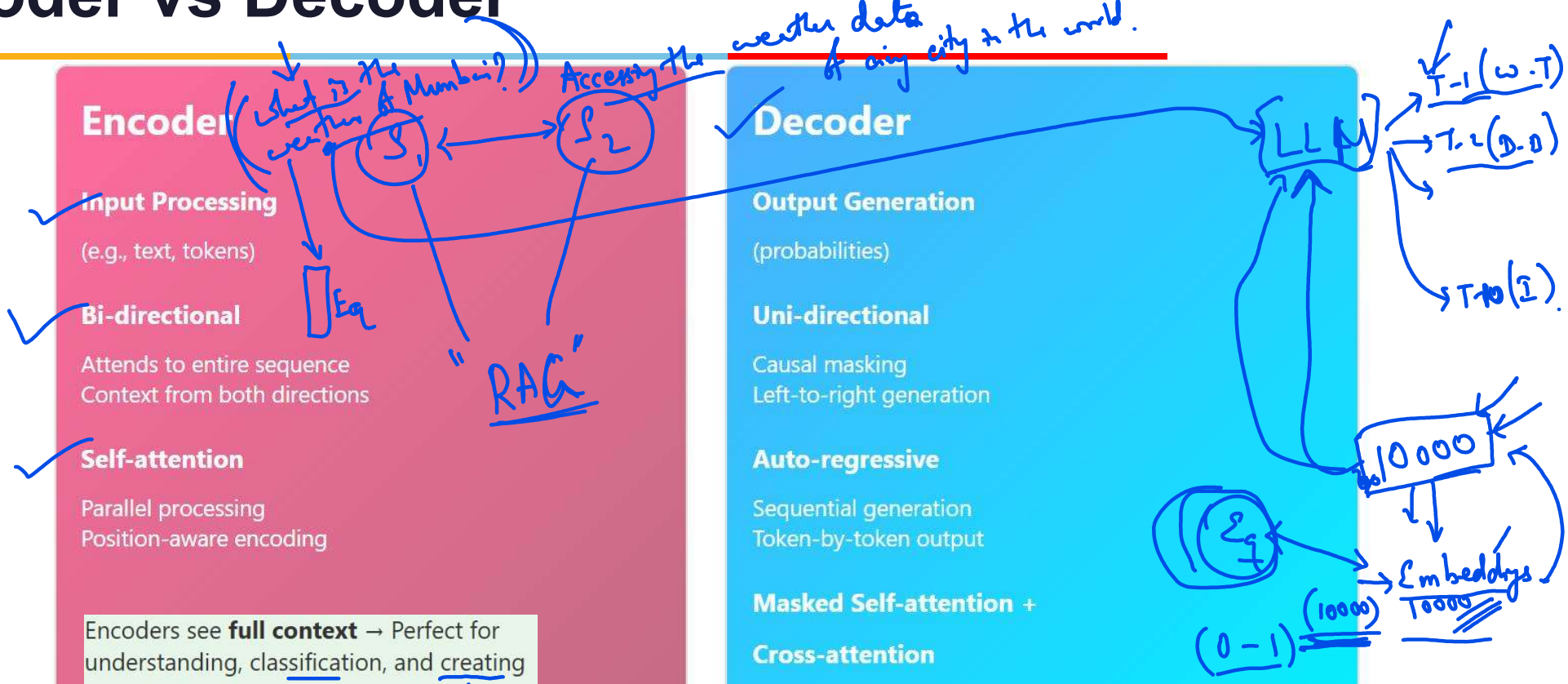
Auto-regressive

Sequential generation
Token-by-token output

Masked Self-attention +

Cross-attention

Attends to encoder output
Prevents future peeking



Encoder vs Decoder vs Encoder-Decoder

Encoder-Only

Core Strength

Bidirectional context understanding. Sees entire input simultaneously, creating rich contextual representations perfect for classification and understanding tasks.

Best Use Cases

Sentiment Analysis
Classifying text emotion: "This movie was terrible but the acting was great" - needs full context to understand mixed sentiment.

Named Entity Recognition (NER)
Identifying entities: "Apple released new products" - needs surrounding words to distinguish company vs. fruit.

Question Answering
Finding answers in passages: Given context and question, extract the specific answer span from the text.

Text Classification
Spam detection, topic categorization, intent classification - needs holistic understanding of entire input.

Semantic Search & Embeddings
Creating dense vector representations for similarity matching and retrieval (e.g., document search, recommendation systems).

Popular Models (2025)

BERT | RoBERTa | DeBERTa | ALBERT | DistilBERT

Decoder-Only

Core Strength

Causal language modeling with autoregressive generation. Predicts next token based on previous context, making it ideal for creative and generative tasks.

Best Use Cases

Text Generation & Completion
Creative writing, code generation, story continuation - excels at producing coherent long-form content.

Conversational AI & Chatbots
Multi-turn dialogue systems (ChatGPT, Claude) - generates contextually relevant responses in conversations.

Code Synthesis
Programming assistants (GitHub Copilot) - generates code based on natural language descriptions or partial code.

In-Context Learning
Few-shot learning with prompts - can adapt to new tasks without fine-tuning through clever prompting.

Instruction Following
Following complex multi-step instructions, reasoning tasks, and tool use - foundation for AI assistants.

Popular Models (2025)

GPT-4 | GPT-3.5 | Claude 3/4 | Llama 3 | Mistral

Encoder-Decoder

Core Strength

Separate encoding and decoding phases with cross-attention. Encoder understands input bidirectionally, decoder generates output while attending to encoded representations.

Best Use Cases

Machine Translation
Language translation (English → French) - cross-attention aligns source and target words effectively for accurate translation.

Text Summarization
Condensing long documents - encoder processes full document, decoder generates concise summary with key information.

Text-to-Text Tasks
Any transformation: paraphrasing, style transfer, format conversion - unified framework for diverse NLP tasks.

Question Answering (Generative)
Generating natural language answers (not just extraction) - encoder processes context, decoder formulates answer.

Document Generation from Structured Data
Converting tables/databases to natural language descriptions - encoder handles structured input, decoder produces readable text.

Popular Models (2025)

T5 | BART | mT5 | PEGASUS | mBART | FLAN-T5

Comparison

Task Type	Encoder-Only	Decoder-Only	Encoder-Decoder	Reasoning
Sentiment Analysis	✓ Best	○ Possible	✗ Overkill	Needs bidirectional context, no generation required
Text Generation	✗ No	✓ Best	○ Possible	Requires autoregressive generation capability
Machine Translation	✗ No	○ Suboptimal	✓ Best	Cross-attention optimally aligns source-target pairs
Named Entity Recognition	✓ Best	✗ Inefficient	✗ Overkill	Token-level classification needs bidirectional context
Conversational AI	✗ No	✓ Best	○ Outdated	Decoder-only scales better for dialogue and instruction following
Summarization	✗ No	✓ Modern	✓ Traditional	Both work; decoder-only now preferred for unified architecture
Semantic Search	✓ Best	○ Possible	✗ Overkill	Encoder creates optimal dense representations for similarity
Code Generation	✗ No	✓ Best	○ Rare	Sequential generation with context, decoder-only excels

How Encoder Transformers Create Embeddings

9 tokens → **Single 768-dimensional vector**

Step-by-Step Process

Input Text: "Machine learning is fascinating"

Step 1: Tokenization
→ [CLS] Machine learning is fascinating [SEP]
→ Token IDs: [101, 8394, 4083, 2003, 17117, 102]

Step 2: Token Embeddings
Each ID → 768-dim vector
8394 → [0.23, -0.15, 0.89, ..., 0.42]

Step 3: Position Embeddings
Position 0 → [0.01, 0.02, ...]
Position 1 → [0.02, 0.03, ...]
Sum with token embeddings

Step 4: Transformer Layers (12 layers for BERT-base)
Each layer: Self-Attention → LayerNorm → FFN → LayerNorm

Step 5: Pooling Strategy
CLS Pooling (most common): $v = h[CLS]$
Mean Pooling: $v = (1/n) \Sigma h_i$
Max Pooling: $v_j = \max(h_{1,j}, h_{2,j}, \ldots, h_{n,j})$

📌 **Default Strategy:** Most pre-trained models (BERT, RoBERTa, DistilBERT) use **CLS token pooling** by default. However, **mean pooling** often performs better for sentence embeddings (used by Sentence-BERT, BGE, GTE).

innovate achieve lead

How Encoder Transformers Create Embeddings

Self-Attention Mathematics

Query, Key, Value projections:

$Q = X W_Q$, $K = X W_K$, $V = X W_V$

Attention scores:

$$\text{Attention}(Q,K,V) = \text{softmax}(QK^T/\sqrt{d_k})\, V$$

Where d_k is dimension of keys (typically 64)

Pooling Strategies

Mean Pooling:

$v = (1/n) \Sigma h_i$

CLS Pooling:

$v = h_{[CLS]}$

Max Pooling:

$v_j = \max(h_{1,j}, h_{2,j}, ..., h_{n,j})$

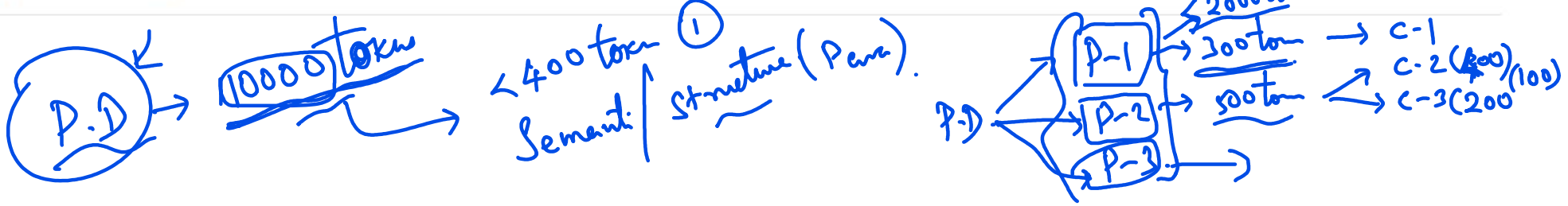
💡 Key Insight

The final embedding is **contextual** - "bank" gets different embeddings in different sentences because self-attention incorporates surrounding context. This is fundamentally different from word2vec or GloVe (static embeddings).

Embedding Models: Key Players

Open Source Models (Recommended for Production)

Model	Dimensions	Context	Best For	Provider
bge-large-en-v1.5	1,024	512	General purpose, high quality	BAAI
gte-large-en-v1.5	1,024	8,192	Long documents	Alibaba
e5-mistral-7b-instruct	4,096	32,768	Instruction-following, very long context	Microsoft
jina-embeddings-v2	768	8,192	Multilingual, fast inference	Jina AI



Embedding Models: Key Players

Commercial API Models (Highest Quality)

Model	Dimensions	Context	Best For	Cost
text-embedding-3-large	3,072	8,191	Highest quality, production	$0.13 / 1M tokens
embed-english-v3.0	1,024	512	Compression support, production	$0.10 / 1M tokens

Selection Guide:

Start with **bge-large-en-v1.5** for general use. Upgrade to commercial APIs if quality justifies cost. Use **gte-large** or **e5-mistral** for long documents (>1000 tokens).

Embedding Models: Complete Reference

Model	Provider	Arch	Layers	Hidden	Output	Training	Context	Type
text-embedding-3-large	OpenAI	Transformer	N/A	N/A	3,072	Contrastive	8,191	API
embed-v3	Cohere	Transformer	N/A	N/A	1,024	Multi-task	512	API
bge-large-en-v1.5	BAAI	BERT	24	1,024	1,024	RetroMAE+Contrastive	512	Open
gte-large-en-v1.5	Alibaba	BERT	24	1,024	1,024	Contrastive	8,192	Open
e5-mistral-7b-instruct	Microsoft	Mistral 7B	32	4,096	4,096	Contrastive pre-training	32,768	Open
jina-embeddings-v2	Jina AI	BERT	12	768	768	Contrastive	8,192	Open

📖 **Reference:** Complete specifications for implementation decisions. See Part 1 for selection guidance.

Key Concepts

- **Base Architecture:** The underlying neural network design (BERT, etc.)
- **Layers:** Number of transformer layers in the model
- **Hidden Size:** Dimensionality of hidden representations within the model
- **Output Dimensions:** Size of the final embedding vector
- **Training Objectives:**
  - *Contrastive Learning:* Learning by comparing similar vs dissimilar pairs
  - *RetroMAE:* Masked auto-encoding with enhanced reconstruction
- **Context Length:** Maximum number of tokens the model can process
- **Multilingual:** Models trained on multiple languages

Training Objective - Contrastive Learning

Core Objective

Train the model to place similar items close together in embedding space while pushing dissimilar items far apart.

How It Works

The model learns by examining pairs or triplets of examples:

Positive Pair (should be close):

• "The cat sat on the mat" ↔ "A feline rested on the rug"

Negative Pair (should be far):

• "The cat sat on the mat" ↔ "How to bake chocolate cookies"

$$\text{Loss} = -\log\left(\exp(\text{sim}(a, p)) \;/\; \Sigma \exp(\text{sim}(a, n)) \right)$$

where: sim = similarity, a = anchor, p = positive, n = negatives

✓ Advantages

- ✓ Creates semantically meaningful embeddings
- ✓ Works well with large datasets
- ✓ Naturally handles synonyms and paraphrases
- ✓ Self-supervised (doesn't need manual labels)

✗ Challenges

- ✗ Requires careful negative sampling
- ✗ Computationally expensive (many comparisons)
- ✗ Sensitive to batch size
- ✗ Hard negatives mining can be tricky

Training Objective - Masked Language Modeling (MLM)

Core Objective

Predict masked (hidden) words in a sentence using surrounding context. This teaches the model deep language understanding.

How It Works

The model sees sentences with some words replaced by [MASK] tokens and must predict what was hidden.

Original: "The quick brown fox jumps over the lazy dog"

Masked: "The [MASK] brown fox [MASK] over the lazy dog"

Model predicts: [$MASK_1$] = "quick", [$MASK_2$] = "jumps"

```
Loss = -Σ log P(masked_word | context)
Maximize probability of correct word given surrounding words
```

✓ Advantages

- ✓ Captures bidirectional context
- ✓ No labeled data required
- ✓ Learns rich linguistic patterns
- ✓ Foundation for BERT and similar models

✗ Challenges

- ✗ Slower training than causal LM
- ✗ Pretrain-finetune gap (no [MASK] at inference)
- ✗ Assumes independence of masked tokens
- ✗ Not optimal for generation tasks

Training Objective – RetroMAE (Retrospective Masked Auto-Encoding)

Core Objective

Enhanced masked auto-encoding that reconstructs the entire input from a heavily masked version, forcing the model to learn more compressed and meaningful representations.

How It Works

Unlike standard MLM which masks ~15%, RetroMAE masks 50-70% and uses two encoders:

Step 1 - Encoder: Process heavily masked input (only 30-50% visible)
Step 2 - Decoder: Reconstruct the ENTIRE original sentence

Example:
Original: "The quick brown fox jumps over the lazy dog"
Masked: "The [M] [M] fox [M] [M] [M] lazy [M]"
Task: Reconstruct all 9 words from just 3 visible ones

```
Loss = MSE(original_embeddings, reconstructed_embeddings)
With asymmetric encoder-decoder architecture
```

✓ Advantages

- ✓ Creates highly compressed embeddings
- ✓ Better semantic understanding than standard MLM
- ✓ Efficient for retrieval tasks
- ✓ Strong performance with less data

✗ Challenges

- ✗ More complex architecture (encoder + decoder)
- ✗ Requires careful tuning of masking ratio
- ✗ Longer training time
- ✗ Higher computational cost

From Embeddings to Search

What We've Learned

✓ Transformer encoders create rich, contextual embeddings
✓ Self-attention captures relationships between words
✓ Different pooling strategies extract sentence-level representations

Next: Vector Databases

Learn how to measure similarity, build efficient indexes, and search at scale using approximate nearest neighbor algorithms.

Vector Similarity: Mathematical Foundations

1. Cosine Similarity

$$\cos(\theta) = (A \cdot B) / (||A||\ ||B||)$$

$\cos(\theta) = \Sigma(A_i \times B_i) / (\sqrt{\Sigma}\ A_i^2 \times \sqrt{\Sigma}\ B_i^2)$

Range: [-1, 1]
Interpretation:

- 1.0 = identical direction
- 0.0 = orthogonal (unrelated)
- -1.0 = opposite direction

2. Euclidean (L2) Distance

$$d(A,B) = \sqrt{\Sigma(A_i - B_i)^2}$$

Range: [0, ∞]
Interpretation:

- 0 = identical vectors
- Larger = more different
- Sensitive to magnitude

Must normalize vectors first!

3. Dot Product (Inner Product)

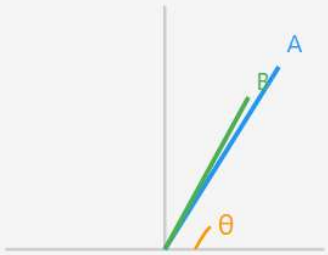
$$A \cdot B = \Sigma(A_i \times B_i) = ||A||\ ||B||\ \cos(\theta)$$

Range: [-∞, ∞] ([-1, 1] if normalized)
Key insight: If vectors are normalized ($||A|| = ||B|| = 1$), then dot product = cosine similarity!

Vector Similarity: Visual Intuition

1. Cosine Similarity

$$\cos(\theta) = (A \cdot B) / (||A|| \, ||B||)$$



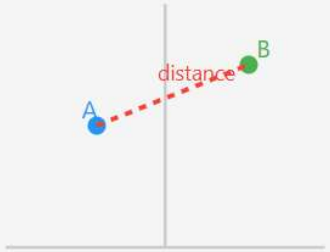
Measures angle between vectors

Range: [-1, 1]

- 1.0 = identical direction
- 0.0 = orthogonal (unrelated)
- -1.0 = opposite direction

2. Euclidean (L2) Distance

$$d(A,B) = \sqrt{\Sigma(A_i - B_i)^2}$$



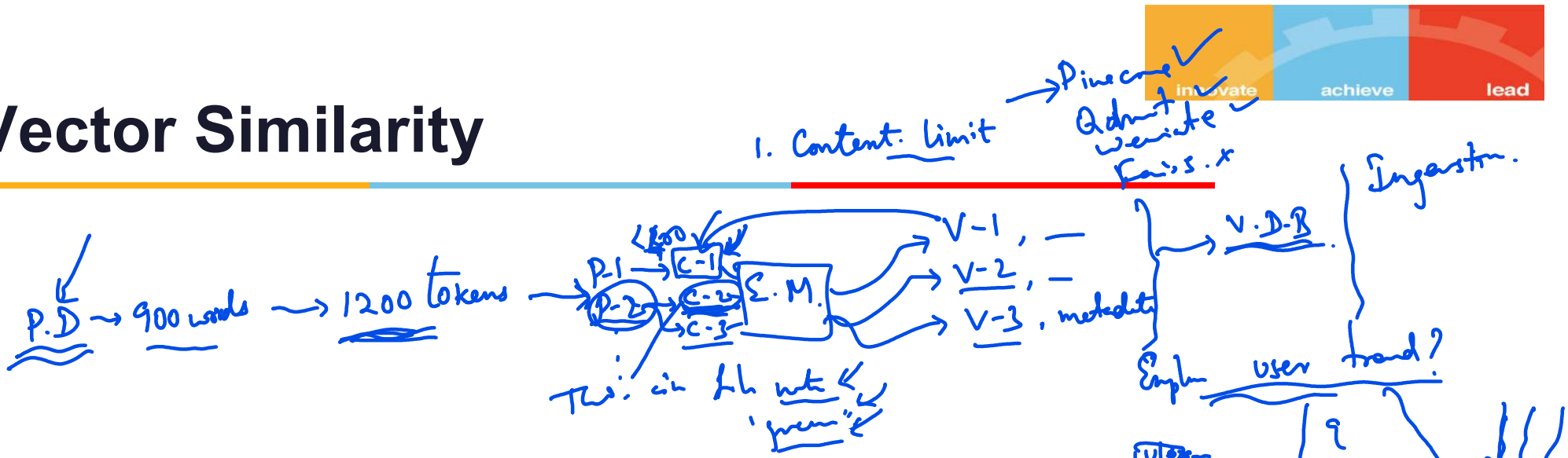
Measures distance in space

Range: [0, ∞]

- 0 = identical vectors
- Larger = more different
- **Sensitive to magnitude**

💡 **Key Insight:** If vectors are normalized (||A|| = ||B|| = 1), then **dot product = cosine similarity**

Vector Similarity



The Computational Challenge

Problem Statement

Given: 10 million document embeddings (768 dimensions each)

Task: Find top 10 most similar to query embedding

Computational Complexity

For linear scan:

- Operations per query = n × d
- n = 10,000,000 documents
- d = 768 dimensions
- Total = 7,680,000,000 multiply-add operations

At 1 billion ops/sec (modern CPU):

Time per query = 7.68 seconds

With 100 queries/sec: Need 768 CPU cores!

Approximate Nearest Neighbor (ANN)

📊 Scale Analysis

Documents	Linear Scan	Cost/month
10K	8ms	$50
100K	77ms	$50
1M	770ms	$200
10M	7.7s ❌	$5,000

✅ With ANN Index (HNSW)

Documents	HNSW	Cost/month
10K	2ms	$50
100K	3ms	$50
1M	5ms	$120
10M	10ms ✅	$250

🎯 The Solution: Approximate Nearest Neighbor (ANN)

Key Insight: We don't need the EXACT top 10 - getting 9/10 correct is often good enough!

ANN algorithms trade tiny accuracy loss (95-99% recall) for 100-1000x speedup by using smart data structures.

ANN Indexing Strategies

1. Graph-Based

Example: HNSW

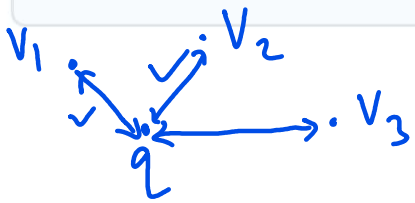
Build a navigable graph where nodes are vectors, edges connect similar vectors

Pros:

- Excellent recall (>95%)
- Fast queries (O(log n))
- No training needed

Cons:

- High memory usage
- Slow inserts



2. Partition-Based

Example: IVF

Cluster vectors into partitions, search only relevant partitions

Pros:

- Balanced performance
- Works with compression
- Scalable

Cons:

- Needs training (k-means)
- Sensitive to nprobe

3. Compression-Based

Example: PQ

Compress vectors to reduce memory, search in compressed space

Pros:

- 8-32x less memory
- Billions of vectors

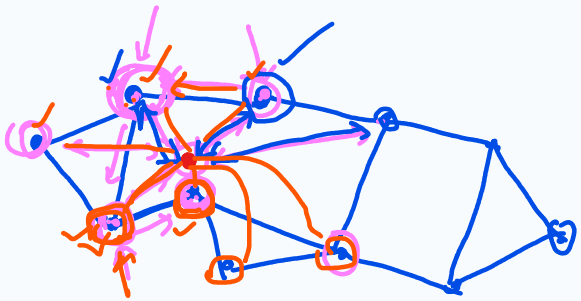
Cons:

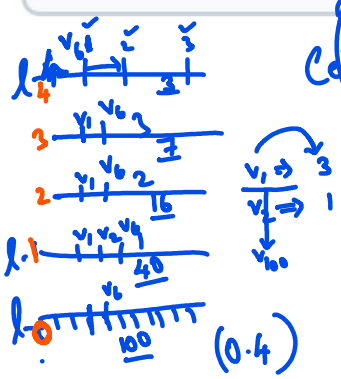
- Lower recall (~90%)
- Needs training

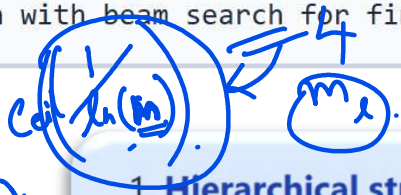
HNSW: Hierarchical Navigable Small World

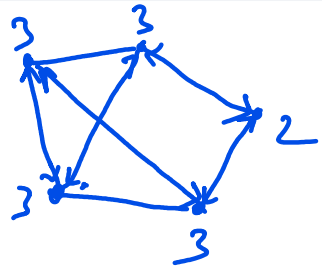
Core Concept: Multi-Layer Skip List for Vectors

```
Layer 2: Entry → [●──────────●──────────●] ← Sparse, long-range connections
Layer 1: [●──●──●──●──●──●] ← Medium density
Layer 0: [●●●●●●●●●●●●●●●●] ← All vectors, dense connections
Search Process:
1. Enter at top layer (random entry point)"
2. Greedy search: move to nearest neighbor
3. When stuck (no closer neighbor), descend to next layer
4. Repeat until Layer 0
5. Expand search with beam search for final k neighbors
```



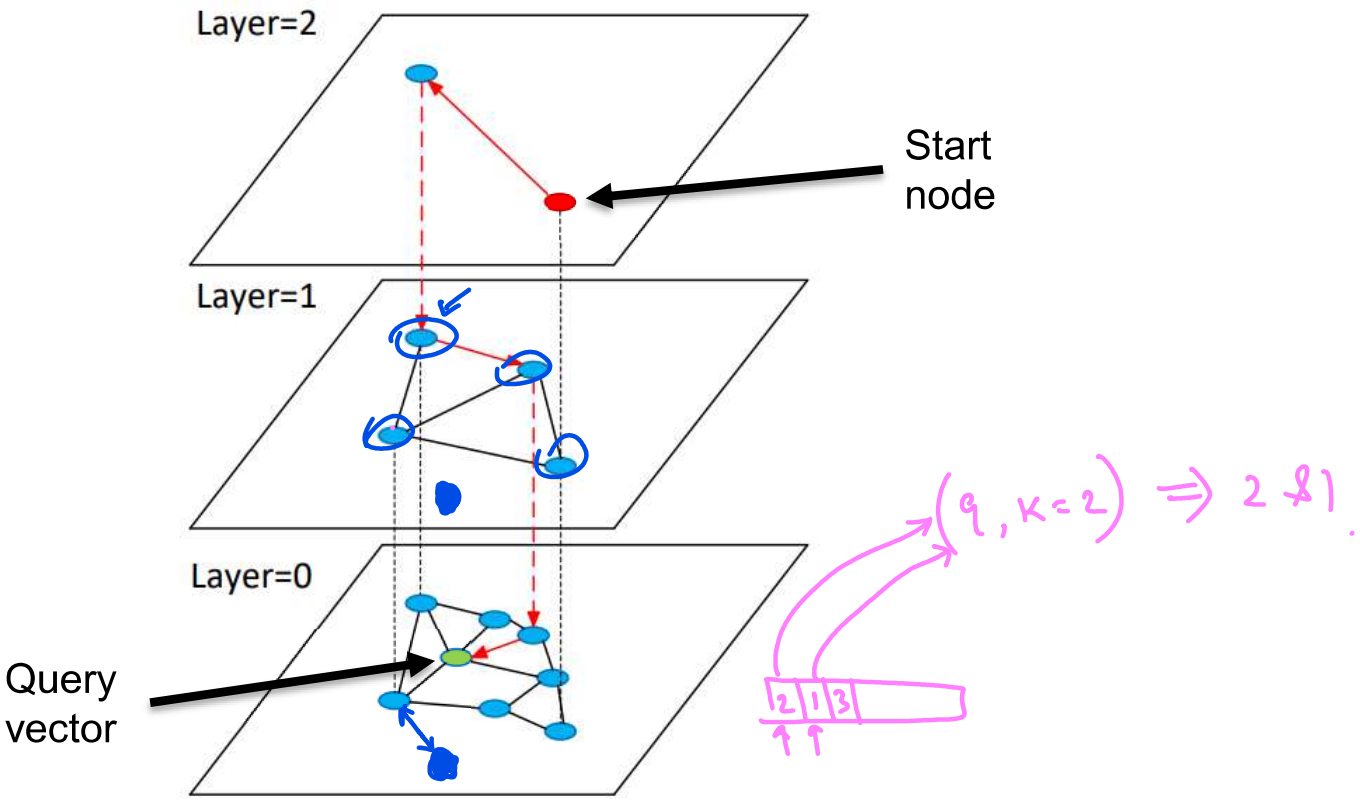






1. **Hierarchical structure:** Top layers skip across dataset for fast navigation
2. **Small world property:** Average path length is O(log n)
3. **Navigable:** Greedy search reliably finds near-optimal path
4. **Robust:** Multiple entry points prevent getting stuck in local minima

HNSW Search: Step-by-Step



① **Start at Top Layer (Entry Point)**
Random entry point from sparse top layer

② **Greedy Search**
Move to nearest neighbor closer to query
Repeat until no closer neighbors found

③ **Descend to Next Layer**
Use current position as entry for denser layer

④ **Repeat Until Layer 0**
Final greedy search on full graph

✓ **Beam Search for Top-k**
Expand search to find k nearest neighbors

HNSW: https://arxiv.org/pdf/1603.09320

HNSW: Memory layout

Per Vector Storage Components

Storage Breakdown

- **Original vector:** d × 4 bytes
- **Layer info:** 1 byte
- **Connections:** M × 4 bytes × layers

Example (768-dim, M=16)

```
Vector: 768 × 4 = 3,072 bytes
Layer: 1 byte
Connections: ~64 bytes avg
_____________________________
Total: ~3,136 bytes per vector
```

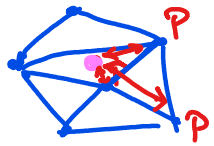
HNSW: Memory Calculation by Scale

Scale	Vector Data	Graph Overhead	Total Memory
1M vectors	~3.1 GB (1.02× raw)	~0.5-1 GB (metadata)	**~3.6-4.1 GB** (1.2-1.3× raw)
10M vectors	~31 GB (1.02× raw)	~10-20 GB (adjacency)	**~41-51 GB** (1.4-1.7× raw)
100M vectors	~310 GB (1.02× raw)	~200-300 GB (multi-layer)	**~510-610 GB** (1.7-2.0× raw)

⚠ **Production Planning: Memory Budget Guidelines**

- **Per-vector data:** Minimal overhead (~1.02×)
- **Graph structure:** 0.4-1.0× additional (depends on M and scale)
- **Practical rule:** Budget **1.5-2.0× raw vector memory** for production HNSW

Parameter Tuning: HNSW



M (Connections per Layer)

16 - 64

Lower (16):
- Less memory
- Faster build
- Lower recall

Higher (64):
- More memory
- Better recall
- Slower inserts

```
Default: M=16 for most cases
```

ef_construction

100 - 200

Lower (100):
- Faster build
- Lower quality index

Higher (200+):
- Slower build
- Better index quality
- Higher recall

```
Default: ef_construction=200
```

ef_search (Query Time)

50 - 500

Tune at runtime!

- ef=50: Fast, ~90% recall
- ef=100: Balanced
- ef=500: Slow, 99% recall

Adjust per query needs

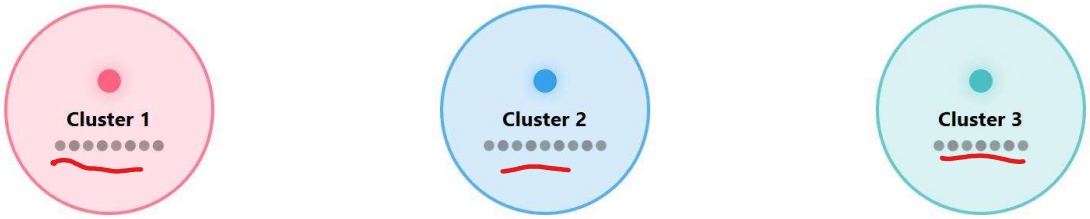
```
Typical: ef_search=100-200
```

💡 **Pro Tip:** Start with defaults (M=16, ef_construction=200, ef_search=100). Profile on your data, then adjust ef_search for latency-recall tradeoff.

IVF: Inverted File Index

📊 Step 1: Training Phase (k-means Clustering)

Partition the vector space into clusters using k-means algorithm



Each • centroid represents the center of a cluster
Small dots represent vectors grouped around each centroid

📌 Step 2: Vector Assignment

Assign each vector to its nearest centroid

```
For each vector v:

1. Calculate: dist(v, c₁), dist(v, c₂), dist(v, c₃), ...
2. Find minimum distance
3. If dist(v, cᵢ) is minimum → add v to listᵢ
```

⬇️

Result: An **inverted index** mapping each cluster to its vectors

- **Balanced:** Good speed/memory/accuracy tradeoff
- **Scalable:** Works well with billions of vectors
- **Composable:** Easily combined with PQ compression
- **Flexible:** nprobe tunable at query time

IVF: Inverted File Index - Search

Query Process:

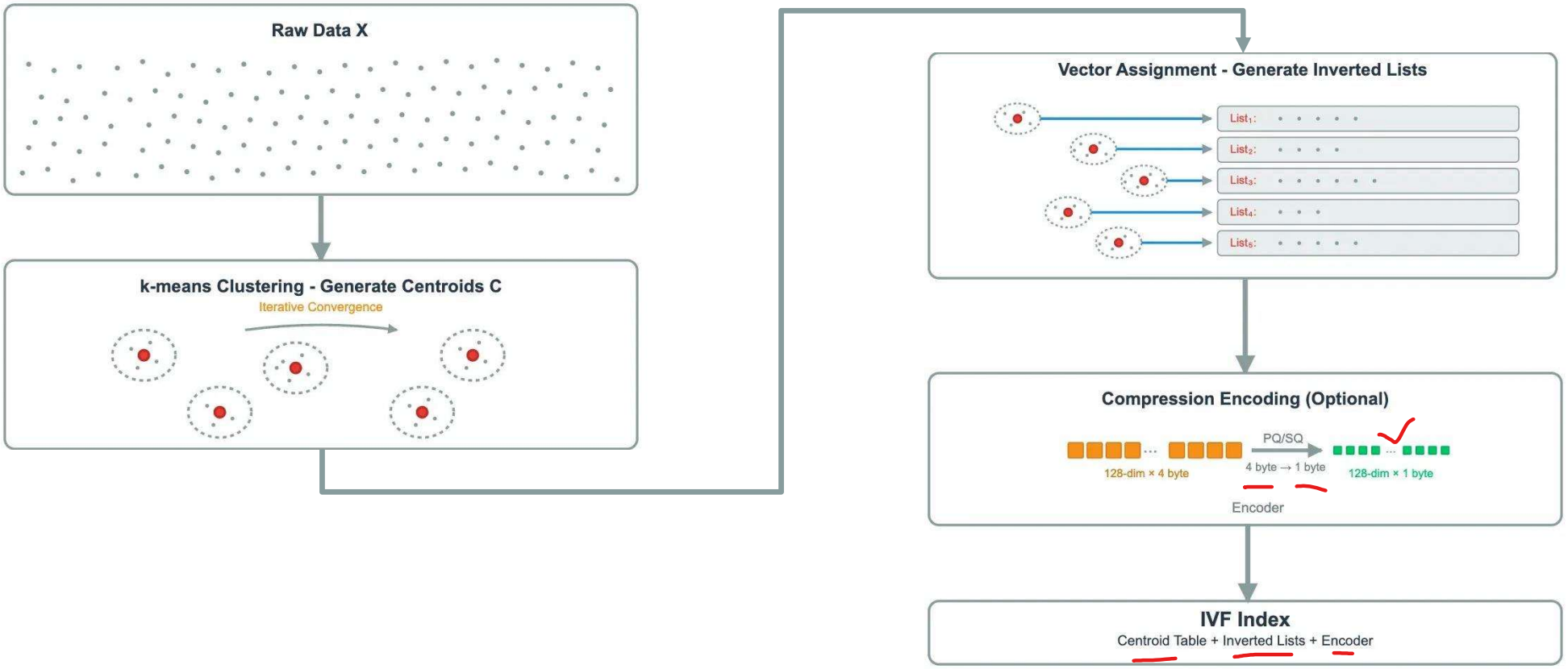
1. Query vector **q** arrives

2. Find **nprobe** nearest centroids
(e.g., nprobe = 3 → search top 3 closest clusters)

3. Search **only those clusters**
(Instead of searching ALL vectors in database!)

4. Merge and rank results across selected clusters

IVF: Inverted File Index + PQ



Parameter Tuning: IVF

nlist (Number of Clusters)

√n to n/1000

Too Few:
- Large partitions
- Slow search

Too Many:
- Tiny partitions
- Many to search

Sweet Spot:
- 4√n often works well

```
1M vectors → nlist ≈ 1,000-4,000
```

nprobe (Clusters to Search)

1 - 100

Lower (1-5):
- Very fast
- Lower recall (~70-85%)

Higher (50-100):
- Slower search
- Higher recall (~95%+)

Tune at query time

```
Typical: nprobe=10-20
```

PQ Subquantizers (m)

d/8 to d/4

More subquantizers:
- Better accuracy
- More memory

Fewer subquantizers:
- More compression
- Lower accuracy

Must divide dimension

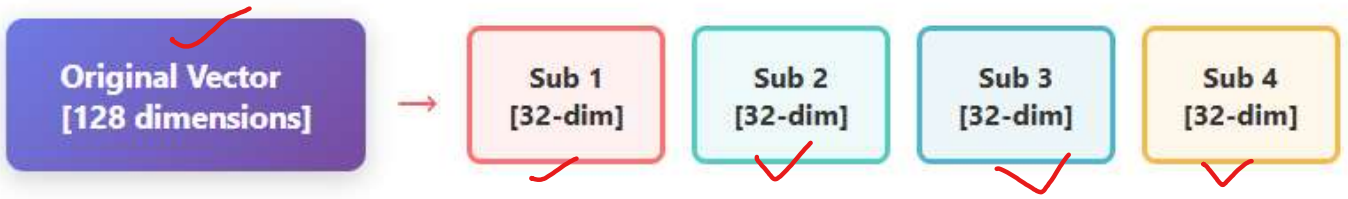
```
768-dim → m=96 (8 per subvector)
```

⚙️ **Training Time:** IVF requires training k-means on sample data (typically 10K-100K vectors). Budget: nlist × 50 iterations × 10 minutes for 1M vectors.

Product Quantization (PQ)

Core Concept: Divide & Conquer

Split high-dimensional vectors into smaller chunks and quantize each independently



Each subvector is encoded independently using a trained codebook

Product Quantization (PQ)

Step 1: Train Codebooks (k-means per Subspace)

For each subvector position, train a codebook with k centroids (typically k=256)

Codebook 1 (Sub 1)

```
ID: 0 → [0.2, 0.5, 0.1, ...]
ID: 1 → [0.8, 0.3, 0.6, ...]
ID: 2 → [0.1, 0.9, 0.4, ...]
...
ID: 255 → [0.4, 0.2, 0.7, ...]
```

Codebook 2 (Sub 2)

```
ID: 0 → [0.3, 0.7, 0.2, ...]
ID: 1 → [0.6, 0.1, 0.8, ...]
ID: 2 → [0.9, 0.4, 0.3, ...]
...
ID: 255 → [0.2, 0.6, 0.5, ...]
```

Codebook 3 & 4...

```
Each subspace gets
its own codebook
trained independently
using k-means
clustering
```

Product Quantization (PQ)

🔢 Step 2: Encode Vectors → Compact IDs

Replace each subvector with the ID of its nearest centroid in the codebook

```
Original Vector (128-dim, 512 bytes):
[0.23, 0.51, 0.82, ..., 0.91, 0.34, 0.67]

↓ Encode with PQ ↓

Compressed (4 IDs, 4 bytes):
[142, 73, 201, 18]

Each ID is 1 byte (0-255) → 128x compression!
```

Centroids index → (x,y)

Before PQ
512 B
per vector

→

After PQ
4 B
per vector

Product Quantization: Step-3: Fast Distance Computation

Asymmetric Distance Computation (ADC)

Step 1: Query Preparation

Query vector **q** arrives (full precision)

Split into subvectors: $[q_1, q_2, q_3, q_4]$

```
[0.23, 0.51, ... ] → splits → 4 chunks
```

Step 2: Distance Tables

Pre-compute distances from each q_i to all 256 centroids in codebook i

```
table₁[256], table₂[256], table₃[256],
table₄[256]
```

Step 3: Database Vector Lookup

Each database vector stored as 4 IDs: $[ID_1, ID_2, ID_3, ID_4]$

```
distance = table₁[ID₁] + table₂[ID₂] + table₃[ID₃] + table₄[ID₄]
```

Just 4 lookups + 3 additions! (vs 128 multiplications + additions)

Speed Gain: Distance computation becomes table lookup instead of expensive dot products. Enables searching billions of vectors in RAM.

Product Quantization (PQ)

Why Product Quantization is Powerful:

Massive Compression
Reduce memory by 32-128x while maintaining good accuracy

Fast Search
Distance = simple table lookups instead of expensive dot products

Scalability
Store billions of vectors in RAM that would otherwise require terabytes

Combinable
Often combined with IVF for even better performance (IVFPQ)

When to Use PQ

- **Billion-scale datasets:** When RAM is the bottleneck
- **With IVF:** IVF+PQ is the standard for massive scale
- **Budget constraints:** Reduce infrastructure costs 10x
- **Acceptable recall loss:** 90-95% recall is sufficient

Complexity Comparison

n = vectors in database | d = vector dimension | k = clusters (IVF) | m = compressed dimension (PQ) | i = k-means iterations

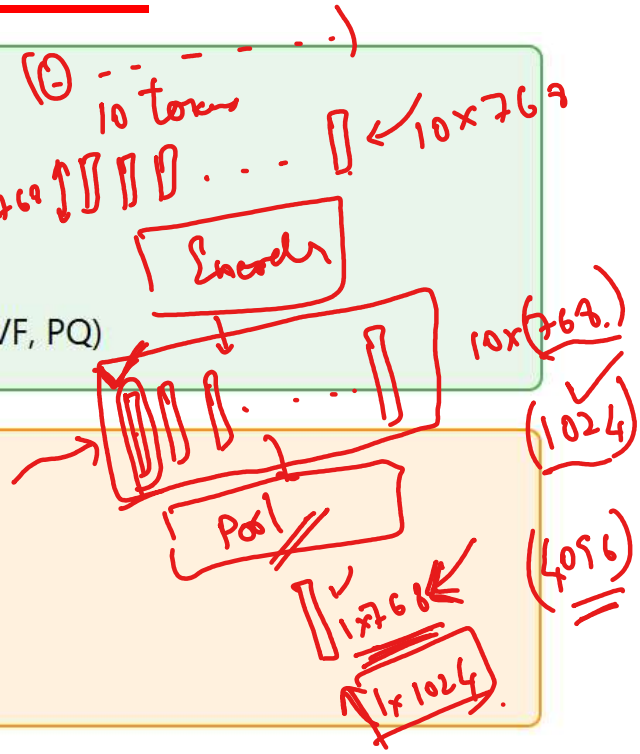
Algorithm	Search Time	Memory	Build Time	Recall
Linear Scan	O(n·d)	O(n·d)	O(1)	100%
HNSW	O(log n)	O(n·d)	O(n log n)	95-99%
IVF	O((n/k)·d)	O(n·d)	O(n·d·i)	90-95%
PQ	O(n·m)	O(n·m)	O(n·d·i)	70-85%
IVF+PQ	O((n/k)·m)	O(n·m)	O(n·d·i)	85-92%
HNSW+PQ	O(log n)	O(n·m)	O(n log n)	90-96%

🎯 **Key Insight:** HNSW trades **memory** for speed. IVF+PQ trades accuracy for **compression**. HNSW+PQ is the sweet spot for production.

From Dense to Sparse: Complementary Approaches

What We've Learned So Far

- Transformer encoders create rich, contextual embeddings
- Self-attention captures relationships between words
- Different pooling strategies extract sentence-level representations
- We can search **billions of vectors efficiently** using ANN algorithms (HNSW, IVF, PQ)



But Vector Search Has Limitations...

- Struggles with **exact keyword matching** (e.g., "ERROR code 500")
- Misses **rare/unique terms** not in training data (IDs, codes)
- Can't handle **out-of-vocabulary** words perfectly

Next: Sparse retrieval methods (BM25)
that complement dense search for hybrid systems

TF-IDF: Foundation of Sparse Retrieval

Term Frequency - Inverse Document Frequency: A statistical measure of word importance in documents

Term Frequency (TF)

Raw count:

TF(t, d) = count of term t in document d

Normalized (common):

$TF(t, d) = f_{t,d} / |d|$

$f_{t,d}$ = *raw count*, $|d|$ = *total terms*

Intuition:

More occurrences = more important

But normalize by document length

Inverse Document Frequency (IDF)

Formula:

$IDF(t) = \log(N / df_t)$

N = *total documents*

df_t = *documents containing t*

Intuition:

Rare terms are more informative

"Qdrant" → high IDF

"the" → low IDF

Combined TF-IDF Score

$$TF\text{-}IDF(t, d) = TF(t, d) \times IDF(t)$$
$$= (f_{t,d} / |d|) \times \log(N / df_t)$$

TF-IDF: Foundation of Sparse Retrieval

Corpus: 1000 documents

Document d: "machine learning is a subset of machine learning"

Query q: "machine learning"

Step 1: Calculate IDF for Each Query Term

Term "machine"

```
f_machine,d = 2
|d| = 9
TF = 2/9 = 0.222
df_machine = 300
IDF = log(1000/300) = 1.20
TF-IDF = 0.222 × 1.20 = 0.267
```

Term "learning"

```
f_learning,d = 3
|d| = 9
TF = 3/9 = 0.333
df_learning = 400
IDF = log(1000/400) = 0.916
TF-IDF = 0.333 × 0.916 = 0.305
```

Document score for query "machine learning":

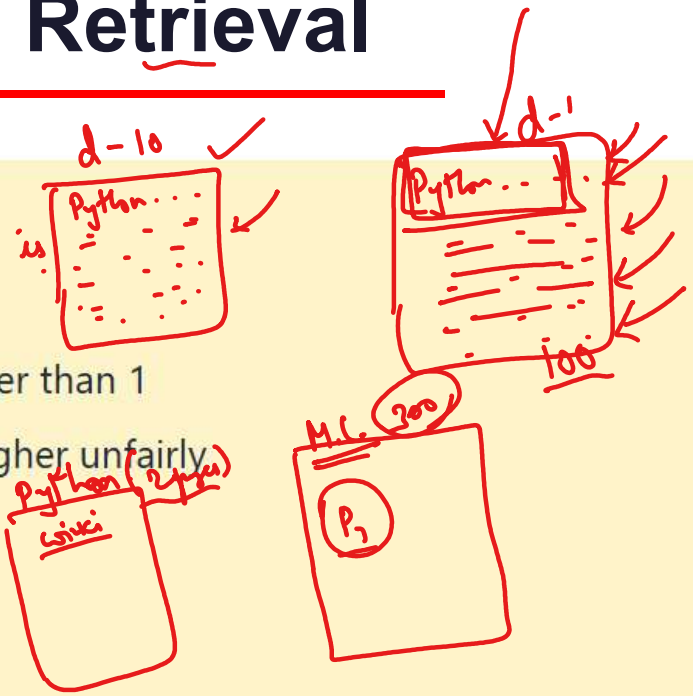
$$score(q, d) = 0.267 + 0.305 = 0.572$$

TF-IDF: Foundation of Sparse Retrieval

✗ TF-IDF Limitations

- **Linear TF:** 10 occurrences should not score 10× higher than 1
- **No length normalization:** Long documents score higher unfairly
- **Bag of words:** Ignores term proximity and order
- **No term saturation:** Repetition keeps adding score

Solution: BM25 fixes these issues!



BM25: Best Matching 25 (Improved TF-IDF)

What BM25 Improves

BM25 is a **probabilistic ranking function** that addresses TF-IDF's limitations with:

1. **Term frequency saturation:** Diminishing returns for repeated terms
2. **Document length normalization:** Fair scoring regardless of length
3. **Probabilistic foundation:** Based on probability ranking principle

BM25 Formula (Full Version)

$$\text{score}(Q, D) = \sum_{i=1}^{n} \text{IDF}(q_i) \cdot [f(q_i, D) \cdot (k_1 + 1)] / [f(q_i, D) + k_1 \cdot (1 - b + b \cdot |D| / \text{avgdl})]$$

BM25: Best Matching 25 (Improved TF-IDF)

IDF Component (Modified)

$IDF(q_i) = \log[(N - df_i + 0.5) / (df_i + 0.5) + 1]$

Components:

- N = total documents
- df_i = docs containing term i
- +0.5 = smoothing (avoid zero)
- +1 = ensure positive score

TF Component (Saturating)

Key innovation: Saturation function

$TF = f \cdot (k_1 + 1) / (f + k_1 \cdot norm)$

Where:

$norm = 1 - b + b \cdot (|D| / avgdl)$

As $f \to \infty$, $TF \to (k_1 + 1) / (k_1 \cdot norm)$
Bounded, not linear!

Parameter	Default	Range	Effect
k_1	1.5	[1.2, 2.0]	Controls TF saturation. Higher = more emphasis on term frequency. **k_1 controls saturation:** With k_1=1.5, going from 1→2 occurrences helps more than 10→11
b	0.75	[0, 1]	Length normalization. 0 = no norm, 1 = full norm **b controls length penalty:** b=0.75 means longer docs get penalized, but not fully

Combined effect: Short docs with focused terms rank high, long docs need more evidence

BM25: Step-by-Step Example

Scenario

Corpus: 1000 documents, average length: 50 terms
Query: "machine learning"
Document D: "Machine learning is a subset of machine learning and deep learning" (12 terms)

Step 1: Calculate IDF for Each Query Term

Term "machine": appears in 300 documents
IDF = log[(1000 - 300 + 0.5) / (300 + 0.5) + 1]
IDF = log[700.5 / 300.5 + 1]
IDF = log[2.331 + 1] = log[3.331] = **1.203**

Term "learning": appears in 400 documents
IDF = log[(1000 - 400 + 0.5) / (400 + 0.5) + 1]
IDF = log[600.5 / 400.5 + 1] = log[2.499] = **0.916**

BM25: Step-by-Step Example

Step 2: Calculate TF Component

For "machine" (f=2, k_1=1.5, b=0.75):

norm = 1 - 0.75 + 0.75 × (12/50)

norm = 0.25 + 0.18 = 0.43

TF = [2 × (1.5 + 1)] / [2 + 1.5 × 0.43]

TF = 5.0 / 2.645 = **1.890**

For "learning"

(f=3, same norm=0.43):

TF = [3 × 2.5] / [3 + 0.645]

TF = 7.5 / 3.645 = **2.058**

Step 3: Combine Scores

$$\text{BM25}(Q, D) = \text{IDF}(\text{machine}) \times \text{TF}(\text{machine}) + \text{IDF}(\text{learning}) \times \text{TF}(\text{learning})$$
$$= 1.203 \times 1.890 + 0.916 \times 2.058$$
$$= 2.274 + 1.885 = \mathbf{4.159}$$

BM25: Step-by-Step Example

Understanding the Difference

```
TF-IDF score (normalized by document length):
"machine": (2/9) × log(1000/300) = 0.222 × 1.20 = 0.267
"learning": (3/9) × log(1000/400) = 0.333 × 0.916 = 0.305

Total = 0.572

BM25 score (with saturation & length normalization):
score(q, d) = 4.159
```

📌 Why BM25 Scores Higher:

- **Document length normalization:** BM25 considers document is shorter than average (12 vs 50 tokens) → less penalty
- **Term frequency saturation:** 3 occurrences aren't 3× better than 1 → diminishing returns applied
- **Probabilistic foundation:** Based on probability ranking principle → better ranking properties

Why Hybrid Search? Dense + Sparse

❌ Dense-Only Failures

Example 1: Exact Keywords

```
Query: "ERROR code 500"

Doc A: "Server error 500 occurred"
Dense score: 0.72

Doc B: "Something went wrong"
Dense score: 0.85 ← Wrong ranking!

Why? Embedding trained on general text
doesn't know "500" is crucial
```

✅ Sparse (BM25) Catches These

Example 1:

```
Query: "ERROR code 500"

Doc A: "Server error 500 occurred"
BM25 score: 8.3 (high IDF for "500")

Doc B: "Something went wrong"
BM25 score: 0.0 (no matching terms)

Correct ranking!
```

Why Hybrid Search? Dense + Sparse

❌ Dense-Only Failures

Example 2: Unique IDs

```
Query: "AIMLCZG521 schedule"

Doc A: "Course schedule for AI/ML"
Dense: 0.88 ← Wrong!

Doc B: "AIMLCZG521 timing"
Dense: 0.75

Unique terms not in training data
```

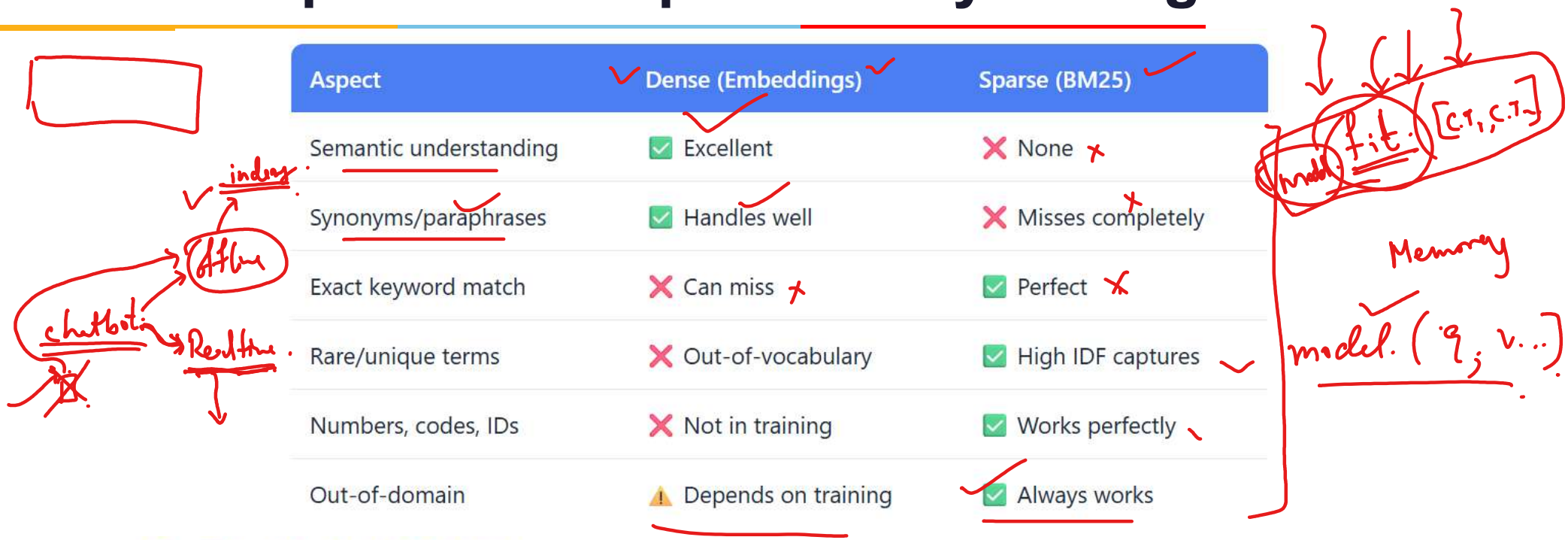
✅ Sparse (BM25) Catches These

Example 2:

```
Query: "AIMLCZG521 schedule"

Doc A: "Course schedule for AI/ML"
BM25: 3.2 ("schedule" matches)

Doc B: "AIMLCZG521 timing"
BM25: 12.5 (exact ID match!)

Correct ranking!
```

Dense + Sparse - Complementary Strengths

Aspect	Dense (Embeddings)	Sparse (BM25)
Semantic understanding	✅ Excellent	❌ None
Synonyms/paraphrases	✅ Handles well	❌ Misses completely
Exact keyword match	❌ Can miss	✅ Perfect
Rare/unique terms	❌ Out-of-vocabulary	✅ High IDF captures
Numbers, codes, IDs	❌ Not in training	✅ Works perfectly
Out-of-domain	⚠️ Depends on training	✅ Always works



💡 The Hybrid Solution

Use BOTH retrieval methods and combine their results!

Dense finds semantically similar content, Sparse ensures exact matches aren't missed.

The Challenge: Combining Different Score Ranges

Dense retrieval gives cosine similarities [0, 1]

BM25 gives unbounded scores [0, ∞]

Problem: Can't just add them! Need score-agnostic fusion.

Solution:

Min-Max Normalization:

score' = (score - min) / (max - min)

❌ Sensitive to outliers

Z-score Normalization:

score' = (score - μ) / σ

❌ Assumes normal distribution

Reciprocal Rank Fusion (RRF):

✅ No assumptions about score distributions

Reciprocal Rank Fusion (RRF): The Math

RRF Formula

$$\text{RRF}(d) = \Sigma_{r \in \text{rankings}} \; 1 \; / \; (k + \text{rank}_r(d))$$

Where:

- d = document being scored
- rankings = set of ranking lists (e.g., dense + sparse)
- $\text{rank}_r(d)$ = position of document d in ranking r (1, 2, 3, ...)
- k = constant (typically 60) to prevent division by small numbers

Why k=60?

Empirical finding from TREC competitions:

- k=60 balances contribution from high and low ranks
- Without k: 1/1 = 1.0, 1/2 = 0.5 (too steep drop)
- With k=60: 1/61 = 0.0164, 1/62 = 0.0161 (gentler)
- Prevents first rank from dominating too much

Alternative k values:

- k=0: Maximum emphasis on top ranks (aggressive)
- k=60: Balanced (standard)
- k=100: More weight to lower ranks (conservative)

Properties of RRF

1. **Score-agnostic:** Only uses rank order, not raw scores
2. **Bounded:** Score $\in$ [0, number of rankings / k]
3. **Symmetric:** All rankings weighted equally
4. **Robust:** Works even if one ranking is poor
5. **No training:** No hyperparameters to tune (except k)

🎯 Why RRF Works So Well

Documents that rank high in MULTIPLE systems are likely truly relevant. RRF naturally gives bonus to "consensus" documents without explicit weighting.

RRF: Example

Scenario: Query "machine learning tutorial"

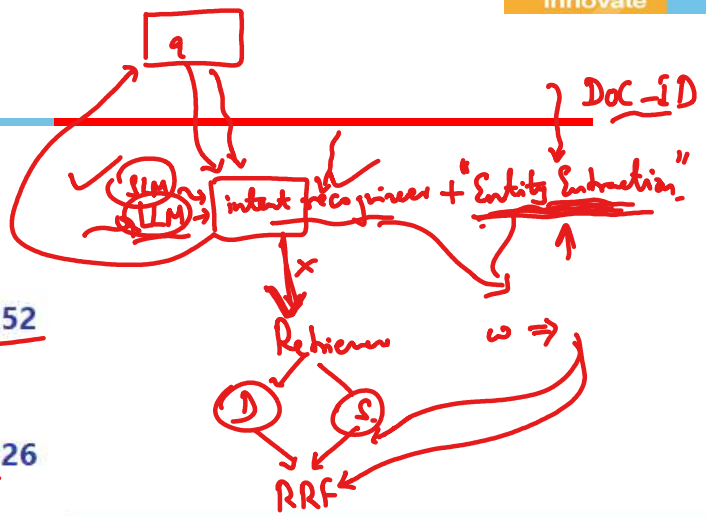
Dense Retrieval Results

Rank	Doc	Cosine
1	Doc A	0.92
2	Doc C	0.89
3	Doc B	0.85
4	Doc E	0.82
5	Doc D	0.79

Sparse (BM25) Results

Rank	Doc	BM25
1	Doc B	87.3
2	Doc A	82.1
3	Doc D	79.5
4	Doc F	71.2
5	Doc C	68.9

RRF: Example



RRF Score Calculation (k=60)

Doc A:
Dense rank: 1, Sparse rank: 2
RRF = 1/(60+1) + 1/(60+2) = 1/61 + 1/62 = 0.01639 + 0.01613 = **0.03252**

Doc B:
Dense rank: 3, Sparse rank: 1
RRF = 1/(60+3) + 1/(60+1) = 1/63 + 1/61 = 0.01587 + 0.01639 = **0.03226**

Doc C:
Dense rank: 2, Sparse rank: 5
RRF = 1/(60+2) + 1/(60+5) = 1/62 + 1/65 = 0.01613 + 0.01538 = **0.03151**

Doc D:
Dense rank: 5, Sparse rank: 3
RRF = 1/(60+5) + 1/(60+3) = 1/65 + 1/63 = 0.01538 + 0.01587 = **0.03125**

Doc E:
Dense rank: 4, Sparse rank: not in top 5 (treat as ∞)
RRF = 1/(60+4) + 0 = 1/64 = **0.01562**

Doc F:
Dense rank: not in top 5, Sparse rank: 4
RRF = 0 + 1/(60+4) = 1/64 = **0.01562**

Final Ranking

Rank	Doc	RRF Score	Dense Rank	Sparse Rank
1	**Doc A**	**0.03252**	1	2
2	Doc B	0.03226	3	1
3	Doc C	0.03151	2	5
4	Doc D	0.03125	5	3
5	Doc E, F	0.01562	4, -	-, 4

Key Insight: Doc A wins because it ranks high in BOTH systems (consensus), even though it wasn't #1 in sparse.

Performance Characteristics (Typical)

Pipeline Stage	Latency	Recall	Precision
BM25 only	20ms	70%	60%
Vector only	50ms	75%	65%
Hybrid (BM25+Vector+RRF)	70ms	90%	75%

Hybrid Search Implementation

Code Demo

Key Takeaways

1. **Encoder Models:** Bidirectional transformers create contextual embeddings through self-attention and pooling
2. **Vector Similarity:** Cosine similarity (or normalized dot product) measures semantic closeness in embedding space
3. **ANN Algorithms:** HNSW (graph), IVF (partitions), PQ (compression) enable fast search at scale
4. **Sparse Retrieval:** BM25 improves TF-IDF with saturation and length normalization
5. **Hybrid Systems:** Dense + Sparse + RRF combines semantic and lexical strengths

Formulae:

- Self-attention: $\text{Attention}(Q,K,V) = \text{softmax}(QK^T/\sqrt{d_k})V$
- Cosine: $\cos(A,B) = A \cdot B / (||A||\ ||B||)$
- BM25: $f(k_1+1) / (f + k_1(1-b+b|D|/\text{avgdl}))$
- RRF: $\Sigma\ 1/(k+\text{rank})$

Resources & Further Reading

- **Dense Passage Retrieval** (Karpukhin et al., 2020)
  Foundation for modern dense retrieval
- **HNSW** (Malkov & Yashunin, 2018)
  Efficient and robust approximate nearest neighbor search
- **Product Quantization** (Jégou et al., 2011)
  Vector compression for large-scale search
- **Sentence-BERT** (Reimers & Gurevych, 2019)
  Siamese networks for semantic similarity